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Life Cycle Assessment (LCA) of Light-Weight Eco-composites



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Miao Guo

Life Cycle Assessment (LCA) of Light-Weight Eco-composites

Doctoral Thesis accepted by Imperial College London, UK



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Supervisor's Foreword

This Ph.D. thesis represents a considerable step forward in our understanding important issues in the Life Cycle Assessment (LCA) of new bio-based materials, particularly for the novel wheat starch-PVOH biopolymer used as the main example. Detailed attributional LCA research was conducted to explore important questions regarding the life cycle and environmental profiles of a range of novel and potential products made from starch-PVOH biopolymer in comparison with conventional petrochemical polymer alternatives. Key contributions to knowledge are provided by (1) Clear presentation of transparent and disaggregated Life Cycle Inventory data, (2) New scientific data from laboratory studies on important aspects of the materials e.g., anaerobic biodegradability, (3) New modeling outputs and data assemblies on, for example, N₂O emissions using a modified Denitrification-Decomposition (DNDC) biogeochemistry model, on AD plant operations and, (4) Novel insights on the environmental profile of starch-PVOH biopolymer, on bio-based materials in general and on methodological issues, such as uncertainty analysis, in the use of LCA for such evaluations.

The LCA models developed in the thesis were used to identify the major contributors to the environmental profiles of novel starch-PVOH biopolymers and to compare these with petrochemical counterparts. Underlying this was a desire to address the question 'Is there a general environmental advantage for starch-PVOH biopolymers over petrochemical polymers'. The thesis presents well-supported arguments for the need for specific, case-by-case assessments rather than reliance on a blanket 'always better' perspective when addressing this question. A hierarchy of critical parameters for LCA-based decision making on biopolymers is also offered as a general outcome of this research.

An innovative aspect of the work was use of the process oriented, biogeochemistry model DNDC to explore the factors involved in the nitrogen and carbon cycles in agro-ecosystems (e.g., soil quality changes, crop rotation) in the context of the system boundary of the LCA research. The output of the DNDC model was compared with the empirical Tier 1 approach of the Intergovernmental Panel on Climate Change (IPCC) which has been widely used in LCAs. Furthermore, the methodology for Monte Carlo simulation of DNDC was improved in this Ph.D.

work and statistical methods were introduced to present a formal analysis of uncertainty in the DNDC and IPCC Tier 1 N_2 O outputs, again within an LCA framework. This work has inspired ongoing developments with DNDC to support its application in LCAs of a wider range of crop types relevant to bio-based materials and energy products.

The LCA case studies in this thesis were used to understand some important (but rarely addressed in depth) issues concerning data quality in LCA research e.g. a lack of uncertainty analysis. The method developed combined uncertainty with the sensitivity analysis and enabled a more transparent basis for the degree of confidence placed on the LCA results. The approaches used were:- (i) comprehensive sensitivity and uncertainty analysis, (ii) integration of statistical methods (maximum likelihood estimation, and goodness of fit) into the LCA research to analyze uncertainty in the industrial and computer-simulated datasets and, (iii) calibration of probabilities arising from uncertainty in the inventory and from data variation characteristics for the biopolymer products. Taken together, these measures enabled confidence levels to be attached to the Life Cycle Impact Assessment (LCIA) outcomes in specific impact categories for the comparisons undertaken between the biopolymer and petrochemical polymers.

Finally, the complete primary LCI datasets developed for the novel wheat starch-PVOH biopolymer are presented in a clear, transparent, and disaggregated form in the thesis. This is of real practical value for other LCA practitioners, because it helps to fill a number of knowledge gaps e.g. inventory data for PVOH production, behavior of the biopolymer under an AD end-of-life scenario. The LCI was supplemented where necessary (and clearly indicated) with secondary data from recognized, publicly available sources. The quantity, transparency, and completeness of the data used, together with the statistical and sensitivity analyses, are important elements that give strong support to the overall LCA conclusions reached and to the scientific value of the work. This thesis presents an integrated and complete body of knowledge on the research program undertaken, and together with the publication of specific aspects in the scientific literature, it is hoped that it will provide a valuable reference for LCA practitioners and the bio-polymers community.

London, UK, August 2012

Dr. Richard Murphy

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Miao Guo Division of Biology Imperial College London

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Abbreviations

AD Anaerobic digestion ALCA Attributional LCA

AR4 Fourth Assessment Report

BIS Department for Business Innovation and Skills

BMP Biochemical methane potential

CFC-11 Trichlorofluoromethane
CHP Combined heat and power
CLCA Consequential LCA

CLO Compost-like output
COD Chemical oxygen demand
CV Coefficient of variation
1, 4-DB 1, 4-Dichlorobenzene

Defra Department for Environment, Food and Rural Affairs

DNDC Denitrification-Decomposition model
DTI Department of Trade and Industry
ECO European Containerboard Organization

EPS Expanded polystyrene

FEFCO European Federation of Corrugated Board Manufacturers
GEO European Association of Makers of Corrugated Board Base

Papers

GHG Greenhouse gas GOF Goodness of fit

GWP Global warming potential
HDPE High density polyethylene
HRT Hydraulic retention time

ISO Internation Organization for Standardization IPCC Intergovernmental Panel on Climate Change

K-S test Kolmogorov-Smirnov test LCA Life Cycle Assessment

LCI Life cycle inventory/life cycle inventory analysis

LCIA Life Cycle Impact Assessment

xviii Abbreviations

LDPE Low density polyethylene
MBT Mechanical biological treatment

Montreal Protocol Montreal protocol on substances that deplete the ozone layer

MLE Maximum likelihood estimation
MSBF Maize starch based foam
MSW Municipal solid waste

NMVOC Non-methane volatile organic compound

NSRI National Soil Research Institute
ODP Ozone depletion potential

OFMSW Organic Fraction of Municipal Solid Waste

OLR Organic loading rate

PDF Probability density function
PHA Polyhydroxyalkanoate
PHB Polyhydroxybutyrate
PLA Polylactic acid

PM2.5 Particulate matter with aerodynamic diameter less than

2.5 µm

PM10 Particulate matter with aerodynamic diameter less than

10 µm

POCP Photochemical ozone creation potential

PP Polypropylene

PSBF Potato starch based foam

PVAc Polyvinyl acetate PVOH Polyvinyl alcohol

RAINS model Regional Air Pollution Information and Simulation Model

RDF Refuse derived fuel SD Standard Deviation

SETAC Society of Environment Toxicity and Chemistry

SMPR Specific methane production rate

SOM Soil organic matter
SRT Solid retention time
TPS Thermoplastic starch

TS Total solid

TSP Total suspended particulate
TSS Total suspended solid

USES-LCA model Uniform System for the Evaluation of Substances Model

VAC Vinyl acetate VFA Volatile fatty acid

VOC Volatile organic compound

VS Volatile solid

VSS Volatile suspended solid WBF Wheat based foam

WRATE Waste Resources Assessment Toolkit for the Environment

Chapter 1 Introduction

1.1 Scope of the Research

The thesis is based on research carried out within a DTI (now BIS) funded project "Lightweight eco-composites based on renewable materials" (Project No: TP/2/MS/6/1/100118), involving a consortium of academic institutions, research organisations and companies. The research reported here is an investigation of the environmental profiles of novel wheat-based foams (WBFs) in a variety of applications compared with conventional petroleum-based foams. The WBF utilises wheat flour—essentially starch with its protein—as the primary ingredient blended with biodegradable components such as polyvinyl alcohol (PVOH), some plant oil and additives.

This introduction provides a background on biodegradable polymers with emphasis on starch-based polymers and their blends, followed by information about Life Cycle Assessment (LCA) methodology and a consideration of previous LCA studies on biopolymers. This consideration pointed out a number of key issues in biopolymer life cycles and these are then explored specifically e.g. modelling greenhouse gas (GHG) emissions in the wheat agro-eco-system, biodegradability and the end-of-life phase. The biodegradability of starch-based polymers under different conditions and the potential environmental impacts of the end-of-life stages are reviewed in some detail as they were specifically investigated in laboratory research in order to generate data inputs to the LCA. Inventory data quality is also considered towards the end of this introduction to provide insight on the assessment of uncertainty and on sensitivity analysis approaches that formed a basis for those applied in the research. This review is therefore a selective and detailed treatment of the literature considered to be of particular relevance to the aims of this study.

1.2 Biodegradable Polymers

1.2.1 Conventional Polymers Versus Bio-Degradable Polymers Based on Renewable Resources

Since the first industrial scale production of petroleum-based polymers (plastic) took place in 1940s, global demand for plastic has increased considerably [5]. According to statistics from Plastics Europe [272], the average annual increase in global production and consumption of plastic has reached 9 % since 1950; total global production increasing from 1.5 million tonnes in 1950 to 245 million in 2008 with applications in almost every sector of life and industry. Consumption on a per capita basis has now grown to approx 100 kg per year in North America and Western Europe and the consumption is estimated to rise to 140 kg per capita by 2015. The UK accounted for nearly 8.5 % of the demand for the 48.5 million tonnes plastic used in Europe in 2008. Another potential area for rapid growth in plastic consumption is the Asian developing countries where average per capita consumption is currently around 20 kg. As shown in Fig. 1.1, amongst 20 distinct groups of plastic, five plastic families accounted for approximately 75 % of European plastic consumption: polyethylene (PE), polypropylene (PP), polyvinylchloride (PVC), polystyrene (PS) and polyethylene terephthalate (PET) [272]. Packaging remained as the largest consumer of plastic, followed by the building and construction sector, accounting for nearly 60 % of Europe and 57 % of UK plastic consumption (Fig. 1.2) [272, 340].

Increasing demand for petroleum-based polymers in packaging as well as other sectors, is not only a resource depletion issue (finite oil and gas reserves), but also environmental and waste management issues. In the EU 24.9 millions tonnes of post-consumer plastic was generated in 2006 [272]. In the UK, plastic waste generated was estimated to be nearly 3 million tonnes [340]. In the UK packaging materials sector, whilst materials such as metal and paper decreased in the waste stream, the share of plastic increased from 17 % in 1998 to 21 % in 2007: plastic waste grew by over 400 thousand tonnes during this ten-year period [325].

Although very few petrochemical polymers are water soluble, such as polyacryl amide, polyethylene oxide, PVOH etc. [56], most are insoluble and non-biodegradable; thus their disposal in soil or via composting is untenable. Alternative degradation routes have been explored such as photo degradation and thermal oxidative degradation for non-biodegradable plastics; however, they are either environmentally unacceptable or too expensive [292]. On the whole a biodegradation option is more favoured if suitable polymers are available at appropriate cost. In a number of cases the effective recycling of plastics waste is also inhibited by factors such as disadvantages in transportation caused by the bulky nature of such waste [251]. The rates for mechanical recycling and energy recovery of post-consumer plastic waste also vary between countries. Although Switzerland, Germany, Sweden and Denmark have almost completed their strategies for diversion-from-landfill, none have reached a recycling rate of above

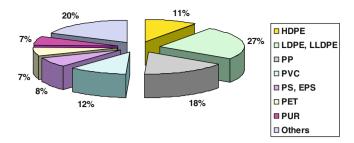


Fig. 1.1 Plastic consumption by types in Europe [272]

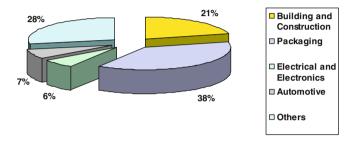


Fig. 1.2 Plastic consumption by sectors in Europe [272]

35 %. In the UK, recycling and recovery rates are also not ideal: only approx 25 % of plastic waste generated in 2008 was recycled or recovered [272], which was much lower than other packaging materials (total recycling rate 57 % in 2006) [325].

Actually, to help solve the problems in plastic waste treatment, scientists have started research on biodegradable plastics since the 1980's [292, 308]. Biodegradable polymers opened new ways for waste management since they can degrade under either natural environmental conditions or in municipal/industrial biological waste treatment facilities. To define biodegradable polymers, a concept summarized by Wang et al. [337] is cited here: 'biodegradation of polymer is deterioration of polymer's physical and chemical properties and a decrease of its molecular mass down to the formation of CO₂, H₂O, CH₄ and other low molecular-weight products under the influence of micro organisms in both aerobic and anaerobic conditions'. They further stated that during this process all carbon should be accounted for carbon balance, residues produced should be non-toxic to the environment and residues along with microbial biomass should be eventually incorporated into the geochemical cycle. Specifically, biodegradable polymers can be categorized as being of natural origin, synthetic origin (petroleum-origin polymers) and biodegradable polymer blends [56, 72, 337]. Very few synthetic plastics are biodegradable. Compared with synthetic origin polymers, biopolymers based on naturally-occurring long-chain molecules e.g. polysaccharides, proteins, lignin, shellac, etc., have been suggested to be more environmentally 'friendly' as

they are derived from renewable feedstock. The blending of biodegradable polymers with synthetic polymers has also received considerable R&D attention as this approach can be used to attain various levels of mechanical and other properties and degradation rates [337].

1.2.2 Starch-Based Polymers

Amongst various natural feedstocks for biodegradable polymers, starch, the second most abundant renewable polysaccharide in nature [140], has been recognized as one of the most promising substitutes for petrochemical plastics for a variety of applications [49, 297]. Composed of repeating D-glucopyranosyl units, starch can be separated into amylose which is linear linked by α (1–4) linkage, and amylopectin which has α (1–4)-linked backbone and α (1–6)-linked branches [10]. Amylose which has a molecular weight of several hundred thousand, shaped in the form of helix, is a minor component typically ranging between 20–30 % of starch; whereas amylopectin with molecular weight in the order of several million presenting in double helical crystalline structure is the major part of starch [337]. Starch is biodegradable as it can be easily metabolized by a wide range of microorganisms. Starch-based materials derived from corn, potato, wheat, tapioca and rice etc. have been widely developed [346]. The various starch-based polymers can be classified into five categories [72, 358]:

- starch filled plastics,
- chemically modified starch,
- plasticized thermoplastic starch,
- biopolymers synthesized from starch and
- starch compounded with biodegradable polymers

In starch-filled plastics, starch is used as biodegradable filler in synthetic polymers, such as starch-filled LDPE film [195] or PS sheet [194]. Generally the starch filler component is lower than 20 % [123]. However, the starch filler only enhances the disintegration of these blends in nature not necessarily its biodegradation [72, 123, 194]. Quite often the properties of native starch are inadequate for the application and chemically modified starches have been developed to overcome the shortcomings [3]. An example of this is the series of papers/patents describing the copolymerization of starch and other polymers such as polyacrylamide-starch complex [149, 150] and the starch esters prepared by a non-aqueous process [180]. Thermoplastic starch (TPS) is processed in the presence of plasticizers such as water, selected amino acids, or glycerol [180, 227]. There has been increasing interest in the utilization of TPS for biodegradable materials and the biodegradability of TPS has been broadly researched [123, 337]. The synthesized biopolymers from starch are either produced via chemical synthesis or fermentation by microbes. Polylactic acid (PLA) is a leading example of a biodegradable biopolymer synthesized from lactic acid derived from dextrose from starch via fermentation. Starch polymers compounded (blended) with other polymers have also developed rapidly in the last decades such as the blends commercialized under the Mater-Bi[®] [16].

1.2.3 Starch-Based Blends

The starch/flour components in the present research are blended with other components and this represents the current mainstream approach to utilising starch in biopolymers.

Although the biodegradability of starch together with its low cost and wide availability offers several advantages [286], its applications are limited by poor mechanical strength, hydrophilic nature and susceptibility to microbial attack. Since the first application of starch in thermoplastics (starch-filled polyethylene) was developed by Griffin [337] these limitations have been overcome by successfully blending starch with various synthetic polymers [124, 161, 227]. Blends of starch with biodegradable synthetic polymers have been of particular interest [16, 161, 218, 226, 229, 263, 279, 281, 294, 296, 317, 345)). These have included blends of starch/PVOH, starch/PCL (polycaprolactone), starch/PLA, and starch/PHAs (polyhydroxyalkanoates). These blends can offer similar mechanical properties to conventional petrochemical polymers such as PE and PS [337]. Lipids have also played a role in the development of starch-based blends and starch-oil composites blended with glycols or polyester have been studied since the 1990s [67, 68, 110, 201].

Amongst all these starch-based composites, starch: PVOH blends are of interest because of the excellent compatibility and processability of the two components [124, 256] and the improved properties of blends [287].

1.2.4 Polyvinyl Alcohol

Since 1924 when PVOH was first discovered by Herrman and Haechel it has been applied in various fields such as textile sizing, adhesives, emulsion polymerization and paper sizing etc. [115, 228]. Nowadays, PVOH is a very widely used, water soluble synthetic polymer [56].

PVOH is not directly produced from the corresponding monomer but instead from a polymerized ester known as polyvinyl acetate (PVAc) [116]. Vinyl acetate (VAC) derived from acetic acid and ethylene is polymerized into PVAC then further hydrolyzed to PVOH. Different technologies have been developed for PVOH manufacture and properties such as solubility can be varied depending on the degree of hydrolysis and polymerization [115, 116]. Generally, commercially available PVOHs fall into a range of degree of hydrolysis of 70–99 % [56] and are only soluble in polar solvents such as water and glycols [228].

PVOH has been considered as biodegradable and soluble since the early 1930s [57] and so PVOH was widely utilized in blends and composites with several natural renewable polymers, including starch, cellulose, lignin, gelatin etc. It offers excellent strength and flexibility [337]. Amongst these blends, starch-PVOH composites have attracted great interests since the 1980s [256, 124]. Many products based on different technology have been developed and reported, including starch-PVOH based films in the presence of a plasticizer e.g. glycerol [54, 122, 227, 247], extruded foams containing up to 10 % of PVOH and baked starch-PVOH foams [56, 297].

However, introducing PVOH may lead to the decrease of biodegradation rate of the blended biodegradable polymer [56, 337]. Some studies have been conducted on the biodegradability of PVOH and PVOH/starch based blends under various environmental conditions [56, 232, 276, 287]; a detailed review is presented below.

1.2.5 Biodegradation of Starch/PVOH Blends Under Different Conditions

As discussed in Sect. 1.2.2, starch is highly biodegradable as it can be easily metabolized by a wide range of micro-organisms [337]. However, in comparison with starch, PVOH only can be assimilated by specific microbial strains [187]. Around 55 species of micro-organism have been reported to participate in PVOH degradation [180]. Generally the metabolism pathway consists of two steps i.e. oxidation of hydroxyl groups and cleavage of C–C linkages [116, 187]. Research on the biodegradation of PVOH dates back to 1936 when the first observation of PVOH degradation was reported [56, 187]. Due to its increasing utilization in the textile and paper industries, the environmental fate of PVOH keeps attracting research interest. Although PVOH has been believed to be non-toxic to organisms during biological disposal, it has surface activity and produces foams preventing O₂ recovery in water [187].

With the introduction of PVOH into bio-polymers nowadays, biodegradation research has not only focused on PVOH polymer but also has expanded to include PVOH blends. A review of previous studies is presented below:

1.2.5.1 Biodegradation of PVOH-Based Blends Under Anaerobic Digestion

As a widely applied technology for the waste treatment of solid organic waste, anaerobic digestion (AD) is also considered as an option for PVOH-based polymers. Although so far no anaerobic PVOH-degrading microbes have been isolated [187], a few studies have been carried out on the degradation of PVOH or PVOH/starch blends under anaerobic conditions [56, 232, 276, 287].

It was found that the rate of PVOH biodegradation was mainly dependent on inoculum and molecular weight. Matsumura et al. [232] tested the digestibility of PVOH with molecular weights of 14000 and 2000 co-digested with river sediments or anaerobically treated activated sludge under anaerobic conditions. Their results indicated that the low molecular weight polymer tended to biodegrade rapidly and river sediments gave higher degradation rates than activated sludge (after 125 days' incubation, the biodegradation of PVOH-2000 was over 60 % and approx 25 % when co-digested with river sediments and sludge respectively under anaerobic conditions). In contrast, other studies have found that PVOH only degraded to a minor extent in sludge when tested according to standard methods (below 12 % in 77 days) [133].

Limited studies have been conducted on the anaerobic digestibility of PVOH-based blends. The degradation of varying starch/PVOH blends was studied by Russo et al. [287] who concluded that after 900 h of digestion PVOH was the predominant residue and that the PVOH inhibited the degradation of the starch. Their explanation for the inhibition of starch degradation was a possible formation of a continuous PVOH phase that encapsulated the starch and the inter-chain mixing and partial phase miscibility between the PVOH and starch [287]. Alternatively, high degradation rates of PVOH under anaerobic conditions (66 % in 22 days) have been found with PVOH/starch blends [219]. Liu et al. [219] concluded that PVOH degradation was suppressed by high glucose concentrations as starch started degrading before PVOH.

The methodologies applied in most of the studies reviewed above was the biochemical methane potential (BMP) assay developed by Owen et al. [259] or the ISO standard method [169]. However, the source of inoculum in these studies varied, including digested sludge from active reactors or the laboratory feeding digesters; in addition, some key parameters such as the activity of the inoculum, load of substrate, ratio of substrate to inoculum are not indicated clearly [276, 287]. These parameters affect the biodegradability and the repeatability and comparability of results. Negligible biodegradation of PVOH by non-adapted cultures has been reported in comparative studies, whereas, after acclimation of micro-organism populations, efficient removal of PVOH has occured [56, 116]. There is no study available on acclimation of inocula to PVOH-based blends. Moreover, no publicly available study was found on AD of PVOH or its blends concerning either the influence of inoculum/substrate ratios or the characterization of the inocula used.

1.2.5.2 Biodegradation of PVOH/Starch Blends Under Aerobic Composting

Several studies have concerned the biodegradability of PVOH and PVOH/starch polymers under aerobic conditions [56, 57, 179, 292]. Although one previous study reported that PVOH tended to biodegrade more rapidly under aerobic conditions

than anaerobic conditions (Matsumura and Toshima [233], the results from other studies indicate that PVOH underwent limited biodegradation under aerobic composting. David et al. [70] showed that moderate biodegradation of PVOH occurred in compost extract; interestingly, it was found that after incubation in composting above 50 °C for over 50 days, 88 % hydrolyzed PVOH showed slightly higher biodegradability than 98 % hydrolyzed PVOH (24 and 15 % biodegradation respectively). The low extent of biodegradation of PVOH was confirmed by another study on PVOH film in which film samples based on PVOH with a hydrolysis degree of 88 % reached only 7 % biodegradation after 48 days in a temperature-controlled composting experiment [57]. The research was also carried out on PVOH blends. A study conducted on the biodegradability of starch/PVOH/glycerol blended film showed that over 45 days composting, most of the starch was degraded but the PVOH was left essentially intact [179].

1.2.5.3 Biodegradation of PVOH/Starch Blends in Other Environments

Investigations on the degradation of PVOH in natural soils date back to 1970s' when the first microorganism capable of assimilating PVOH was isolated from soil samples and identified as *Pseudomonas* species [56, 313]. Despite the isolation of PVOH-degraders, limited degradation of PVOH in natural soil has been reported repeatedly [64]. In a simulated soil burial test only 8–9 % degradation of PVOH was observed within 74 days irrespective of the PVOH concentration and physical state (film or powder) [57]. Similar results were obtained in another soil burial experiment with longer incubation periods [305]. Similar results have been obtained for PVOH blends—limited biodegradation in soil environments [64]. Chiellini et al. [56] offer two possible explanations for the negligible biodegradation of PVOH in soil burial or aerobic composting (1) insufficient numbers of PVOH-degrading microorganisms in soil and (2) adsorption of PVOH by inorganic or organic components present in soil inhibiting the biodegradation process.

The biodegradation of PVOH and starch/PVOH composites has also been investigated in aqueous environments and landfill. Limited PVOH biodegradation has been observed in aerobic liquid cultures [56]. An interesting study conducted by Ishigaki et al. [167] tested biodegradability of PVOH/starch blends in both aerobic and anaerobic landfill reactors. Film breakage did not occur in either aerobic or anaerobic reactors which, together with results from SEM observation and weight loss tests, indicated that the PVOH component remained [167]. Another biodegradability test on PVOH/starch/glycerol and urea blends indicated that after 18 days of inoculation with micro-organisms isolated from landfill, starch and the amorphous part of PVOH were firstly degraded but the crystalline regions of PVOH remained [323].

1.3 LCA of Starch-Based Bio-Composites

A main driver for the development of biodegradable polymers, including starch-based bio-composites, is the increasing interest in environmental sustainability. However, to determine whether biodegradable polymers deliver progress in achieving this goal, quantitative and reproducible environmental assessments are needed to avoid inadvertent 'problem shifting' or lack of a holistic assessment. Life Cycle Assessment (LCA) is a cradle-to-grave modelling method that offers a systematic approach for such overall environmental assessment of materials, products and services, including biopolymers [335].

1.3.1 LCA Framework and Approach

1.3.1.1 LCA Framework

Under the ISO 14040 series of standards, LCA consists of four phases (Fig. 1.3): goal and scope definition, life cycle inventory analysis (LCI) [168], impact assessment (LCIA) [170], and interpretation [172]. The first stage is the foundation, upon which the LCA study is laid out; all the stages interact with each other [252]. As a cradle-to-grave approach, LCA has been widely acknowledged as one of the optimal decision support tools for identifying the important environmental factors in product systems [269, 314].

The guiding principles in conducting LCA are life cycle perspective, transparency and completeness [174]. LCAs usually attempt to take every stage of product life cycle into account [269] from raw material acquisition to final disposal. Importantly, transparency in the assumptions and methodologies used ensures a reproducible analysis and proper interpretation of results [174] and a comprehensive consideration of several aspects of the natural environment, human health and resources helps to give a holistic assessment. LCA is also a relative approach with all the inputs-outputs and the environmental profile generated being related to the functional unit [174]; thus the functional unit forms the basis for LCA comparisons between different product systems.

According to the general LCA framework, in the first phase of the assessment the study goals (e.g. intended applications, audience) are described and fundamental modelling elements are described, including the product system, the system boundaries and the functional unit. The principles and main methodologies to be applied are defined, including data quality requirements, allocation approach, impact categories concerned and impact assessment methods (characterization, normalization methods). At the LCI phase, inventory data are collected on each unit process of the product system within system boundary and the data quality assessed LCI results are then further analyzed in the LCIA, which comprises the mandatory element of characterization and possibly other optional ones

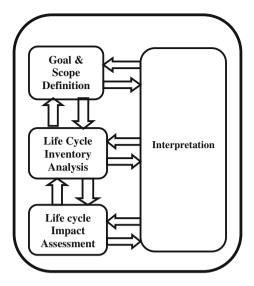


Fig. 1.3 Framework of LCA [174]

(normalization, weighting). During the LCIA phase, LCI outputs are associated with impact categories and converted to category indictors by using defined characterization factors; the aggregated indicator results provide characterized profiles of the studied products, which can be further normalized to give information on relative magnitude of each indicator result. Finally, LCI and LCIA outcomes are presented in the interpretation phase in accordance with the study goal and scope to reach conclusions and recommendations. However, as indicated in Fig. 1.3, the four LCA phases are not independent but interact. For instance, the inventory data are collected for the initial system boundary definition whereas the results of sensitivity analysis at LCIA phase can indicate a need to redefine the system boundary and develop the assessment further.

1.3.1.2 LCA Approaches

The ISO 14040 series of standards provide a framework for undertaking LCAs and indicate generic methods and approaches. They do not specify the exact LCA methodology that must be used for a given product systems. Generally, two types of LCA have been distinguished: attributional LCA (ALCA) and consequential LCA (CLCA) approaches. The former is focused on describing the environmentally relevant flows to and from a life cycle and its subsystems; the latter aims to study how environmentally relevant flows change in response to possible decisions [119]. These two types of LCA have been emerged from previous studies that were described in other terms such as retrospective and prospective [320], descriptive and change-oriented [119]. As stated by Tillman [320], the different characteristics

	Attributional LCA	Consequential LCA
System boundary	Completeness	Parts of system affected
Choice of data	Average technology	Marginal technology
Allocation approach	Physical/economic/system boundary expansion	System boundary expansion

Table 1.1 Characteristics of two LCA approaches

of ALCA and CLCA are reflected in their methodological choices, i.e. choices of data, system boundary and allocation principles and this has received general consensus in the literature [69, 119]. Data used in ALCA represent the average process, thus the average environmental profiles of a product system are evaluated (Table 1.1). Conversely, in CLCA marginal data is used to reflect the influence of changes in the environmental aspects of the product systems. In addition, their allocation methods differ.

For multiple-product systems, three main allocation approaches are applicable to partition the material/energy flows and their associated environmental impacts between the main and co-products: allocation by physical relation (e.g. mass, volume etc.), allocation by economic value or system boundary expansion [168]. As shown in Table 1.1, it is well recognized that allocation by mass or economic value can always be avoided by applying system boundary expansion in CLCA [119, 342]. But there is no universal agreement on the allocation method in ALCA. System boundary expansion is indicated as the prefered approach in ISO 14041 and 14044 [168, 175] as well as in PAS 2050 [40]; together with the economic allocation it is widely applied in ALCA studies [343]. On the contrary, some LCA practitioners state that system boundary expansion is not applicable to ALCA as ALCA studies seek to describe status quo situations in which there are no change in outputs [342].

ALCA is the 'traditional' method on which most existing LCA studies are structured [69]; whilst CLCA as a relatively new approach is still at the exploration stage. Attempts have been made to apply both methods to the same products to illustrate the applicability of consequential approach, e.g. the study carried out by Thomassen et al. [318] and Dalgaard et al. [69]. However, as pointed out by Finnveden et al. [119], CLCA studies are likely to be more conceptually complex and less transparent than static models based on the traditional ALCA approach; furthermore, results from CLCA can be more sensitive to assumptions. The choice over which LCA approach should be used depends on the goal and scope of the study. Tillman [320] and Finnveden et al. [119] suggest that for a decision between alternatives or when modelling future technologies/systems ALCA can provide the best support by modelling the overall influence, whereas for evaluating improvement possibilities, CLCA can be more relevant. Under the current study, the LCA research focused on an attributional approach, thus the following sections mainly concentrate on this traditional LCA approach. CLCA will be explored in future research.

1.3.2 LCI and LCIA

1.3.2.1 LCI Database

Besides direct measurements, other approaches are also used to develop LCA inventories for sub-processes, such as expert judgements, evaluations based on empirical observations and computer models [119]. Amongst them, the estimation approach has been widely applied, for example in the Eco-invent inventories for infrastructure [126], energy consumption and CO₂ estimation of organic chemicals [266]. In addition, computer simulation has also been used to derive LCA inventory elements, especially those concerning complex bio-chemical processes such as agricultural field emissions [152] and landfill gas emissions [8]. By using the above approaches, the datasets representing the average processes for certain regions or industries have been developed, which are generally used to complement site-specific data in LCA models.

Publicly available datasets can be classified into: national or regional and industrial datasets. The former are developed by incorporating regional datasets to present national or international inventories for products or services: such as the EU LCA platform developed by European Comission [109], NREL US LCI databases [255]. Industrial datasets are developed by industrial associations generally to represent industry-average processes or products e.g. the datasets for plastic products established by Plastics Europe (2005), EU corrugated board database [113].

Some of the databases discussed above have been incorporated into commercially available software for LCA modelling, such as SimaPro, GaBi, etc. which include a range of wordwide datasets e.g. Eco-invent [126], Buwal and ETH-ESU etc. [275], covering various regions and industries.

1.3.2.2 LCIA Methodology

The LCI results are associated with environmental categories and category indicators in the LCIA phase; in some cases they are further linked to category endpoints defined as 'attribute or aspect of natural environment, human health or resources identifying an environmental issue' [171]. Thus LCIA methodologies can be categoried as midpoint and endpoint-oriented approaches which are also termed as 'problem-oriented' and 'damage approach' respectively [274]. The former is chosen along with environmental mechanisms between the LCI results and endpoints [171] and the latter is defined at the level of protection area [119]. As stated by Bare et al. [13], these two approaches are differentiated by the way in which the environmental relevance of category indicators is taken into account: unlike the midpoint approach, at the end-point level the environmental relevance of category indicators do not need to be dealt with separately, instead, they are quantified to provide an understandable insight for decision-makers.

CML 2 baseline^a Eco-indictors 99b LCIA element Characterization Characterization Normalization Normalization Weighting LCIA approach Midpoint/problem-oriented Endpoint/damage-oriented Abiotic depletion Minerals (resource depletion) Impact categories concerned Fossil fuels (resource depletion) Global warming potential Climate change (human health) Ozone layer depletion Ozone layer (human health) Acidification Acidification/eutrophication (eco-Eutrophication system quality) Human toxicity Carcinogens (human health) Aquatic eco-toxicity (fresh water Eco-toxicity (eco-system quality) and marine) Terrestrial eco-toxicity Respiratory organic (human health) Photochemical potential Respiratory inorganic (human health) Radiation (human health)^c Land use (eco-system quality)^c

Table 1.2 Comparison of CML 2 baseline and Eco-indicators 99

Notes

Actually, a range of LCIA methodologies have been developed and introduced into software tools, such as the midpoint-oriented methods CML 2001 and TRACI 2002+ and the endpoint approaches Eco-indicators 99 and EPS 2000 [274]. Amongst them, the CML (baseline/all impact category version) and Eco-indicator methods are commonly applied. The former were developed by Centre of Environmental Science of Leiden University where a range of environmental categories are taken into account e.g. depletion of abiotic resource, climate change, acidification etc. [142]. Eco-indicators 99 and earlier versions were derived from a collaboration between Swiss and Dutch LCA experts whereby midpoint impact categories are further integrated into three end-points in a 'damage assessment step', i.e. damage potential to human health, ecosystem quality and resources [137]. The comparison in Table 1.2 indicates that although the impact categories evaluated in two methods are not identical, most of them overlapped. As shown in Table 1.2 the CML 2 baseline method represents eco-toxicity in three sub-categories whilst Eco-indicators 99 uses only one integrated eco-toxic indicator result. Equivalent to photochemical potential in CML 2 baseline (summer smog), Ecoindicators 99 includes a respiratory organics impact category where respiratory effects resulting from exposure to organic compounds in summer-smog are evaluated [137, 274]. Eco-indictors 99 also accounts for winter smog (respiratory inorganic), damages induced by radioactive radiation and conversion and occupation of land [274] all of which are not in the scope of CML baseline method.

^a [142, 274]

^b [137]

^c Brackets in Ecoindicators 99 indicate the category end-point concerned in damage assessment

1.3.2.3 Characterization Models

Generally, two input-related categories are considered in LCA studies—abiotic resource and biotic resource depletion potentials [173]. Additionally, land use may also be considered as another resource input [235]. The other impact categories presented in Table 1.2 are output-related.

For each impact category, the environmental impact mechanism is defined in characterization models that describe the relationships between LCI results and category indictor/category endpoint [171]. In-depth research has been carried out to develop understanding of these mechanisms, a prime example being the worldwide recognized Intergovermental Panel on Climate Change (IPCC) models [125]. However, for certain impact categories either relatively little knowledge exists or there is no widely accepted characterization method(s) available, such as for land use or biotic depletion [119, 173].

Biotic and Abiotic Depletion

The main differences between these two impact categories are: abiotic depletion involves deposits (fossil resources, minerals), environmental resources (ground water soil etc.), and natural flow resources (solar, air, water) [137]. Biotic depletion is associated with fauna and flora [182]. Audsley et al. [9] cite farmland as an example of biotic depletion, stating that farmland contains a variety of species and that the farming system influences biodiversity e.g. via the removal of habitats, application of fertilizer/pesticides. However, previous authors tend to agree that biotic resources grown and harvested on a sustainable basis (e.g. arable crops) should not be considered as a biotic depletion [96, 151] and, as pointed out by PRé Consultants [274], the biotic depletion category is more intended to represent impacts on rare animals and plants. However, defining this biotic resource depletion potential category has been highly complex due in part to the absence of scientific consensus on biodiversity definition or measurement [9]. Whilst some biotic depletion characterization models have been presented, e.g. the factors developed by Heijungs et al. [151], biotic depletion is generally excluded from LCIA models [274]. Thus, it is evident that further research and development is necessary to make this impact category generally applicable in LCA.

On the contrary, abiotic depletion is one of the most frequently discussed impact categories, and there are a variety of methods available. All the methods generally fall into two groups [119, 137], i.e. the methods based on measurement of available resources and extraction rates and the methods based on exergy consumption and entropy production [241]. The former is commonly applied and the available methods have been summarised by Guinée et al. [142]. This approach was adopted in the CML baseline LCIA method where the extraction of minerals/ fossil resources are determined according to the concentration of ultimate reserves and rate of de-accumulation [142]. The exergy/entropy approach has been put forward since the 1990s. After the applicability of exergy in LCIA studied by

Finnveden and Ostlund [121] a range of models based on evaluation of cumulative exergy extraction from natural environment were developed, e.g. indicator cumulative exergy demand introduced by Bosch et al. [30] and LCIA approaches proposed by Dewulf et al. [97] which aggregated the exergy data on fossil resources, nuclear and metal ores, minerals, air, water, land occupation, and renewable energy sources. This exergy consumption based LCIA approach was also applied to Eco-invent datasets [127].

Global Warming Potential

Another frequently discussed issue is climate change and the increase in the global average temperature accompanied with widespread melting ice and rising average sea level [125]. To evaluate the influence of factors relating to climate change, the concept of radiative forcing quantified in terms of 'rate of energy change per unit area of the globe as measured at the top of the atmosphere' was introduced. To further evaluate the overall and potential climate change responding to GHGs, parameters such as the lifetime of forcing agents were used to develop 'Global Warming potentials' (GWPs) as a simplified index defined by the IPCC and adopted in the Kyoto Protocol. GWP is based on time-integrated global mean radiative forcing of a unit mass emission relative to that of one unit of mass of the reference gas CO₂ [125]. In the IPCC model, direct GWP values of GHGs are given under different time-horizons (20, 100, 500 years). This means that longlifetime compounds tends to contribute more to total GWP in 'forward-looking' perspective e.g. CClF₃, whereas compounds with short-lifetimes become less important after removal/depletion over a longer time-horizon e.g. CH₄. Generally GWP100 horizons are applied in LCAs.

In addition to direct GWPs, approaches to evaluate indirect GWPs are also discussed, which take into account the effects of degradation products or the radiative effects of changes in GHG concentrations due to the presence of an emitted gas or its degradation products [125]. The compounds involved include CH₄, CO, H₂, NO_x non-methane volatile organic compounds (NMVOC) and halocarbons. Their indirect radiative effects mainly concern ozone formation/depletion, production of CO₂, change in stratospheric water vapour levels, and enhancement of CH₄ life-times via change in the concentration of OH⁻. Although the suggested indirect GWP values are given in the IPCC Fourth Assessment Report [125], they are not commonly applied at the LCIA stage, except for CH₄. In the IPCC characterization model, most of the indirect radiative effects of CH₄ were taken into account in direct GWP100 estimation, except CO₂ production due to oxidation of CH₄. A study by Boucher et al. [31] suggests that CO₂-induced effects should be included in GWP calculations for fossil-derived CH₄ as it was found to make a significant contribution.

Besides the generally accepted IPCC model, alternative metrics for assessing GHGs have been developed such as index GTP (global temperature potential)

suggested by Shine et al. [295] and revised GWP formulae proposed by Fuglestvedt et al. [130].

Ozone Depletion Potential

The concept of Ozone Depletion Potential (ODP) introduced by Wuebbles in 1981 and developed by the World Meteorological Organisation (WMO) has been used to evaluate the effects of compounds on stratosphere ozone [45, 353]. The main identified ozone depleting substances are halogenated compounds (e.g. CFCs, HCFCs, halons); their ODP value released in the Montreal Protocol [327] provided a foundation for the characterization models given in the Scientific Assessment of Ozone Depletion [350], on which the CML 2 baseline method for ODP characterisation is based.

Actually, ODP calculations are often based on the assumption of steady state with constant emission independent of the time horizon [350], e.g. the ODP model adopted in CML 2 baseline is infinite time based. Although most of the ODP substances are long-lived compounds, their lifetime varies substantially (1–3,000 years). Thus time-dependent ODP have also been estimated in previous studies: the semi-empirical approach proposed by Solomon and Albritton [306] covered a 5–500 year time-scale where the ODP of compounds having a shorter lifetime than the reference gas CFC-11 decrease with increasing integrated time. This semi-empirical approach was used by WMO to compare with their ODP model and the ODP values suggested by Albritton (1992) under different time horizons were incorporated into the CML 2001 method library.

Acidification Potential

The acidification problem relating to the long-term exposure of ecosystems to acid inputs leads to forest decline and depletion of wildlife [17]. It is mainly caused by the release of protons or the release of the corresponding anions, e.g. SO₂, NO_x, NH₃, Cl [182]. Some approaches linked H⁺ release and molar mass to estimate Acidification Potential (AP) value of each acidifying substances with SO₂ as the reference substance, such as the models presented by Jensen et al. [182] and Kemna et al. [191] which are applied in the CML 1992 version. In some cases, moles of H⁺ release are directly used as the indicator result [182]. But as pointed out by Bates et al. [17], these AP methods considered the characteristic of pollutants but failed in estimating the fate of substances in different environments. Thus a more complex computation model RAINS (Regional Air Pollution Information and Simulation) was introduced, concerning parameters such as sensitivity of receiving ecosystem, spatial differences, the fate of substances and the extent of background deposition. The adapted RAINS-LCA version is currently amongst the most internationally accepted AP models [17, 156] and the average EU AP values derived from RAINS were incorporated in the CML 2 baseline method 2000.

However, the RAINS model only considers three acidifying gases (NH₃, NO_x, SO₂), thus the CML 2 baseline does not reflect other pollutants e.g. HCl, HF, or H⁺ [17]; but their acidification potentials (without fate) were modelled in CML 2001 version by linking H⁺ release and molar mass to estimate AP value [274].

Eutrophication Potential

Eutrophication is normally referred to as the enrichment of aquatic ecosystems with nutrients resulting in the increased production of phytoplankton, algae and higher aquatic plants, which deteriorate the water quality and reduce the utilization value of aquatic ecosystem [182]. Eutrophication can take place in both aquatic and terrestrial eco-systems; surplus N and P are the most important nutrifying elements [151] which, together with the degradation of organic compounds, are the major causes of Eutrophication Potential (EP). One indicator of aquatic eutrophication is toxic H₂S released from the anaerobic zone in sediment at the bottom of lakes, which is due to O₂ depletion by algal growth and decomposition of organic material/substances. Terrestrial eutrophication can be seen from the changes in diversity of species due to atmospheric N deposition [182].

The methodologies for EP calculation can be classified as the aggregation method and the scenario-based approach. The former leads to single indicator results (e.g. total N, total P or NO₃⁻ equivalents) and is commonly applied in LCIA methods e.g. CML, Eco-indicators 99. In contrast, the scenario-based approach distinguishes between different receiving eco-systems and EP is divided into two sub-categories (aquatic and terrestrial), e.g. the characterization model suggested by Detzel et al. [96]. Although RAINS-LCA also applied the second approach (scenario-based) considering both receiving ecosystems and spatial differences, only critical loads in terrestrial ecosystems were calculated; except NO_x and NH₃ fluxes, water emissions were not accounted for [156]. Thus to model aquatic EP in RAINS-LCA [156], the methods presented by Heijungs et al. [151] was recommended to be supplemented. Heijungs et al. [151] mainly considered substances containing N and P and developed a model on the basis of stoichiometric procedures and the average C: N: P ratio of algae; this method was modified and incorporated in CML methods [274].

Human Toxicity and Eco-Toxicity

Toxicity related impact categories are recognized as being amongst the most difficult to model in LCA due to the limited coverage of inventory, lack of consensus on characterization models, and the lack of toxicological and physicochemical data necessary for impact assessment [119]. Generally, in LCA characterization models, ecotoxicity is divided into sub-categories differentiating aquatic and terrestrial ecosystems but the approaches to handling human toxicity vary between models. The CML approach, (adapted from USES-LCA) aggregates

toxicity potential of all the substance into a single indicator result [142] whereas the Environmental Design of Industrial Products (EDIP) model divides human toxicity into sub-categories according to the exposure routes [274].

Both human and eco-toxicity not only depend on the effects and fate of substances but also the exposure process [182, 283]. A number of models accounting for these parameters have been published since the 1990s; they are commonly based on the multi-media fate models developed for computation of toxicity potential [160] such as the USES 1.0 (Uniform System for the Evaluation of Substances) [330], and the CalTox Model developed by McKone [236]. However, due to the fact that these models were originally developed for regional risk assessment, there are some drawbacks in terms of their realistic properties [157], e.g. the open character of modelled system, the limited coverage of compartments. After alteration [157], these models were further adapted for LCA modelling purpose: such as USES-LCA [157]. Besides, other methods adopting environmental multi-media, multi-pathway modelling approach include Impact 2002+ [183], Eco-indicator 99 [137] have been developed. The EDIP characterization method also considers fate and exposure [344] but it is developed from the key properties of substances [99, 283].

Great efforts have been made in comparison between different multi-media models at both the chemical fate level and the exposure/toxic effects levels [283]. Comparisons have also been conducted by testing models with hypothetical chemicals, through which, the most sensitive model parameters influencing outputs were identified [341]. Studies on the comparison of multi-media models in the LCA context reveal that models vary substantially in terms of scope, modelling principles and, most importantly, can fail to arrive at consistent characterization factors [99, 262]. This introduces potentially great uncertainty into LCA results.

To harmonize modelling approaches and characterization factors, a life cycle initiative was launched in 2002 by UNEP (United Nations Environment Program) and the Society of Environmental Toxicology and Chemistry (SETAC) [147]. By using an identical representative substance database the differing characterization factors generated by different multi-media models were compared in order to identify the influential parameters and sources of differences [147]. Based on a range of existing models (e.g. Impact 2002, EDIP, USES-LCA, Caltox) a scientific consensus model USEtox was developed [283]; USEtox not only gives the largest coverage of toxic chemicals but also uncertainty has been taken into account [283].

Time-dependency effects are another issue concerning calculation of toxicity potential. Generally, the methods reviewed above are steady state models with infinity as the time horizon [142, 160]. However, Huijbregts [158] stated that there are drawbacks in such models e.g. shorter-term toxic impacts could be misestimated, dominated by persistent substances which actually take effects after long-time exposure. Therefore, time horizon-specific toxicity potentials (20, 100 and 500 year horizons) were introduced in dynamic characterization models where metal and organic substances showed greater time-dependency due to their longer residence time in comparison with inorganic [158]; this approach was also adopted in the CML 2001 method library [142].

Smog

Two different smogs can be differentiated: summer smog and winter smog. Summer smog is also termed photochemical smog and refers to photochemical ozone formation resulting from the reactions between NO_x and hydrocarbons or volatile organic compounds (VOCs) in the presence of sunlight. Photochemical ozone is highly reactive and known to affect human health (e.g. eye irritation, respiratory problems) and plants (e.g. damage to leaves and photosynthetic function) [17, 182]. Winter smog, also referred to as acid smog, is caused by urban pollutants SO_2 and SPM (suspended particle matter) together with involvement of NO_x , CO and organic substances [274]. The most well known winter smog was the London smog taking place in December 1952, which was believed to have resulted in approximately 12000 deaths [32].

Photochemical ozone precursors include NO_x, CO, CH₄, and a number of nonmethane VOCs (NMVOCs). There have been several well-developed approaches for evaluation of their environmental impacts since early 1990's, e.g. the model developed by Heijungs et al. [151]. Jensen et al. [182] summarized these methods but also pointed out although they are scenario-based i.e. with different EU regions considered, they only cover organic but not inorganic precursors (e.g. NOx, CO). Thus, the approach with two subcategories was suggested to evaluate impacts of NMVOCs and inorganic compounds separately [182]. Models converting and aggregating the impacts of all precursors into a single indictor result were also developed, such as the method introduced by Derwent et al. [94]. This method adopted the concept of photochemical ozone creation potential (POCP) and derived the POCP index from a photochemical trajectory model [93-95]. The methods reviewed above generally adopted C₂H₄ as the reference compounds, the POCP of a particular chemical is quantified by the effects of a small increment in its emission on ozone formation relative to that resulting from an identical increase in the emission of C₂H₄ [17]. A model with indicator results expressed as kg ozone formation was also developed e.g. the POCP model presented by Guinée et al. [142], which was derived from the experimental data reported by Carter et al. [50].

Compared with summer smog, very few LCA methods concern winter smog. In Eco-indicators 99 the impact category respiratory inorganics is introduced which is equivalent to winter smog (defined in Eco-indicator 95) [137]. The winter smog model adopted in Eco-indicator 99 was originally developed by Hofstetter [154], which covers the pollutants SO_x NO_x and SPM and takes the fate of substances into account. But in most of the other widely accepted LCIA models, winter smog is not included e.g. CML 2001.

Land Use

Land use is an environmental concern in LCA with a group of impact categories involved [119]. However, although this issue has been widely discussed since the 1990s, there is no agreed approach incorporating land use in LCA [119, 235].

In previous studies, generally four areas of protection affected by land use were suggested: human health, natural environment, natural resource and man-made environment [291]; a range of potential impacts were proposed to quantify land use in the LCA framework, such as land occupancy, land transformation, impacts on biodiversity, impacts on soil quality [37, 119, 235]. Amongst the methodologies developed, some concerned one impact category e.g. the characterization model presented by Michelsen [242] which focused on the impacts of land use on biodiversity. Other studies covered several environmental impacts but focused on one protection area e.g. the characterization model given by Scholz [291] which quantified damages on the natural environment from land occupation and transformation by introducing an end-point impact indicator EDP (Ecosystem Damage Potential). Apart from characterization models, normalization and weighting factors for land use were also proposed in methodologies like Eco-indicators 99 [137]. Normalization and weighting land use is a controversial topic [242].

General guidelines for methodologies of land use impact assessment have been presented [47, 325] and research on the applications of characterization models has been carried out [235, 242, 243]. However, there is a lack of study concerning comparisons of land use models and their general applicability. Together with other issues on land-use such as the lack of consensus on characterization models this indicates a demand for greater efforts and further in-depth research is under way (e.g. the working panel formed within UNEP/SETAC Life Cycle Initiative) to address these issues [119].

1.3.2.4 Time Horizon

Temporal effects are an important source of uncertainty in LCA study [119]. In contrast to the steady-state, time independent LCA models, a dynamic approach incorporating dynamic effects at both the LCI and LCIA levels has been considered to improve the accuracy of LCA [208]. This section mainly focuses on the characterization LCIA methods.

As discussed in Sect. 1.3.2.3, the time-dependency of GWP, ODP, and toxicity potential has been taken into account in previous studies, amongst which the time scale of GWP has been the most commonly discussed. It is known that the time-horizon can produce significant influences on the characterized GWP outcomes [15, 192, 208]. The characterization models reviewed here were addressed at the midpoint level and actually most of them have been incorporated into the CML 2001 method library [142]. Besides this, dynamic endpoint models were also developed, such as the time-dependent acidification characterization model presented by Zelm et al. [356]. A good example of consideration of the time horizon in the damage-oriented approach is the 'perspectives' function in Ecoindicators 99 where three different perspectives are available i.e. E (egalitarian), H (hierarchist), I (individualist). The former two apply the longest time horizon (100,000 years) whereas the latter (individualist) integrates the exposure over 100-year with the proven effects included [137]. Generally, assumption of infinite

time (except for GWP) is suggested as the baseline approach for impact assessment with other time horizons applied in a robustness analysis [137, 142].

1.3.3 LCA of Biopolymers

A literature review was conducted to consider recent evaluations of biodegradable polymers derived from renewable resources on a life-cycle basis; the main focus of this was on starch-based biopolymers.

1.3.3.1 LCA of Renewable Resource-Based Biopolymers

LCAs have usually shown biodegradable polymers made from renewable resources to compare favourably with conventional petrochemical plastics. However, depending on the processing choices, number of recycling loops and end-life scenarios, the impacts of biodegradable foams may be equivalent or even higher than those of petrochemical systems [249].

A comprehensive review was carried out by Shen and Patel [293] covering polysaccharide-based bio-composites applied in packaging, textiles and engineering materials. It was found that generally the polysaccharide-based products deliver better environmental profiles than virgin petrochemical polymers in terms of non-renewable energy use and GWP at each life cycle stage. But they pointed out that when considering the recycled content, polysaccharide biopolymers can hardly compete with petrochemical polymers; furthermore, the comparisons also depend on the functional units defined. A higher mass input of polysaccharide polymer is often required to fulfil equivalent functions to petrochemical polymers, which can give different outcomes from comparisons carried out at the cradle-togate, per kg basis [293]. Furthermore, Shen and Patel [293] report that comparison results were sensitive to the end-of-life scenario: polysaccharide polymers showed environmental advantages over petrochemical products in life cycles with incineration scenarios but this was not the case in landfill scenario due to the long-term stability of fossil C in non-biodegradable petrochemical polymers in landfill.

Synthesized biopolymers derived from renewable resources such as those produced via fermentation by microbes have also not always been found to present more favourable environmental profiles to petrochemical polymers in LCA studies. These can be related not only to factors in the polymer production processes (feedstock or technology adopted) but also varied according to the LCA scope (system boundary, impact categories). Kim and Dale [197] reported that under current technology, corn grain-based PHA appeared to have higher impacts than PS (per kg basis) in terms of GWP, energy use, acidification, eutrophication and POCP but that better GWP and energy consumption profiles for PHA than PS could be expected via improvements in fermentation technology or changes in

feedstock (corn stover). Another study carried out on PHA carrier bags found that the outcome of comparison of PHA with PP was driven by the energy source used in PHA production [193]. Comparison of Polyhydroxybutyrate (PHB) or PLA with petrochemicals has also been found to depend on feedstock and the LCA scope. Harding et al. [146] considering production process only concluded that PHB derived from sugarcane sucrose was environmentally superior to PE and PP over almost all impact categories. Conversely, in a plastic bottle case study, Rebitzer et al. [280] concluded that corn-based PHB caused higher environmental impacts than its petrochemical counterparts due to corn-glucose production and heating requirements. Rebitzer et al.'s [280] results have been supported by Pietrini et al. [270] who also pointed out that expanding the system boundary from factory gate to grave led to PHB having a higher impact than PP even though on per kg of polymer (cradle-to-gate) basis PHB had a lower impact than PP. PLA compared to PET, PS and PP on per kg basis was reported to be environmentally superior to [334] but in a following study taking the final product into account, PLA was presented as environmentally disadvantageous over PS in most impact categories [222].

1.3.3.2 LCA of Starch-Based Blends

Relatively few full LCA studies (in English) on starch-based blends were found as publicly accessible [107, 176, 250, 331, 338]. Furthermore all these were on packaging case studies. Except for the PLA-dominated starch blend modelled by Vidal et al. [331], other studies mainly focused on wheat or maize-derived starch-based polymers blended with polyesters or other fossil-based polymers e.g. Ecoflex.

Vidal et al. [331] found that starch/PLA based blends delivered better profiles than PP films in GWP and fossil energy depletion but not on acidification or eutrophication. Similar conclusions were also reached by James and Grant [176]: various starch-based grocery bags were indicated as environmentally superior to conventional PE bags on abiotic depletion and GWP but not eutrophication. Estermann et al. [107] report similar observations on starch-PVOH blended loosefills which incurred lower burdens than EPS on most impact categories except ODP, eutrophication and aquatic ecotoxicity where impacts of bio- and fossil-based loosefills was comparable.

These studies have some limitations notably in the selective impact categories used and in the end-of-scenarios modelled. Except for two studies [107, 338] which covered a range of environmental aspects and modelled both aerobic and anaerobic degradation, the other studies either mainly concerned only one biological waste treatment or evaluated only GWP, abiotic depletion, acidification and eutrophication. Moreover, the data quality, especially uncertainties in both the LCI and LCIA results, were not interpreted in any of the studies reviewed. For instance, the inventory developed for PVOH was based on German producers and patent specifications with a high degree of uncertainty [107, 267].

1.3.4 LCA of Agro-Ecosystems

LCA has been applied to agricultural systems since late 1990s such as the studies on wheat carried out by Hanegraaf et al. [144], Cowell [66], Hansson and Mattsson [145]. A number of crops have been studied, amongst which wheat and its derived products will be the main focus of the current review.

1.3.4.1 LCAs of the Wheat Agro-Ecosystem

Although LCA was primarily developed in applications of industrial production systems, substantial effort has been made to develop the methodology for agricultural systems [9]. Some studies focus on the general methodology aspects, where wheat has been a main example [9, 34, 35]. In addition to ALCAs, application of CLCA in wheat farming systems have also been explored [289]. Based on the general LCA framework, regional LCA models for wheat were developed e.g. the UK model developed by Cranfield University [347]. Moreover, methods to integrate land use change in the LCA of agro-ecosystem have also been discussed, e.g. the approach reported by Kloverpris et al. [200], the method and case study presented by Hillier et al. [153] where soil C turnover resulting from land use change was integrated into LCA. In previous studies, estimates for agricultural field emissions of GHGs using IPCC Tier 1 approaches have commonly been applied. Biswas et al. [24] suggested using regional N₂O field emission estimates rather than IPCC default values as this led to an over 30 % decrease in total GHGs of wheat farming. Yu and Tao [355] used a regional simulation model to estimate field emissions in China and Hillier et al. [153] have also pointed out that IPCC Tier 1 approaches lack spatial precision thus effects of soil texture and climate remain unaccounted. Hillier et al. applied the process-oriented model Roth C to estimate the soil C emission due to land use change.

Some studies indicate that wheat is less energy efficient than other crops such as maize [51, 336] and a number of LCA studies were carried out to evaluate the different farming practices to improve the environmental profiles of wheat. Many aspects were covered in previous LCAs, such as the application of different pesticides [134, 148], weed management [185] fertilizer application rates [36, 52], choice between organic and artificial fertilizers [319] etc. Besides this, different farming systems were also examined by using the LCA approach e.g. comparison of organic farming with conventional systems [237, 268] or different cropping systems to explore environmentally efficient ways to utilize crop land [135].

In terms of applications of wheat grain and straw, a few LCA studies have concentrated on either animal feed [105, 329], or human food [21, 359] and several have focused on bio-fuel from wheat grain [19, 206, 223, 224, 231]. Two studies on wheat straw as a feedstock for bioethanol production have investigated impacts on soil [207] and land use change [55]. In addition, an interesting study explored gasified wheat straw utilized as feedstock for NH_4NO_3 fertilizer production [4] and Wang el al. [338] have studied wheat-based biopolymers [338].

1.3.4.2 LCA Approach and Environmental Concerns

ALCA has been commonly applied to wheat-based LCAs to date. Audsley et al. [9] have presented a guideline to a number of important system boundary issues: temporal boundary, capital equipment, human labour, soil, atmospheric deposition, crop rotation (referred to as the interaction between crops) and land use, but the specific methodology was not given. Amongst these issues, the importance of including capital equipment in LCAs of agricultural production was been widely emphasised. Atmospheric deposition has been modelled in a few studies e.g. the model presented by Williams and Audsley [347] and although whole crop rotations have been investigated [135, 153] relatively little attention has been given to the effects of previous crops on the crop modelled; in other words, the system boundary expansion by including the interactions between rotated crops has not been addressed. Only one study applied a process-oriented model to estimate soil C emission from wheat farming [153]. Apart from it, no study was found on the application of process-oriented models in LCA to estimate other field emissions from the wheat agro-ecosystem.

In addition to the system boundary, Audsley et al. [9] also indicated the importance of impact category selection, amongst which, GWP, abiotic depletion, eutrophication, and acidification are the most commonly modelled in LCA studies [24, 131, 135, 136, 268, 347].

In reviewing the literature it is apparent that data quality and data gaps limit the extent to which comparisons between studies can be reliably undertaken. Although quantitative results differ, some similarities have emerged between different LCAs. For instance, four studies conducted in the UK, USA and Germany indicate some common outcomes: the dominant contributor to the total energy input was fertilizer manufacture (50-52 % in UK), especially nitrogen fertilizer (39, 47, 40 % in UK, USA, Germany respectively), followed by diesel fuel (31–35 and 25 % in UK and USA respectively) [202, 271, 324, 348]. The comparison of reviewed studies has led to following key findings for wheat grain production: for wheat production, fertilizers and fuels are the main causes of environmental impacts. Fertilizer production, field operations, especially cultivation, and harvesting are the predominant fuel consumers. Fertilizer application and manufacture dominate GWP; other main sources include GHGs emitted from soil or fuel combustion in field operation. Field emissions and leachates due to nutrient application and fuel combustion are significant contributors to both eutrophication and acidification potential.

1.3.4.3 Field Emissions and Leachate

Since the IPCC's First assessment report released in 1990, agriculture has been recognized as an important source of GHGs. CO₂ emitted from microbial decay of crop residues and soil organic matter (SOM) or burning of crop litter is one of the GHGs concerned. The other two important GHGs from agricultural land are CH₄

and N_2O . The former is released from the decomposition of organic materials under anaerobic conditions; while the latter is generated during the microbial transformation of nitrogen in soils, enhanced by the available N which exceeds plant requirements, especially under wet conditions [300]. Apart from GHG fluxes, other field emissions from agricultural land have also attracted more and more attention in recent years including N gases (NH₃/NO/N₂) and C/N/P/K leaching as well as trace emissions e.g. pesticide run-off [9]. Although pathways for these emissions vary, most of them are products from C/N cycles within agro-ecosystems and are highly related to nutrient applications: e.g. NH₃ is regulated by volatilization and the equilibrium between NH₃ and NH₄⁺; NH₄⁺ and NO₃⁻ leaching are dependant on N fertilizer supply and biochemical processes (e.g. NH₄⁺ oxidation, nitrification and denitrification).

Agriculture plays an important role in both the global and UK emission profiles. According to the IPCC Fourth assessment report [300], agricultural CH₄ and N₂O emissions have increased globally by 17 % from 1990 to 2005; in 2005, agriculture accounted for 10–12 % of total global GHGs, approximately 60 % of N₂O and 50 % of CH₄. In the UK, agriculture is recorded as a major contributor to N₂O and CH₄ emission (75 and 38 % in 2007 respectively) [92]. As for other trace gases/leaching from agriculture in UK, over 90 % of NH₃ emission is attributable to agriculture, where soil emission accounts for 10 % [92] and approx 60 % of nitrate and 25 % of phosphate in waters in England originate from agricultural land [91]. These increasing emissions affect several environmental issues, i.e. global warming, acidification and eutrophication.

1.3.4.4 Modelling Approach for the Simulation of Field Emissions

To simulate field gas fluxes/leaching, generally there are two modelling approaches applicable: empirical models such as the IPCC methodology [209] and process-oriented models e.g. DNDC (Denitrification–Decomposition). The latter take into account more factors involved in C and N cycles in a specific ecosystem such as soil, climate and fertilizer type [209]: thus it is more site-specific and offers an option to expand the LCA system boundary. The biochemical processes simulated can also be different between the 2 model types. Take N₂O simulation as an example: the current IPCC methodology (second phase) extends the previous method (phase one) to include both direct N₂O emissions and indirect N₂O emissions (indirect N₂O via two pathways: NH₃/NO_x deposition and N leaching) [164, 166, 209], whereas DNDC includes direct N₂O emissions.

To date, the major process-oriented models for GHG emissions from agricultural systems include DNDC [209], Daycent [265] which was developed based on the Century model [190], Roth-C 26.3 [62] and its new version RothPC-1 [181], Sundial [33, 138] expert N [186] and Ceres [132].

DNDC Model

Amongst process-oriented models, DNDC is one of the most well-established and has been widely validated [1, 12, 18, 39, 41, 42, 44, 139, 302, 339]. Validation results reported in previous studies generally confirmed a good agreement between DNDC-simulated and field-measured values of N₂O, CH₄, NO₃⁻ for cropland and seasonal emissions [12, 18, 44, 321].

DNDC was originally developed for upland agro-ecosystems in the USA [214]. At the early development stage, soil climate (thermal-hydraulic), denitrification and decomposition (including nitrification processes) and plant growth sub-models were developed to predict N₂O and CO₂ flux [212, 213]. Then the simulation of other trace gases (NO, CH₄, NH₃) and NO₃⁻ leaching was explored and reported [210, 211]. Now the latest version DNDC (version 92/93) is constructed with two interacting components: the first component includes 3 sub-models i.e. soil climate, plant growth and decomposition and the second component consists of nitrification, denitrification and fermentation sub-models [211]. In DNDC, ecological drivers (climate, soil, vegetation) and soil biochemical reactions are linked via soil environmental variables such as temperature/moisture/pH, and available substrates (NH₄⁺, NO₃⁻ and dissolved organic carbon) to simulate trace gas fluxes and leaching from agricultural land.

Data Quality of DNDC Output

To test the data quality of model output and performance of DNDC, most previous studies analyzed the sensitivity of model output to input parameter variation relating to climate, soil crop parameters and farm managements. Based on the sensitivity analysis results reported, the main input parameters affecting DNDC outputs are summarized in Table 1.3.

Another data quality assessment—uncertainty analysis is only addressed in very few publications on DNDC [214, 277]. In those studies, the Most Sensitive Factor (MSF) method was adopted to determine the uncertainty of DNDC output. Although MSF was verified by running against Monte Carlo simulations [214], MSF only gave a range as results; whereas Monte Carlo generates a set of results which represent samples from a frequency distribution. A Monte Carlo simulation function has been built into the current DNDC model but it splits the range of ecological variable into eight intervals, within which random samples are generated. This could lead to a discrete frequency distribution as the uncertainty result. Thus, more efforts could be made to modify the Monte Carlo method built into the DNDC model.

The built-in Monte Carlo function offers an approach to obtaining quantified uncertainty information (e.g. variability, probability distribution) of model outputs which can be further introduced into the LCA model to estimate the uncertainties of LCIA indicator results. So far, no publicly available study has been found on this topic and it was therefore investigated in the current research.

Table 1.3 Sensitive factors affecting DNDC model

Trace gas emission/leaching	Highly sensitive factors	References
$ m N_2O$	Soil clay content/texture	[1, 18, 212]
	Soil organic C	
	Annual temperature	
	Soil pH	
	Annual precipitation	
	Soil temperature	
	Soil nitrate	
	Fertilizer type	
	Water management	
N_2	Annual precipitation	[212]
	Soil pH	
	Annual temperature	
	Soil organic C	
CO ₂	Soil organic C	[212, 214]
	Soil clay content/texture	
	Annual temperature	
	Crop rotation crop residue	
	Annual precipitation	
CH ₄	Soil texture/clay content	[12, 214]
	Soil pH	
	N fertilizer application rate	
	Crop rotation	
NO ₃ ⁻	Initial organic carbon	[211, 212]
	Soil temperature	
	Annual precipitation	
	N fertilizer application rate	
	Soil moisture	

Simulation Models and LCA

Research has been carried out to compare different modelling methods for field emissions [71, 129, 164, 209, 215, 303, 304]. Notably, studies by Li et al. [209] and Hutchinson et al. [164] compared IPCC and DNDC and found that both models gave similar estimations of annual national inventory of direct N_2O emission although geographical patterns differed.

In LCAs the IPCC Tier 1 approach and its default emission factors (EFs) have generally been applied concerning GWP e.g. EBAMM [112], BESS model [216, 217]. However, in the IPCC approach, meta-analysis of available experimental data was undertaken to develop EFs [102], for the purpose of national GHGs inventory reporting rather than for site-specific studies. Thus IPCC is best regarded as a first approximation, applicable worldwide but disregarding of regional or local agro-ecosystem characteristics [102, 163]. Therefore, DNDC and other process-oriented models have been recommended by LCA experts to more closely approach site specific relevance of, for example, N₂O estimation than the

IPCC approach [152, 153]. Only few studies have so far been carried out on the integration of process-oriented models (RothC, Daycent) in LCA studies [2, 153, 199]. However, these mainly focused on GHGs emitted from agricultural lands at region or country scales and the LCA system boundary expansion issues (e.g. soil fertility change, crop rotation) were not discussed. Neither site-specific study on integrating process-oriented models into LCA nor comparisons between process-oriented model and IPCC within an LCA framework were found. In addition, the literature review suggested that the data qualities of model output under an LCA context have not been presented in any previous study. But this issue is worth exploring when integrating process-model into LCA because the robustness of LCI database and LCA findings has been widely recognized as significant in order to deliver unbiased information for decision-making [119].

1.4 End-of-Life

As noted earlier, this phase of the life cycle can have a considerable bearing on the results of comparative studies between biodegradable biopolymers and their petrochemical alternatives.

1.4.1 Waste Treatment Options

In the UK, annual waste production is dominated by construction waste, commercial and industry waste [75], household waste only makes up less than 10 % of the total waste. However, UK household waste makes up 88 % of municipal solid waste (MSW) [90]. Here as defined in the Landfill Directive 1999/31/EC [110] 'municipal waste' is referred to as waste from households, as well as other waste which is similar to household waste in terms of its nature and composition. Generally, MSW is either bulk collected or source segregated [178]. Applied waste treatment routes include AD, composting, recycling, landfill, incineration and mechanical biological treatment (MBT). For the former three options, prior to disposal, a pre-treatment is required; while the latter three routes are suitable for bulk collected MSW [245].

Amongst all these disposal routes, landfill has traditionally dominated in the UK, accounting for 43 % of total waste generated in 2002/03 (including MSW, commercial waste, construction waste), the remainder being mainly recycled or recovered (42 or 10 %) [77]. Regardless of commercial or construction wastes, approx 54.5 % of England's municipal waste stream ended in landfill in 2007/2008, whereas the remaining approximately 12.9 million tonnes were recovered either by recycling, composting or incineration [85]. Although the total annual municipal waste in England increased, there has been a significant decreasing proportion of municipal waste ending up in landfill [84] since 1999 when the EU Landfill

1.4 End-of-Life 29

Directive [110] acted as main driver to divert MSW, especially biodegradable municipal waste (BMW), from this disposal route. Legislation set up targets for England to decrease BMW going to landfill to 11.2 million tonnes in 2010, and 5.2 million tonnes in 2020. The 2010 target was virtually met in 2006/2007, when BMW landfilled in England was reduced by 17.2 % (11.5 million tonnes) compared with 2004/2005 [81].

AD and composting are widely used biological treatment options for BMW. Actually in England, according to the statistics, biodegradable waste is one of the major fractions of municipal solid waste, especially household waste, nearly 60 % of which is contributed by biodegradable components [74]. Typical organic household waste in England consists of nearly 70 % garden waste, 27 % kitchen waste, and a small amount of paper waste [184]. Composting increased considerably during the ten year period 1997/98 to 2007/08 and in 2007/08, approx 12 % of household waste generated in UK was composted [88, 89]. In contrast, AD has developed more slowly with only two AD systems operating in the UK on MSW [245]. However, the total UK capacity of biological treatment (including AD, composting, MBT) has substantially increased; the total capacity for source segregated and mixed waste in 2006/07 was estimated as 5.3 million tonnes at a usage level of 71 %, thus a great potential exists for further treatment of BMW [301].

The mechanisms and classification for each waste treatment option are discussed in detail below.

1.4.1.1 AD

AD Technology Development

AD technology for biodegradable solid waste has primarily followed the conventional approach used for sewage sludge digestion over the last 50 years. AD has played an important role in the EU for treating the organic fraction of municipal solid waste (OFMSW) since the late 1980s when the first full scale AD plants for OFMSW were commissioned. So far a total of 168 AD facilities have been recorded [245]. In contrast, the development of AD technology in UK has been slow, with one system operating on MSW in Leicester treating OFMSW and one pilot scale AD system located in Shrosphire [245].

The AD process involves a dynamic complex system in which microbiological, biochemical and physico-chemical attributes are closely linked [6] to effect a processing of the biodegradable waste into biogas and a reduced volume of sludge. In comparison with other waste treatment options, including biological treatment method, AD has been identified as the most environmentally sustainable option for biowaste treatment as it offers a unique technology which not only diverts biodegradable waste from landfill but also produces bio-energy as well as a beneficial soil conditioner [245]. In addition to biogas-based electricity, another potential

beneficial product is renewable heat yielded from combined heat and power (CHP) systems, which ideally could be used by district or industrial heating schemes [22]. Generally there are four main classifications of AD systems [245]:

- \bullet Classified by temperature: mesophilic (30–40 °C) or thermophilic (50–65 °C) digestion
- Wet digestion (feedstock with less than 15 % dry solid) or dry digestion (feedstock with dry solid content 20–40 %)
- Single step (one vessel) or multiple step digestions (system with several digestion vessels, usually two-step digestion i.e. hydrolysis and methanogenesis)
- Batch digestion (after loading feedstock, the digestion vessel is sealed until thorough degradation occurs) or continuous digestion (vessel is fed continuously and degraded material is continuously removed)

AD Biological Process

Although AD systems differ, generally five trophic groups are considered to be relevant to the process i.e. hydrolysing bacteria, acidogenic bacteria, acetogenic bacteria, aceticlastic and hydrogenotrophic methanogens [285]. They are involved in different metabolic steps. Firstly the carbohydrates, lipids, proteins, etc., are hydrolyzed by extracellular enzymes released by hydrolytic bacteria; then, in the acidogenesis step, the molecules produced from the first stage, such as sugars and fatty acids, are converted into volatile fatty acids, alcohols, CO₂ and H₂ [310]; simple molecules created in the acidogenesis step are then converted in the next phase by acetogenic bacteria mainly into acetic acid, H₂ and CO₂; finally, all these intermediate products are converted into CH₄, CO₂ and water in the last step where the methanogenic bacteria are involved [322].

Biodegradability of Substrates

According to the extent to which the degradation of a substrate is achieved, the biodegradability under anaerobic conditions can be specified as ultimate (fully converted to inorganic forms), primary (converted to inorganic and other products in specific metabolic process) or inherent (potentially degradable if action is taken such as increasing the inoculum ratio) [285]. Generally two methodologies have been adopted in previous studies for testing the biodegradability of an organic material under anaerobic conditions: (1) the BMP assay developed by Owen et al. [259] or (2) the ISO standardized method [169]. Both methods are batch-feeding techniques with biodegradability determined by monitoring the CH₄ yield from samples incubated anaerobically in a chemically defined medium.

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Key Factors Influencing AD Process

Many factors influence the AD processes, such as pH, temperature, organic loading rate (OLR), and the presence of inhibitory substances. Amongst all the parameters, the ratio of inoculum to substrate (I/S) and the biodegradability assessment are amongst the most important, especially for high solids, batch digestions [253, 278]. An I/S ratio of approx 1 proposed by Owen et al. [259] was applied in BMP assays as standard which is expressed in terms of volatile suspended solid (VSS): chemical oxygen demand (COD), but an increasing ratio was stated as necessary for some substrates, and a ratio of 2 was suggested [58]. Raposo et al. [278] studying I/S ratios between 1 and 3 found that biogas production was inversely proportional to the I/S ratio and a ratio of 1 gave a higher maximum specific methane production rate (SMPR).

Temperature and pH also play important roles. The methanogenesis is reported to be found within the temperature range of 4–100 °C [310], generally AD is operated at mesophilic temperature (35–37 °C) or under moderate thermophilic conditions (50–60 °C) [245]. However, thermophilic AD was considered less preferred than mesophilic as it is more sensitive to environment change giving lower CH₄ yields [322]. Monson et al. [245] note that mesophilic AD systems contain greater diversity of micro-organisms. An optimum pH can enhance bacterial activity as well. For methanogenic bacteria, the optimum pH is around neutrality or slightly alkaline [205]. For acidogens and acetogens in the AD process pHs above 5.5 have no inhibition effects [245]. Therefore neutrality or slightly alkaline pHs are suggested for AD operations i.e. pH range of 6.5–8.2 [310] or even a narrower range of 6.8–7.2 [245].

As optimum parameters like temperature and pH differ for specific anaerobic trophic groups, therefore compared with one stage digestion, two (multiple) stage digesters can provide optimum environmental conditions for each bacteria group leading to better performance [245]. Actually by buffering OLR in the first tank, two-stage AD system provides a constant feeding rate to methanogens which is the dominant group in the second stage and is one of the most sensitive groups in the anaerobic consortium [310]. Consequently, there is a great benefit in two stage AD giving accelerated digestion rates, better stability and increased CH₄ yield [332].

Another process parameter is retention time which includes hydraulic retention time (HRT) and solid retention time (SRT). The former is referred to the mean time that any proportion of liquid feed remains in a digestion system; the latter is defined as the mean time for which any portion of solid feed or microbial biomass remains in the digester. In single stage digestion system, SRT and HRT are the same; while in two-stage AD system longer SRTs are achieved, thus higher degradation rates and biogas yields are obtained [245]. This proportional relation between degradation rate/biogas production and SRT was confirmed in a previous study [258].

In addition, OLR is also critical, which is measured in terms of COD or volatile solid (VS) of feed to a unit volume of digester per unit time [245]. Maximum OLR

in OFMSW range between 6 and 9.7 kgVS/day/m³ varying with biodegradability of feedstock and AD system [322].

Apart from the organic carbon source for microorganisms' growth, a medium containing multiple nutrients especially nitrogen is also needed for cell synthesis. Optimum C:N ratios are between 20: 1 and 30: 1; other nutrients such as S, Mg, K, P, Ca, Fe, Zn, Al, Ni, Co, Cu and vitamin B12 are necessary for synthesis of new cells [245]. In large-scale AD plants those nutrients are contained in the OFMSW, while in lab-scale AD systems, such as BMP assay, these nutrients and vitamins are supplied in the media [259].

The feedstock provides nutrients but also may contain compounds which could be toxic or inhibitory to the AD process. Methanogens are usually the most sensitive bacteria groups [310]; the toxins for them include NH₃, NH₄⁺, soluble sulphides and soluble salts of metals etc. For instance, NH₃ is a product from biodegradation of protein content present in kitchen waste or garden waste [188, 189] and it is generally accepted that NH₃–N concentrations exceeding 1,500–3,000 mg/L at a pH higher than 7.4 are inhibitory [245], as the high pH can shift the equilibrium towards the unionized NH₃ form [322].

During digestion of biodegradable solid waste volatile fatty acids can be inhibitory at high concentrations and their inhibitory effects have been widely studied. However, in a well-balanced AD system VFAs should not accumulate; moreover, the digester's alkalinity conditions—regulated by either naturally occurring components of waste or pH buffer (e.g. lime)—have buffering effects on VFA accumulation [245].

1.4.1.2 Composting

Composting is a high solids aerobic microbial degradation process [230], offering a route for recycling organic matter and nutrients from the BMW [245]. Composting can be carried out at various scales, including large-scale centralized systems, small-scale on-farm or community composting and home composting [178]. The biological processes of decomposition operating at these different scales are similar: an initial mixing phase with mesophilic growth, followed by a thermophilic phase, and a longer stabilization phase with lower temperature [254].

The composting industry has a long development history, its concept originated in Holland in 1929 [299]. Since 1984, when pilot projects were initiated in Germany, Austria, Switzerland and the Netherlands, separate collection and composting of BMW has been implemented in several EU countries, especially since 1996, when the EU took further steps to divert BMW from landfill [273].

According to a survey on centralized composting of source-segregated waste [301], by 2006/07 the number of composting sites and the amount of source-segregated waste composted in the UK had increased to over 222 sites and 3.6 million tons respectively. 82 % of the composted waste was MSW; and over half of it was disposed of in centralized biological treatment or composting sites with a smaller proportion was treated at farm-scale composting facilities.

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Amongst different industrial centralized composting methods, generally windrow composting systems are the most widely applied as they offer a practical and economic approach. In-vessel composting systems are also used such as tunnel composting, housed bay piles, composting in vertical towers, rotating drums [78]. In the UK, open-air mechanical turned windrows (piles) still dominate accounting for 79 % of composted waste in 2007 [301], though in-vessel composting has increased, making up 11 % of composted waste.

In addition to centralized composting, local authorities also introduced composting schemes for the community sector. According to a survey conducted by Jones et al. [184], home composting in the UK represent as a commonly applied composting method, making up 45.7 % of composted household waste; other important compost routes are kerbside collection and civic amenity collection operated by local authorities.

During composting, microorganisms use the organic matter as a food source, producing heat, CO₂, water vapor, and humus as a result of their growth and activity [61]. During the composting process, initially mesophilic bacteria predominate and decompose the readily degradable organic matter such as proteins, starches, and fats. The heats released by these bacteria raises the temperature of compost pile and above 40 °C thermophiles dominate the bacterial community. During this stage, most of the organic matter is converted to CO₂ and humus and the temperature of an unventilated composting pile can reach 70 °C while in a aerated pile, the temperature typically achieves between 55 and 65 °C. Some compost piles can attain an 'over-heat' level (above 75 °C) and in such cases microbial activity virtually ceases only spores survive and germinate when favorable temperature is restored. In the final stage, the compost temperature slowly reverts to mesophilic levels initiating the stabilization phase where mainly lignin and humic materials are left coupled with a decline in bacterial activity but in which fungi dominate [61].

The final compost products can be used as soil conditioners, mulch, or top soil for sectors such as agriculture, landfill restoration, horticulture, sports turf etc. It is estimated that in 2007, 2.17 million tons of compost was produced in the UK from 3.6 million tons of source-segregated waste and primarily used for agriculture (especially cereal crops) (53 %), landfill restoration (15 %) and landscaping (12 %) [301]. Quality cured compost not only provides nutrients to soil but also introduces diverse microorganisms combined with organic matter to benefit the soil nutrient cycle. However, an incompletely cured compost which maintains a higher microbial activity can compete with plant roots for oxygen and high levels of soluble organic matter in poorly prepared composts can induce phytotoxicity problems in horticultural applications [61].

1.4.1.3 Incineration

Incineration is another disposal route diverting MSW from landfill. Together with biological treatment, it provides options for separate waste streams i.e.

bio-degradable and non-biodegradable wastes [245]. But compared with waste recovery/recycling routes, this energy recovery route is listed as the second choice in EU and UK legislation [110]. In fact, incineration has undergone substantial development since the beginning of the twentieth century. The share of MSW incinerated in the Europe varies from 0 % in Greece to high percentage (almost 100 %) in Switzerland [282]. In the UK incineration with energy recovery accounts for the treatment of only 2.3 % of total waste generated (including MSW, commercial and construction waste) [77]; and in 2007/08 only 11 % of MSW produced in England was incinerated [86].

Incineration involves the combustion of unprepared (raw or residual) waste in a sufficient supply of O_2 . As the fuel is fully oxidized the waste is mostly converted to O_2 and O_2 with about 20–30 % by weight remaining as bottom ash—a noncombustible solid material [80]. Incineration produces heat with a thermal generating efficiency of approx 80–90 % which can then be used via a boiler to raise steam (recovery rate generally 80 %) and the steam generated is further used either through a steam turbine to produce electricity or for heating purpose [80]. A modern incinerator producing electricity only can achieve a maximum electrical generating efficiency of 27 %, typically ranging between 14 and 24 % [80].

Whilst energy-recovery is an advantage of incineration, the release of pollutants including CO₂, SO₂, NO_x, CO, HCl, particulate and especially products from incomplete combustion such as polychlorinated dibenzo-p-dioxins are the main concerns [245]. Therefore, minimum temperature and residence time for OFMSW are regulated to achieve complete combustion and strict emission limits are set [80].

1.4.1.4 Recycling

Recycling is the preferred approach for EU waste treatment [110]. The average MSW recycling rate in the EU reached 37 % in 2007 [288]. In the UK, approx 22 % of household waste generated in England was recycled in 2007/08 [88]; recycling rate for commercial waste and construction waste in England was much higher (45 and 50 % respectively) and in 2002/03 the average recycling rate for total waste generated in UK already reached 42 % [76, 77, 79].

The largest component of UK household waste that is recycled is paper, followed by co-mingled material, glass and metals; plastics only occupied a small fraction [82]. The UK recycling rate for paper and cardboard doubled from 32 % in 1993 to 71 % in 2007 [87], and the glass recycling rate in 2008 was over 50 % [86]. The recycling of post-consumer plastic waste in the UK has increased since 2001 but was still less than 20 % in 2008 [272].

Actually the recycled plastics include two sources: one is plastics arising from industrial 'process scrap', i.e. polymers left over from production; the second one is post-consumer plastic waste which is recycled after its first full service life. The former shows high recycling rates—95 % in UK; whereas the latter is much lower. Across the EU, from 2007 to 2008, average recycling rate for post-consumer plastic only increased by less than 1 %, achieving 21.3 % [272]. This can be

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explained by factors such as the difficulties in collection of post-consumer plastics, contamination of the plastics and the need, ideally, for recycling technologies able to separate distinct plastics groups.

Recycling technologies can be broadly classified as mechanical or chemical (feedstock) recycling [340]. The former refers to processes that involve the melting, shredding or granulation of pre-sorted waste plastics; the latter refers to technologies to break down polymers into monomers which are used again in refineries, or petrochemical and chemical production. Mechanical recycling is the most commonly applied technology in the UK and EU: 98.6 % of EU recycled post-consumer plastic is treated via mechanical recycling and only 1.4 % by feedstock recycling [272].

Different mechanical recycling technologies have been developed for distinct plastics. For instance, in UK, a successful NIR sorting system has been developed for HDPE bottles and applied in two newly established recycling plants to produce food-grade recycled HDPE [272, 352]. Other mechanical recycling systems have been developed for PS and PP rigid plastic trays, plastic films, etc. [272]. As for feedstock recycling, new technologies attracting increasing attention include pyrolysis and gasification. The former is a thermal degradation under anaerobic conditions and the latter involves partial oxidation of the substances. They show advantage over mechanical recycling in terms of flexibility of input material and tolerance to impurities [340] though the energy released may be less than combustion of waste in incineration [80].

1.4.1.5 Landfill

Landfill can be considered as the 'conventional' disposal route for bulk collected MSW and, globally it is estimated that 1.5 billion tones of MSW are landfilled annually [316]. The UK has relied on landfill for disposal of MSW due to its availability and low operational costs [178]. There were 19,196 known, open or closed landfill sites in Great Britain in 2000 [65, 177] and in 2001, 2300 landfill sites were in operation [264]. The EC Landfill Directive introduced three main classes (inert, non-hazardous and hazardous landfills) [110]. Specifically classified landfills in the EU include [257]:

- Open dump landfill to dispose of untreated municipal waste, no safety measures
- Sanitary landfill to dispose of untreated municipal waste but with physical barriers to protect public (liners and caps, CH₄ oxidation layer)
- · Landfill for hazardous waste
- Landfill for non-hazardous waste including MBT and incineration residues
- Landfill for inert waste including excavated earth and construction waste

The first two types represent the conventional landfill systems where no active measures were taken to enhance waste degradation. In the future landfills may only accept waste that has been either pre-treated via incineration or by mechanical/biological treatment [257].

Landfill process include four phases [14, 240, 316]. Landfilled MSW firstly undergo biochemical processes in the presence of oxygen, the organic waste near the surface of landfill is oxidized aerobically, CO₂ and water vapor are produced. But the main biochemical process in landfill is similar to AD whereby complex organic matter is hydrolyzed by fermentative bacteria to soluble molecules, which are further converted to simple organic acids, CO₂ and H₂; in the final stage, mainly methanogenic bacteria break down fatty acids to CH₄ and CO₂. CH₄ makes up over half of landfill gas yielded either by bacteria digestion or reaction of CO₂ with H₂.

In modern landfill sites equipped with landfill gas collection systems, the landfill gas is captured and recovered to generate electricity and heat. It was reported that until 2001, globally there were 955 landfills with biogas recovery systems and the UK ranked as the third in the world in terms of the number of landfill gas recovery plants (135 landfill sites) [316]. Based on a conservative estimation of 50 m³ CH₄/tonnes MSW landfilled, Themelis and Ulloa [316] have shown that annual potential CH₄ generation from global MSW landfilled (1.5 billion tonnes per year) is 75 billion m³ of which less than 10 % is captured. In addition to the landfill gas collection, landfill leachate produced is also treated prior to discharge to surface water [225]. Besides these collection systems, cover layers are also applied in landfill management e.g. CH₄ oxidation layer to reduce CH₄ emissions, or the water retention layer to minimize the entry of rainwater and further reduce leachate [238, 257]. A new design referred to as 'bio-reactor landfill' is equipped with leachate re-circulation system to accelerate the biochemical degradation of MSW [238]; in another semi-aerobic technology introduced, combinations of aerobic and AD can be applied: once the CH₄ generation reaches a level too low for energy recovery, the aerobic step is activated by injecting air from bottom of landfill site [225].

1.4.1.6 MBT

MBT is a generic term for an integration of a range of processes commonly found in other waste management technologies, it incorporates two core stages, i.e. mechanical and biological treatments for residue MSW [83, 114]. Actually, the first MBT plants were developed with the aim of reducing the environmental impacts of landfilling residual waste, therefore, MBT supplements rather than replaces other waste treatment technologies [83].

Currently there are more than 70 MBT plants operating in the EU [83, 114] with over 40 plants and most MBT technologies being developed in Germany. Only 7 MBT plants are operated in the UK, such as the Biffa MBT plant located in Leicester, the SITA plant in operation at Byker and the smaller scale Premier plant in County Durham [78, 83].

A typical MBT system is illustrated in Fig. 1.4. Before biological treatment or a sorting process the waste is prepared; mechanical techniques such as ball milling, hammer milling or shredding are generally employed for waste preparation. Then,

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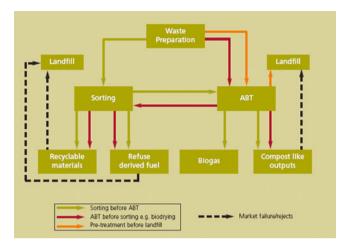


Fig. 1.4 MBT system [83]. *Notes* ABT (advanced biological treatment) includes in-vessel composting and AD or bio-drying [78]

the mixed wastes enters a sorting process where various separation technologies are applied and finally the separated fractions are distributed to further processes e.g. recycling, landfill, or biological treatment [7].

As indicated in Fig. 1.4, MBT processed waste contains recyclable material (metal/plastics/glass), compost-like output (CLO), refuse derived fuel (RDF), biostabilized landfill waste and biogas [7]. Generally, the CLO products from MBT are applied as landfill cover or in land restoration rather than as soil improvers for crops as CLO derived from mix waste is considered as lower quality than compost because of contamination and toxic elements [7, 83]. Another product is electricity. Although it can be generated from both RDF and biogas, the energy derived from RDF is very limited due to the advanced conversion technology required, which includes advance thermal treatment (pyrolysis gasification), or a conventional combustion facility with high-quality CHP system. Only two plants operating in UK utilize RDF to generate electricity [83].

1.4.2 LCA and End-of-Life Scenarios

LCA has been widely applied to waste management, either to investigate the waste management system in a region [103, 141, 260, 357] or to compare different MSW treatment options. But most comparisons of disposal routes have focused on landfill, incineration, recycling, rather than on composting and AD. Generally the LCA results agreed with waste hierarchy i.e. recycling is environmentally preferable over incineration and further over landfill [26, 120, 248, 290].

1.4.2.1 LCA of Recycling

Amongst different waste treatment options, recycling is one of the most commonly studied disposal routes in LCAs and generally considered as an option offering more environmental benefits than landfill or incineration. A comprehensive review undertaken by WRAP [351] covered the majority of materials which are often collected in UK for recycling, including paper/cardboard, plastics, aluminium, steel, glass, wood etc. This concluded that in almost all LCAs of paper/cardboard reviewed, recycling was found to be environmentally preferable to landfill, but the comparison of environmental profiles between recycling and incineration varied with impact categories. Similar conclusions were reported by a another review conducted on paper/cardboard [333]: all studies under their review showed recycling offers more environmental benefits than landfill and incineration.

In the case of plastics, three scenarios were examined [351]: scenario 1 closed-loop with 1:1 ratio of recovered material to substituted virgin material, scenario 2 closed-loop with ratio of 1:0.5, and scenario 3 assuming substantial washing of plastic before recovery. WRAP [351] concluded that recycling is environmentally preferable to landfill and prevailingly better than incineration in scenario 1, but, incineration might be found environmentally equal or better than recycling in scenarios 2 and 3. In fact, in most of LCA studies, a 1:1 substitution ratio is assumed, such as those of Finnveden et al. [120], Eriksson et al. [106] and as presented in the Eco-invent database (Version 2). Moreover, most of LCA studies concern mechanical recycling technology with only one found involving chemical feedstock recycling of plastics. Perugini et al. [269] found mechanical recycling to be more environmentally preferable than feedstock recycling except in the energy consumption impact category.

WRAP [351] point out two knowledge gaps in the LCA of mechanical recycling i.e. significance of sorting separation process in recycling of mono-material, and open-loop recycling. Although methodologies applied in open-loop recycling were discussed [118, 143, 354], the limited case studies applying open-loop recycling mainly focused on metal products such as the study conducted by Matsuno et al. [234].

1.4.2.2 LCA of Landfill

A main concern in LCAs that include landfill is the temporal system boundary, this often being a substantial difference between landfill and the other processes [117, 118]. Finnveden [118] discussed this issue and summarized two principles in terms of time-boundary definition i.e. defined number of years or critical time period. The latter refers to the period until all emissions fall below acceptable or background concentration levels although this was considered to be a restricted approach due to uncertainties in future acceptable emission loads and the times taken to reach that level [118].

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Thus, an approach differentiating two time frames were proposed: surveyable time-period (a century) and a hypothetical infinite time-period [118]. This approach was also recommended by SETAC: if the first choice of infinite time is not applicable, 100-year should be considered as the second choice [257]. The time horizon defined in previous LCAs has varied, Menard et al. [238] defined infinity as their temporal boundary, Obersteiner et al. [257] and Manfredi and Christensen [225] adopted a 100 year time frame; less than 30-year time periods have also been investigated or compared with other time horizons [46, 118]. As for the Eco-invent database v2.0, two emission categories are included i.e. short term and long-term, which are defined as a 100 and 60,000 years after present respectively [128].

Most LCAs have concentrated on short-term landfill emissions [98, 203]. Laner [203] pointed out that the time boundary could be a critical parameter and a main source of uncertainty in some impact categories, especially impacts caused by metal emissions and leachate. This is consistent with earlier work by Finnveden [117]: the fraction of metal emitted within 100-years only reaches between 10^{-5} and 10^{-3} [120]. Thus metallic emissions under infinite-time need considering. However, Obersteiner et al. [257] argued that the uncertain parameters over the 100-year time horizon such as the technical innovation, change in climate condition etc make it impossible to ascertain the future characterization values which should be applied to long-term emissions; moreover, they proposed an assumption that leachate from sanitary landfill after 10 years decrease to the level of bottom ash landfills. Thus Obersteiner et al. [257] concluded that the waste remaining in a landfill was not a crucial factor for the difference in long-term emissions from different landfill types. However, when comparing landfill with other waste treatment options, [203] suggests that the long-term emissions from landfill should be incorporated into sensitivity analysis.

Actually, the generation of landfill gas and leachates not only depends on the composition of the waste, but also relies on the landfill design and operations. In addition to top soil cover, leachate treatment system, landfill gas collection and treatment system, which can effectively reduce GHG emissions and support energy recovery, technical barriers such as bottom liner also prevent the interaction of the landfill with the general environment [98, 203]. The influence of such technical barriers and operations should be included within the LCA system boundary, e.g. as in the LCA models presented by Doberl et al. [98], Menard et al. [238] and Binaghi et al. [23]. But the effects of barriers are limited to a certain period, which should be considered especially in LCA models based on medium or long-term period; often a maximum 100-year life time was assumed for barriers [98, 203]; whereas a 20 or 30-year operation period for leachate treatment and landfill gas collection systems were modelled in previous studies [225, 238, 257].

Various landfill technologies have been studied using LCA. Menard et al. [238] compared sanitary landfill and bio-reactor landfill; Obersteiner et al. [257] modelled four types of landfill; the study carried out by Manfredi and Christensen [225] concerned six landfill types and in these special emphasis was placed on the comparison of various new technologies e.g. bio-reactor.

1.4.2.3 LCA of Incineration

Literature reviews by ETCWMF [108] and WRAP [351] indicate that, in certain cases, incineration is more favourable than recycling e.g for paper/cardboard and plastics. However, this was highly dependent on the assumptions and methodologies applied in the particular LCA study. This is confirmed by Börjesson and Berglund [29] and Merrild et al. [239] who found that ranking of recycling and incineration of paper is very sensitive to assumptions and system boundary defined. Therefore, recycling versus incineration has no conclusive answer [29] and sensitivity analysis should be conducted to test the effects of key assumptions on the comparative LCIA profiles between recycling and incineration.

The main environmental benefit brought by incineration is energy-recovery from waste combustion and its substitution for other sources of energy generation e.g. grid average. Interestingly, two LCAs compared incineration and an advanced thermal treatment technology pyrolysis [11, 269]. Although different wastes were modelled, both studies indicated that pyrolysis gives more favourable environmental profile than incineration for MSW treatment in terms of energy consumption/recovery. Perugini et al. [269] also investigated other impact categories, i.e. resources consumption and climate change and pyrolysis was also shown as a better choice than incineration for plastic waste.

1.4.2.4 LCA of Biological Treatment

Only limited numbers of LCAs have been conducted to compare biological treatments with recycling, incineration and landfill. Composting and AD were examined by Eriksson et al. [106], composting led to higher impacts than AD in four impact categories studied; in comparison with landfill and incineration, AD showed better environmental profiles in energy consumption and GWP, but in acidification and eutrophication incineration was more favourable. Similar results were also reported in another study based on the same region and model method [307], in both energy and GWP impact categories, AD gave better profiles than both composting and incineration. In two studies carried out on OFMSW [100, 101], it was concluded that energy played an important role in comparison of incineration, composting and AD; by comparing LCIA single scores, AD (with energy recovery) was represented as the best disposal option, while open windrow composting gave similar environmental profiles to incineration. However, the comparison results discussed above were mainly focused on selective impact categories or on a single score, which do not represent an overall characterized LCIA profile. Moreover, methodologies and assumptions applied in these LCA studies were not clarified; this lack of transparency makes it difficult to compare and interpret the results presented in different studies.

This review of LCAs of composting of BFMSW has found that mainly industrial composting was studied, not home composting. Amongst a range of

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industrial composting technologies, the main focus has been on open-windrow composting [43, 100, 101, 307] with only limited study on other composting technologies [27, 43]. Cadena [43] compared different composting systems and concluded that open windrow composting was an environmentally preferable choice over in-vessel tunnel composting in most impact categories assessed (GWP, acidification, eutrophication and human toxicity) [43]. Based on results from very limited LCAs concerning home composting, aerobically operated home composting was indicated as a more environmentally friendly option for kitchen waste than industrial composting in all impact categories examined (GWP, toxicity, acidification, eutrophication) [220]; but the authors pointed out that poorly maintained home composting with anaerobic zones dominating can release significant quantity of GHGs emissions. Besides kitchen waste, no LCA study was found on home composting of other organic waste fractions.

Limited LCAs have been undertaken on AD, with most focused on waste water treatment [155, 165, 312, 315]. Only 7 out of 24 studies reviewed concern solid waste digestion e.g. [53, 100, 106, 307]. Few of these publications defined the AD systems they simulated—those that did concerned two models—a continuous single-stage AD digester operated at mesophilic temperature [307] and multiple stage, thermophilic dry batch digester [101]. However, there have been several LCAs carried out on the AD system design to assess the environmental impacts of various biogas production systems [20, 28, 29] and, in these studies LCA methodological aspects were also explored e.g. allocation method.

1.4.2.5 LCA Models

Mathematical models have been developed since the early 1990s to provide tools for decision-makers and waste managers to apply LCA methodology to specific waste treatment systems [349]. Some of models concerning different disposal routes were developed to identify the optimal waste management strategies such as the ORWARE applied in Sweden [307] and the EASEWASTE model developed in Denmark [225]. Six widely applied models were compared by Winkler and Bilitewski [349] and it was found that variations in the LCA results deriving from different models were substantial with different models even giving contradictory findings. They concluded that, although the all six modelling approaches to LCA were comparable at a general level, the specific details implemented in each model differed greatly [349].

Focusing on regional characteristics, UK-based models have been developed, e.g. WISARD, which was used by UK Environmental Agency, municipalities and waste management industry [73] and the WRATE software, which is recommended by Environmental Agency [104] as an LCA tool for waste management. In addition to these models, others have been developed, concentrating on one disposal route, such as the GasSim [8] and LandSim [298] models simulating gas

emissions and leachate from landfill. They have been applied in previous studies to assess potential environmental impacts caused by a specific waste stream [298], or assess the environmental benefits or disadvantages brought about by a waste treatment method such as MBT [261].

1.5 Data Quality Analysis in LCA

Data quality analysis is standardized as an optional element of LCIA where two techniques are concerned i.e. sensitivity and uncertainty analysis [171]. The specific methodologies have been broadly discussed since the 1990s, e.g. the guidelines developed by USEPA [328].

Björklund [25] reviewed the approaches for sensitivity analysis, amongst which scenario analysis is a widely applied approach. It has been applied to test system boundaries [55, 198], allocation approaches [136, 196, 221, 246], parameter values [107, 204] and the characterization methods adopted [99].

In contrast, uncertainty analysis is not commonly performed in LCAs [25, 159, 284] although great efforts have been made on the investigation of classification, definition, and source of uncertainty as well as the methodology aspects for expressing uncertainty. A SETAC-Europe LCA working group was established [38] and developed a framework for modelling uncertainties in LCI, where data uncertainties were classified into lack of data and data inaccuracy; furthermore, a pedigree matrix approach was recommended for the estimation of data inaccuracy [159]. The Pedigree matrix approach is also suggested for application to literature-based data by Sugiyama et al. [311] who further proposed to use standard statistical methods to quantify the uncertainties of industrial inventories i.e. using maximum likelihood estimation (MLE) ang goodness of fit (GOF). Unlike the use of the Pedigree matrix approach, which has been introduced into LCA database such as Eco-invent [275], statistical methods have only been used in a few LCAs to improve data quality [48, 60, 311].

A range of available approaches for uncertainty analysis in the LCIA phase were reviewed by Björklund [25]; amongst them, Monte Carlo simulation was the most commonly recommended, and specific methodologies have been developed [59, 63, 162]. Moreover, Monte Carlo simulation has been built into some commercial LCA software such as SimaPro [275] and applied in LCAs [15, 244, 309].

1.6 Aims and Objectives of this Study

Overall, the aim of this thesis is to investigate the cradle-to-grave environmental profiles of novel wheat based foam materials (WBFs) by using LCA and to address the general question 'Is there a general environmental advantage for WBFs over

petrochemical foams?' In addition, this study aims to seek an insight into the application of LCA approach on crop-based bio-products. The objectives of the study were:

- To develop a cradle-to-grave LCA model for WBFs by using primary data collected from industry and laboratory experimentation, supplemented with secondary data from publicly available sources and, via contribution analysis to identify the major drivers of category indicator results of WBFs (contribution analysis refers to identification of the extent to which the different life cycle stages and groups of processes contribute to the total result by expressing their contribution as a percent of the total [175]). Additionally, the scope was widened to explore briefly the LCIA profiles of two additional starch-based foams derived from potato and maize.
- To use LCA case studies to compare the environmental performance of WBFs with petrochemical polymers (HDPE/LDPE/EPS) in various applications
- To explore expansion of the LCA system boundary by applying process-oriented models instead of empirical models to simulate field emissions from the
 specific wheat agro-ecosystem and to analyze the influences of both modelling
 approaches on the LCIA profiles of WBFs.
- To model diverse end-of-life scenarios for the waste treatment of WBFs, including landfill, home composting, industrial composting and AD; to conduct laboratory research to obtain missing data on WBFs for LCA modelling, including physico-chemical parameters and biodegradability and energy recovery under AD conditions.
- To conduct data quality analysis to (1) evaluate the sensitivity of the results to methodologies, key parameters and scenarios and (2) quantify the levels of uncertainty for the LCA results due to the input uncertainty and data variability.

This thesis is structured to focus on key issues associated with the life cycles of bio-based, biodegradable foam products. Chapter 2 presents the general materials and methodologies adopted throughout the work. Chapters 3–7 present specific aspects of the research and each includes introduction to literature and background relevant to their topics. Each chapter presents primary data developed/used in the overall LCA work. A principle adopted throughout this thesis has been to present such primary data and assumptions in a justified, transparent and complete way so that it can be of maximum benefit to other practitioners. Elements of secondary data and mined or reviewed data that are more widely available to practitioners are detailed in relevant Appendices.

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Chapter 2 Materials and Methods

2.1 LCA Modelling Methods

In the current study, an attributional LCA approach was applied. As indicated in the introduction, LCA is a systems analysis approach, assessing the environmental aspects and impacts of product or service systems over their whole life cycle in accordance with the stated goal and scope of the study. Based on the initial unit processes and associated definitions in study scope, the LCI concerned with data collection and calculation procedures is conducted. In conjunction with LCI, the LCIA phase provides a systematic characterisation of the environmental and resource issues for the systems. In the LCIA phase, LCI results are assigned to impact categories and based on the category indicator selected, the indicator result for each impact category is calculated. Then, the conclusions drawn from the findings of LCA are identified, qualified, and evaluated in the interpretation phase, in relation to the aims declared in the goal and scope of study.

Definition of the goal and scope is therefore the basis for all LCA studies. In this chapter the goal and scope for the LCA research presented in this thesis are set out together with discussion of specific aspects of the data development undertaken in order to address this scope. The other phases of LCA are presented in Chaps. 3–7.

2.1.1 Goal of LCA Study

The LCA research set out to explore the environmental attributes of using starch-based foams (primarily WBF) as alternatives to conventional petrochemical foam materials. A variety of product systems were examined to determine whether a 'generic' set of LCA conclusions could be established for starch-based foams and their comparison with petrochemical alternatives or whether the outcomes were

specific to the individual product systems and comparisons being studied. These goals were addressed through the following objectives:

- To determine the environmental profile of the production of starch-based foam derived from a specific variety of winter wheat (Soisson).
- To assess the environmental profiles of WBF in case studies representing the packaging, display and construction industries.
- To compare environmental burdens of WBF with those of 'conventional' petroleum-based foams made from EPS/HDPE/LDPE in the case studies.
- To model and compare diverse end-of-life scenarios for WBF.
- To explore two additional starch-based foams derived from potato and maize starches (PSBF/MSBF).

2.1.2 Scope of Study

2.1.2.1 Function of Product System and the Functional Unit

Case studies were developed for four product systems. Amongst the product systems modelled, WBF cool-box has been tested in the lab and through commercial trials and has been verified as a marketable product in the short-term; the other three products were potential products at lab-test stage and are simulated as concept products in the LCA modelling. Their function and functional units are defined below.

Insulated Corrugated Box

This case study modelled a corrugated-board box insulated with WBF (density 25 kg/m³) or PE foam (density 35 kg/m³) designed to provide packaging and a degree of thermal insulation for shipping of temperature sensitive products (*e.g.* perishable foods, pharmaceuticals).

The functional unit was: "a single 8.5 l capacity corrugated box insulated with WBF or PE foam to maintain a temperature below 5 °C for 24 h for the transport of temperature-sensitive contents (see Fig. 2.1)".

Display Board

Conventional HDPE display boards are used for outdoor or indoor display purposes, such as posters, bulletins or advertisements. In this case study, conventional HDPE display boards with a 20 % recycled content and WBF concept products were compared.

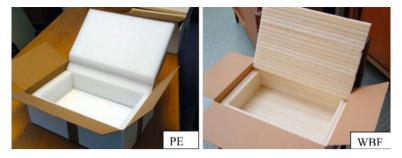


Fig. 2.1 PE coolbox (Hydropac Ltd. UK) vs. WBF coolbox (prototype)

Fig. 2.2 EPS trough mould [18]



The functional unit was "a single display board used for indoor advertisement application with 2 m^2 surface area, 10 mm thickness and 3-month service life (excludes the artwork on the film rolled on to the board)".

Trough Mould

As shown in Fig. 2.2, conventional reusable trough mould products manufactured by bonding PP skin to solid EPS core are used as a void-formers for constructing in situ ribbed concrete floor [18]. Generally after construction, the EPS trough moulds are left in situ for less than 6 months and then disposed, so in environmental terms they have medium-term life cycle. This design provides a cost efficient method to reduce concrete volume used and achieve longer spans than flat slabs.

Various grades of EPS with different density and compressive characteristics are used in trough moulds depending on the depth and side slope of the trough. Five case studies were conducted to compare WBF and two EPS grades (under trade name Filcor $20^{\$}$ and Filcor $45^{\$}$), both of which contain recycled-EPS (30 and 15 % respectively) and have density of 15 and 20 kg/m³ respectively.

The functional unit was "EPS/WBF used as a specified trough mould core to deliver equal physical property and provide 6-month service life."

Concrete Formwork

EPS foams are applied as formwork to construct simple or complex geometric structures such as spiral staircases, shaped columns, or external curved structures [17]. Generally EPS derived from virgin material are precisely cut off-site to provide a template for on-site concrete casting, but it has short life cycle—after a single use, they are disposed. Some EPS former products are lined with a coating to achieve a smooth surface. In this LCA study, Refractory lining and an EPS formwork for the 'Doha Villa' were modelled to compare virgin EPS (trade name Filcor 70°) and WBF used as short-life-cycle construction products. The functional units of the 2 case studies were:

A dome-shape single-use refractory former with $2.4~\text{m}^3$ volume, made from virgin EPS (density $25~\text{kg/m}^3$) or WBF (density $70~\text{kg/m}^3$)

A special-shape single-use formwork for the Doha Villa with a supplied volume of 335 m^3 (approx an area of 670 m^2 and an average depth of 500 mm) made from virgin EPS or WBF.

2.1.2.2 Product System and System Boundary

The product system and unit processes presented here are those which are general to the life cycle of WBF in the case studies; the detailed unit processes specific to an individual, life-cycle-phase are presented in subsequent chapters.

The generic product system for WBF products is illustrated as Fig. 2.3. The following unit processes are considered within the system boundary: production of wheat grain, flour milling, and production of WBF production of the finished products using the WBF (the insulated cardboard boxes, display boards, trough moulds and refractory formers), distribution, end-of-life and transportation.

The inputs/outputs for the product system(s) included raw/ancillary material inputs, process energy input, other inputs and final or intermediate products, coproducts, by-products, emission to atmosphere, water, and land. Environmental burdens associated with land use and human labour were excluded from the system boundary.

Unit processes either producing the inputs (*e.g.* production and delivery of process energy) or receiving the outputs (*e.g.* recycling of waste paper) were also included, but in some circumstances not every input and output can be modelled [49]. The criteria used to include inflows and outflows in the study were:

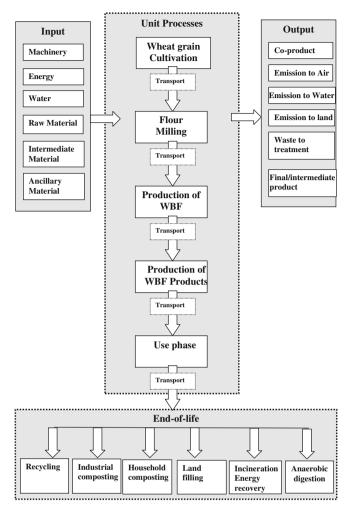


Fig. 2.3 Diagram for WBF products life cycle

- Data availability for the given input or output. Data were not available for all the inputs/outputs—these are defined as missing data. Such missing data are listed below, and their potential significance was considered in the sensitivity analysis and the interpretation phase.
- No specific cut-off rule (e.g. 2 % by mass) was applied. Instead, during the LCI development as much relevant data as possible for the product systems were sought and it is estimated that approximately 95–98 % of the mass and energy flow for all systems was achieved.

Based on these criteria, the following material/aspects were omitted:

- Energy consumption, infrastructure and other inputs in conversion of HDPE/ WBF block to display board.
- Energy consumption, infrastructure and other inputs in conversion of EPS/WBF block to trough moulds and refractory former.
- The same artwork printing technology for WBF and HDPE display boards were assumed, so the production of artwork-film rolled on to the display boards were not included in system boundary.
- The same skin/coating materials for WBF and EPS trough moulds/concrete former were assumed, therefore, the production of skin/coating materials was not taken into account.
- The models for production of LDPE/HDPE/expandable PS were based on EU average data [10]. Some transportation operations are stated to be omitted from the Plastics Europe database [11].

Besides, infrastructure was another concern. Although the effects of these components on the products they produce are usually negligible due to the large throughput achieved in their lifetime, the environmental impacts of capital plant and buildings could be high. Thus the baseline approach in the current study was to include infrastructure, its exclusion was explored in the sensitivity analysis. Surrogate processes for infrastructure were applied for the production of WBF and its end-of-life.

2.1.2.3 Allocation Procedures

Several industrial processes in the present study yield more than one product (multi-output system) and, therefore, an allocation procedure needs to be applied so that upstream environmental interventions and wastes can be correctly shared amongst these products. A number of methodological options exist for such allocation in LCA [49]. Briefly, these are (a) to avoid allocation by system expansion, (b) to partition the inputs and outputs either by physical relationship (i.e. mass etc.) or other relationship such as economic value [56]. As discussed in Sect. 1.3.1.2, the selection of allocation approaches for ALCA remains a controversial issue. Although the relevance of system boundary expansion to ALCA has been questioned by some LCA practitioners [102], in the current ALCA study system boundary expansion was applied in the cases where energy related co-products occurred (e.g. electricity from CHP, electricity from AD biogas) or closed-loop recycling occurred. This was based on the following considerations:

- 1) this approach is generally accepted to be relevant to ALCA and moreover is recommended as the preferred approach in PAS 2050 [14, 27].
- 2) for the energy co-products examined, hypothetical historical changes were investigated.

Besides, in this study, allocation by economic relationship (accounting for price and quantity) (except CO₂, see Sect. 2.1.2.3) was adopted for most of the stages where multiple-products occurred. Examples are discussed in detail below:

'Avoided Burdens' Approach for the Allocation of Co-Produced Energy from the CHP System and Bio-Gas Plant

The 'avoided burdens' approach, i.e. allocation by substitution [56, 71] was applied in the paper production processes and the end-of-life scenarios (landfill, AD, incineration). The surplus electricity produced in the CHP system and sold to the national grid [25] is a co-product of the paper/cardboard manufacturing process. In the case of waste treatment processes, including landfill, AD and incineration, electric and/or thermal energy are produced; electricity is sold to the national gird whereas thermal energy is wasted. In these processes, the inputs and outputs for the equivalent quantity of electrical power generated by the average electricity generation supply mix for the UK grid are allocated as a 'credit' to the modelled systems.

Allocation by Economic Value

Allocation by economic value was adopted for all inputs and outputs (except CO₂-see below) in the flour milling process according to the respective value and quantity of flour and its co-product (wheat feed). The same approach was applied to soy flour production process—the environmental burdens were allocated among the soy flour and soy oil based on the yield and price.

Carbon Counting

Economic value-based allocation was not adopted in accounting for the biogenic CO₂ inputs and biogenic carbon-based emissions in the life cycle because attempt to allocation carbon by economic value introduces serious distortions in the predicted carbon sequestration and release between main product(s) and co- and by-products. In order to 'track' the carbon footprint during the life cycle of WBFs, a stoichometric carbon counting approach was applied to determine (1) carbon sequestration into the wheat flour component of the WBF (during the crop growth phase of the life cycle) and, (2) the downstream release of this carbon during subsequent processing, product use and final disposal stages of the life cycle. Based on the carbon content in wheat starch and protein, the carbon sequestered into the wheat flour used for WBF was calculated in terms of its CO₂ equivalents. The 'sequestration' of this amount of carbon during the crop growth phase of the life cycle thus represents a 'negative' GHG balance at this stage which is then returned to the environment in various ways dependant upon the subsequent 'fate'

of the WBF product(s). This carbon-accounting approach enables clear recognition of the stages of the life cycle where GHG emissions are either mitigated or exacerbated and also facilitates identification of various options for enhancing GHG mitigation strategies.

Closed-Loop Allocation

The recycled EPS/PE/cardboard may be re-used within the same product system, or used in other product systems (recycled material undergoes changes in inherent properties, *e.g.* recycled EPS used as plastic wood). The former is referred to as "closed-loop recycling" the latter as "open-loop recycling". In this study the close-loop allocation approach was applied—virgin material for the life cycle is assumed to be displaced by recycled material within the same product system.

2.1.2.4 Data Categories

The data categories applied in this study include:

- Raw material inputs, e.g. CO₂ from atmosphere, cooling or process water.
- Energy inputs or outputs such as electricity, natural gas, and heavy fuel oil (to calculate GJ from m³ or tonnes of fuel, the net calorific value published by DTI was used [22].
- Intermediate products: such as wheat grain, pesticides, NPK compound fertilizer, flour, corrugated board.
- Final products, such as insulated coolboxes with PE foam or WBF.
- Emissions to air water or land: CO₂, N₂O etc.
- Wastes to be treated e.g. paper rejects, wood waste to be recycled.

2.1.2.5 Data Quality Requirements

Data Quality Parameters

The three data quality parameters [51] used in this study are defined as:

- Time-related coverage: in this study the reference years are 2006–2008. Primary data collected from specific companies are no more than 5 year old prior to 2008. Secondary data from published sources are generally within 10 years prior to 2008.
- Geographical coverage: primary data has been collected from the site-specific manufacturers under study; for the secondary data, UK sources were preferred, if not available, EU or global data was used.

Technology coverage: primary data was from defined processes from consultations and visits to manufacturing sites; secondary data have been collected from trade associations and government reports which are representative of the process. If neither was available, data from a different technology (surrogates) or laboratory scale (data development) was used.

Data Quality Indicators

The indicators to characterize the quality of the data used in this study are: (1) precision: a measure of the variability of data values for each data category; (2) completeness: indicated by the percentage of locations out of the total number in existence; (3) representativeness: an indicator of the degree to which the data set reflects the true measurement of the population of interest [51], it involves geographic, temporal and technological dimensions.

The quality and nature of data were characterised by both qualitative and quantitative aspects: the data sources were clarified and the uncertainty of either industry-based or literature-based data were analyzed by the method indicated in Sect. 2.3.2.

2.1.2.6 LCIA Methods

Two LCIA elements are concerned: characterisation and normalization. Characterisation is to assign and convert LCI results (unit process data); the numerical indicator results represent the characterisation outcome. Normalization aims to calculate the magnitude of the category indicator results relative to a reference baseline.

The impact categories, characterisation models and category indicators used are shown in Table 2.1.

Most of the models shown in Table 2.1 are incorporated in the CML 2 baseline 2000 V2.04 characterisation model [34], except IPCC AR4, instead, IPCC AR3 is included [28]. CML 2 baseline 2000 V2.04 adopts a problem oriented (midpoint) approach and is used in the current study as the 'default' LCIA method. However, a second LCIA method—Eco Indicator 99 (a damage-oriented approach) defining impact categories at the endpoint level was also applied to analyse the sensitivity of the LCIA results to the LCIA method choice.

As an optional LCIA element, normalization changes the outcome of the characterisation and gives a normalized LCIA profile for the product system [50]. The reference system provided by CML 2 baseline 2000 V2.04 West Europe 1995 was used as default method [80], but a second normalization method was applied in sensitivity analysis. In West Europe 1995, the total annual emission or resource

Table 2.1 Characterisation models

Impact category	Characterisation model	Category indicator	Indicator result	References
Eutrophication potential	Model based on stoichiometry procedure	Deposition increase divided by N/P equivalents in biomass	kg PO ₄ -equivalents	[38]
Acidification potential	RAINS model	Deposition/ acidification critical load	kg SO ₂ equivalents	[46]
Ecotoxicity and human toxicity potential	USES-LCA model	Predicted environmental concentration increase/ predicted no-effect concontration	kg 1,4- DB (1,4- dichlorobenzene) equivalents	[39, 42]
GWP100	IPCC model	Infrared radiative forcing (W/m2)	kg of CO ₂ - equivalents	IPCC AR4 (fourth assessment report) [29]
POCP	Trajectory model	Quantity of tropospheric ozone formed	kg C ₂ H ₂ equivalents	[21, 52], [20]
ODP	Montreal protocol	Stratospheric ozone breakdown	kg CFC-11 equivalents	World meteorological organisation [105]

use in Western Europe for the given year 1995 are chosen as reference value. All of these reference values have been reported by Huijbregts et al. [40]. However, as pointed out by Heijungs et al. [37], biased normalization profiles can be delivered due to the limitations in the coverage of elemental flows for the product system and for the reference system. A large degree of bias may occur in normalized indicator results for impact categories which are not well-established (e.g. marine eco-toxicity, land use) or that are related to many substances (e.g. human and eco-toxicities). Particularly biased marine ecotoxic results have been observed [37]. Limitation in the characterization factors for toxicity-related impact categories have been discussed in previous studies [39, 42, 85]. It should be noted with regard to the present study that the USES-LCA model for metals is debatable and moreover that missing data and knowledge impose limitations on the toxicity models, especially for the marine eco-toxicity model where no experimental data were available.

2.2 Agro-Eco-System Modelling Methods

Since 1990 when the IPCC first assessment report was released, agriculture has been seen as an important source of GHGs. In addition to GWP, agriculture also contributes to other impact categories such as acidification and eutrophication potentials via leaching or trace gas emissions. To simulate the carbon and nitrogen biogeochemistry in agro-ecosystem, two approaches were applied in this study: the empirical model IPCC approach [62], and a process-oriented model DNDC (Denitrification-Decomposition).

2.2.1 IPCC Approach

To estimate the emissions from the agricultural system, such as N_2O emissions from soil, CO_2 from liming, IPCC tier 1 approaches [48] were applied. Here soil N_2O emission estimation is given as example. The IPCC method accounts for both direct and indirect N_2O emissions (both pathways are defined in IPCC Guidelines) [48]. It utilizes activity data and emission factors (EF) to derive the N_2O emission estimations to the level of N input [48].

However, the IPCC EFs are derived from field measurement at sites in a variety of countries with different soil types, climate and crops [13], and so have a wide range, leading to a large degree of uncertainty in the emission estimation [12]. Moreover, the IPCC Tier 1 methodology is intended to be broadly applicable rather than being site-specific, it does not account for regional difference in agroecosystem characteristics and should be regarded as a first approximation [44].

To estimate the combined uncertainty for the IPCC method-derived GHGs inventory, IPCC guidelines [48] established two approaches: Approach 1 uses a simple error propagation equation; whilst in Approach 2 Monte Carlo simulation is recommended. Monte Carlo Simulation is a computational algorithm method. In the Monte Carlo process, pseudo-random samples of inputs are generated by an algorithm (pseudo-random number generator) [48] from the probability density function (PDF) specified for each input variable; then one random value for each input is entered into the model to arrive at one estimate of the model output. After repeating this process for a number of iterations, multiple estimations representing the sample values from PDF of model output was obtained. By analyzing the samples of model output, the mean, SD (standard deviation), and 95 % confidence interval of output PDF can be inferred.

In this study, Approach 2 was adopted; uncertainties in EF were determined according to uncertainty ranges given in the IPCC Guidelines [48]. RiskAMP Monte Carlo Add-In Library version 2.97 (Professional Edition, Structured Data, LLC) statistical analysis software was used to perform the Monte Carlo simulation.

2.2.2 Process-Oriented Model DNDC

The process-oriented models take into account site-specific factors such as fertilizer type, climate, crop rotation, agricultural management. Described below is the rainfall event-driven process-based model used.

2.2.2.1 DNDC Model Structure

DNDC was selected for this LCA research and its latest version DNDC93 was modified and applied in this site specific study in the UK. DNDC bridges ecological drivers and soil biochemical reactions via linking both to soil environmental factors. In the DNDC model, classical laws of physics, chemistry and biology or empirical equations obtained from laboratory observation were used to parameterize geochemical/biochemical reactions [63, 64]. The original parameters and equations have been published in details [63–66].

The structure of DNDC is presented in Fig. 2.4. The DNDC model comprises two interacting components—the first includes 3 sub-models (soil climate, plant growth and decomposition) and predicts soil environmental variables based on ecological drivers; the second component consists of nitrification, denitrification and fermentation sub-models simulating microbial activity and trace gas fluxes and N leaching [64].

The six sub-models play different parts and interact with each other. The soil climate sub-model integrates climate, soil properties and O₂ profile to simulate soil temperature moisture and Eh [63, 65]. The climate, soil, crop parameters and field operations are integrated in the plant-growth sub-model to estimate crop growth, and its effects on soil temperature, moisture, available N and DOC etc. [66]. The decomposition sub-model mainly models 4 pools of soil organic carbon—microbial biomass, plant residues, active humus and passive humus; in addition, N dynamics during decomposition of organic matter in soil are simulated as well (e.g. nitrogen mineralized enters the inorganic nitrogen pool as NH₄⁺ which is either nitrified to NO³⁻ or is removed via crop-uptake, leaching or volatilization) [62, 63]. The denitrification sub-model is activated by increase in soil moisture or decrease in oxygen level from events like rainfall, flooding, and freezing temperatures (below -5 °C) [62]; when these events occur, the production, consumption and diffusion of NO and N₂O are simulated. Another main source of NO and N₂O, nitrification is included as a sub-model in DNDC and nitrificationinduced NO and N₂O is calculated as a function of predicted nitrification rate and temperature and is influenced by the soil environmental variables. In addition, the NH₄⁺/NH₃ equilibrium and functions for NH₃ production and volatilization are also included in the nitrification model [63]. The release of CH₄ is modelled in a fermentation sub-model, where CH₄ production, oxidation, and transport under submerged conditions is calculated based on fermentation equations [63].

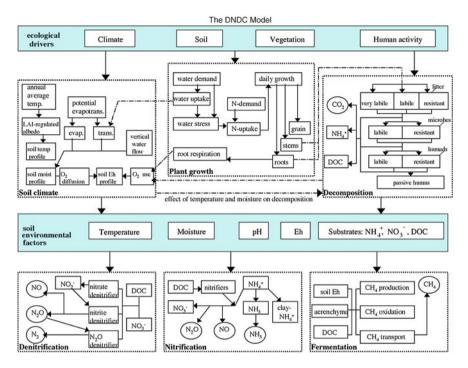


Fig. 2.4 Structure of DNDC model [64]

2.2.2.2 DNDC Input Data

The specific data on soil characteristics, daily climate, crops and farming practice for each of the 6 fields located in Norfolk that produced Soisson winter wheat for WBF manufacture were used as input to the DNDC model. The farming database for the six fields over five years (2003–2007) were obtained in collaboration with Heygates Farm Swaffham Ltd, whose cooperation is gratefully acknowledged.

The soil types and soil properties for the different soil layers at Swaffham farm were obtained based on the National Soil Map/Inventory and provided by the National Soil Research Institute (NSRI) of Cranfield University. This inventory covering over 50 % of arable land and grassland in England and Wales was developed from a soil survey conducted on the basis of a 5-km soil sampling grid. The specific research methods for this soil survey were reported by Bellamy et al. [7]. This soil map/inventory represents the most accurate comprehensive source of data on soil at the national level in the UK [74], and was used as the soil database for the UK-DNDC model [13]. According to this soil map, two soil associations (soil associations present a group of soil types which are typically found occurring together i.e. associated in the landscape) covering an area of 554 km² and accounting for 0.37 % of England and Wales's landmass are present in the Swaffham farm area and comprise multiple soil series(soil types). Soil texture was

identified based on a soil texture triangle [99] and the UK soil classification [73] and it together with the soil composition reported by Swaffham farm were applied in the DNDC.

Besides soil, another important ecological driver is climate. Daily meteorological data for the five year period 2003–2007 were collected from a weather station run by Broom's Barn, which is 30 miles away from the farm modelled. The data include daily maximum and minimum temperature (°C), precipitation (mm) and wind speed (m/second).

Both NH₄⁺ concentration in rainfall and atmospheric NH₃ concentration were derived from a database provided by the Centre of Ecology and Hydrology (CEH). Within UK National Ammonia Monitoring Network (NAMN) operated by CEH, there are 95 sites developed for exploration of concentration and deposition of NH₃/NH₄⁺. Rainfall NH₄⁺ concentration for the Swaffham farm area was estimated based on the 2006 UK map for ammonium ion rain concentration [15]. Atmospheric NH₃ concentration was calculated according to the data collected from a site (Stoke Ferry) closest to Swaffham farm (9.2 miles away) [16]. The sampling methods are described in CEH report [98].

As for the atmospheric CO₂ concentration and its annual increase rate, several data sources were considered and compared—CDIAC website (CO₂ Information Analysis Centre), study conducted by Reay et al. [83], IPCC as well as personal communication with Professor Keith Goulding from Rothamsted Research [32].

2.2.2.3 Sensitivity Analysis and Uncertainty Analysis for DNDC Outputs

Compared with climate data and farming practice, the soil properties are highly variable in spatial terms even within one single field. Averages of the soil survey data cannot solve this issue, as the correlation between modelled trace gas and any of the soil properties is non-linear in the DNDC model [67]. To test the sensitivity and uncertainty of the DNDC simulation to the variability of soil parameters, the following methods were adopted.

In sensitivity tests, a baseline scenario was constructed by using the mean value for soil characteristics, daily climate, crops and farming practice. Alternative scenarios were built up by varying each of the soil parameters across a range provided by NSRI. To quantify the sensitivity analysis and determine the most sensitive factors for modelling trace gas and leaching, a sensitive index [64] was introduced:

$$S = \frac{\left(\frac{O_2 - O_1}{O_{avg}}\right)}{\left(\frac{I_2 - I_1}{I_{avg}}\right)} \tag{2.1}$$

where S is the relative sensitivity index; I_1 , I_2 are the minimum and maximum input values for a given parameter; I_{avg} is the mean value of I_1 and I_2 . O_1 and O_2 are the model outputs corresponding to I_1 and I_2 . O_{avg} is the mean value of O_1 and O_2 . The

higher the absolute value of S, the greater the impact the input parameter has on the output. A negative value of S indicates an inverse relationship between input and output.

Based on the sensitivity analysis results, the two most sensitive soil parameters for each trace gas (N₂O, CH₄, and NH₃) or N leaching were identified and then explored in uncertainty analysis. In this research, the methodology for Monte Carlo simulation in DNDC93 was modified in collaboration with the model originators at the University of New Hampshire. Originally, when DNDC was running in the Monte Carlo mode, the range defined for each ecological variable was divided into eight intervals fitting a discrete distribution. Then random samples were selected from the eight intervals and entered into the model. However, this only represents eight samples from the potential the range of inputs. In the modification of DNDC93 implemented here, the sample size was increased from 8 to 50. In other words, the range defined for each variable was divided into fifty intervals, and then the random sample generated within these 50 intervals was entered into the model. The Monte Carlo simulation was run with an iteration of 5,000. The 5,000 fluxes for trace gases based on the randomized soil parameters were generated and further analyzed by the methods described in the next section. A further modification was to the simulation period. The original DNDC93 did not allow users to define the time period for the outputs from Monte Carlo simulation, only the summary data for one year (365 Julian days) was provided. In the modified DNDC93 flexibility was increased so that the model outputs are given as total gas-flux/leaching for any user-defined period, which allowed uncertainty analysis of simulated results to be conducted based on a time boundary such as one wheat crop cycle which was more appropriate to the scope of this LCA.

2.2.2.4 Statistical Analysis of DNDC Results

In this statistical analysis, the simulated trace gas emissions and leaching from the DNDC model were the observed samples. They were fitted with various hypothesized standard distributions. The GOF of each distribution was assessed and from this analysis the best-fit distribution was selected.

This analysis starts with counting the frequency of the observed samples that falls into a range of equally-distributed intervals or bins. The frequency in each bin is the observed frequency O_i . After that, standard distributions are fitted to the observed samples. A widely used technique known as MLE is applied to assess the characteristic parameters θ_m of each distribution. This technique is frequently used for parameter estimation and fitting distribution to available dataset [97, 104]. Suppose the observed data X_1, \ldots, X_n are independent and identically-distributed random variables with a common standard PDF $f(x_i; \theta)$. The likelihood function is defined as:

$$L(\theta; x) = \prod_{i=1}^{n} f(x_i; \theta), \quad \theta \in \Omega$$
 (2.2)

where $\mathbf{x} = (\mathbf{x}_1, ..., \mathbf{x}_n)$ is the data of the observed sample. θ can be a scaler or a vector, depending on the PDF of the distribution. For instance, the θ for the PDF of the normal and lognormal distribution is a vector consisting of the mean and SD [97]. The maximum likelihood estimator θ_m is the parameter for the distribution that fits the observed sample best. It is the value of θ which maximizes the function $L(\theta)$, which is solved by differentiating the logarithm of $L(\theta;x)$ as follows:

$$\frac{\partial l(\theta)}{\partial \theta} = 0$$

where function

$$l(\theta) = \log L(\theta) = \sum_{i=1}^{n} \log f(x_i; \theta), \quad \theta \in \Omega$$
 (2.3)

Sample size is one of the most important factors affecting the robustness of MLE. The larger the sample size, the smaller is the bias in the parameter estimates [8]. In this study, the sample size was 5,000. The PDF of the hypothesized distribution as a function of x was calculated by MLE and is expressed as $f(x; \theta_m)$. Using this method, the PDF of all distributions were calculated.

In order to identify the best fit distribution, the PDF of each hypothesized distribution was compared with the observed sample distribution of the results using GOF tests. Two non-parametric test methods were applied—the Chi square test and the Kolmogorov–Smirnov test (K–S test). Both address how well the observed samples conform to the hypothesized distributions expressed by a null hypothesis H_0 (i.e. no difference).

The Chi square test statistic is given as

$$\chi^2 = \sum_{i=1}^n (O_i - E_i)^2 / E_i$$
 (2.4)

where n is number of bins; O_i is the observed frequency or number of counts in bin i, E_i is the expected frequency of the hypothesized distribution in bin i. Chi square is used as a measure of how far a sample distribution deviates from a hypothesized distribution; the larger the disagreement between the observed and the expected frequency, the larger is the χ^2 value obtained. Based on the degree of freedom df, defined as n-1, and the χ^2 value, tables for the critical values of the Chi square distribution indicate the probability p for the occurence of a given χ^2 value if H_0 is true. If $p < \alpha$ (significance level, $\alpha = 0.05$ was applied here), then the null hypothesis is rejected.

The Chi squared test above was performed on all the distributions. After that, the χ^2 values were ranked. The distribution with the smallest χ^2 value is the best fit distribution for the observed samples.

The K–S test originally was developed for continuous data, and is more powerful than Chi square when the sample size is small [107]. It quantifies the maximum absolute deviation between cumulative empirical frequencies F(x) and cumulative density function (cdf) for the hypothesized distribution G(x). The test statistic is given as

$$d_{\max} = \sup_{x} |F(x) - G(x)| \tag{2.5}$$

where the data is grouped into bins; sup is the supermum of set of data |F(x)-G(x)| for each bin. According to the total number of data, and the number of bins n, a critical value at significance level α ($\alpha=0.05$ was applied) is given in the critical value table for the K–S test. If $d_{\rm max}$ is greater than critical value, then H_0 is rejected. Using the K–S test critical value table, the probability p can be obtained. In addition, by the K–S test statistics $d_{\rm max}$ for all the hypothesized distributions were ranked. The distribution with the lowest $d_{\rm max}$ value is the best representative of the observed samples. In most situations, the best distributions identified by the two tests are the same. However, when discrepancy occurs, the distribution identified by the Chi square test takes priority as this test is suitable for the large sample size used in this analysis.

The statistical analysis was performed in Matlab in collaboration with Dennis Lee in the Civil and Environmental Engineering Department of Imperial College. The best-fitted distribution identified for the simulated DNDC results was used as input data for the uncertainty analysis of the LCA in Simapro 7 (v 7.1.8).

2.3 Sensitivity Analysis and Uncertainty Analysis of the LCA Results

This section presents the general methodologies for testing the sensitivity of the LCA results to different parameters (such as LCI results, characterisation models), and the uncertainty of LCA results due to the input uncertainty and variability in the LCI data.

2.3.1 Sensitivity Analysis

A series of sensitivity analyses were conducted to analyze the influence of a given parameter on the LCIA results including the characterisation and normalization models. The parameters assessed include unit process data, characterisation factors, allocation rules, system boundary, the omitted unit process and scenarios.

2.3.1.1 Tornado Diagram

Tornado Diagrams were used to assess the sensitivity of the results for one product system to data for a single unit process and to identify the most sensitive parameter [9, 100]. In this approach, the LCA model is run with the extreme values for one parameter while all other parameters are kept constant. The results are presented in bar graphs to indicate the degree to which the outputs vary due to the changes in individual parameters—the top bar represents the most sensitive parameter while the bottom bar shows the least sensitive one.

2.3.1.2 Scenario Sensitivity Analysis

In the case of other parameters, such as the characterisation model, allocation rules, and the system boundaries, sensitivity tests were conducted through scenarios. Here, the scenarios are defined as descriptions of possible future situations, based on specific future assumptions and they are characterised by the choice of parameters listed above [9]. A sensitivity test involves calculation based on all possible scenarios for the tested parameter(s) and analysis of the influences of the relevant parameter(s) on either the characterisation or normalization profiles or the comparison ranking. For one product system, 10 % changes in the characterised or normalized indicator results was chosen as the threshold above which the influences of parameter on the model results were considered to be significant.

2.3.2 Uncertainty Analysis

2.3.2.1 Uncertainty of the LCI Analysis

The uncertainty introduced into the LCI results due to the cumulative effects of input uncertainty and variability of inventory data were quantified by the following methods.

MLE and GOF Methods

In the case of an industry-based inventory data with multiple measurements or a computer-simulated inventory data with information on variability, statistical methods (MLE and GOF) were applied to fit the probability distribution to the observed or simulated data. The specific methodology is described in Sect. 2.2.2.4 where distribution fitting for DNDC simulated data was given as an example.

Pedigree Matrix Method

For literature-based secondary data or industry-based primary data which were only represented as single measurement values, temporal, geographical, or technological gaps are the likely major sources of uncertainty. In such cases, MLE and GOF are not applicable and an expert judgement-based approach termed Pedigree Matrix was applied. The Pedigree Matrix approach was originally developed by Weidema and Wesnæs [103], and was adopted and modified in other studies to represent uncertainty in LCI data [9, 41, 59]. The Pedigree Matrix approach is also introduced in the Ecoinvent database [31], transforms the data quality indicators (such as completeness and representativeness) to probability distributions by representing the data quality indicator value by a 'default' lognormal distribution. Specifically, uncertainty in inventory data is characterised by six characteristics (from U_1 to U_6). Each characteristic is divided to five levels with a score (1–5), and an uncertainty factor in terms of contribution to the square of the geometric SD is given to each score of the six characteristics.

The geometric SD (at 95 % confidence interval) is defined as:

$$\sigma^{2} = \exp \sqrt{[\ln(U_{1})]^{2} + [\ln(U_{2})^{2}] + [\ln(U_{3})^{2}] + [\ln(U_{4})^{2}] + [\ln(U_{5})^{2}] + [\ln(U_{6})^{2}] + [\ln(U_{b})^{2}]}$$
(2.6)

where: U_1 is the uncertainty factor of reliability; U_2 is the uncertainty factor of completeness; U_3 is the uncertainty factor of temporal coverage; U_4 is the uncertainty factor of geographic coverage; U_5 is the uncertainty of technological coverage, U_6 is the uncertainty factor of sample size; U_b is the basic uncertainty factor which is based on expert judgement. The Pedigree Matrix defining criteria for data quality assessment and the uncertainty factors are given in Appendix A.

In this method, the 95 % confidence interval for each inventory datum was estimated based on the mean value μ and the SD σ^2 : (μ/σ^2 ; $\mu \times \sigma^2$) [1].

2.3.2.2 Uncertainty of LCIA Results

Statistical variability in LCI data or the lack of temporal, geographical or technological dimensions in the LCI introduces uncertainty in the LCIA results. As indicated before, uncertainty of LCI data is expressed as a probability distribution, either log-normal-distributed random errors introduced by the Pedigree Matrix method, or PDF identified by statistical methods. Based on these, Monte Carlo simulation was applied to estimate the uncertainties in the LCIA results.

Monte Carlo simulation was built in Simapro 7.0 software and it was run with 1,000 iterations at significance level $\alpha = 0.05$. By analyzing samples of the model output, the mean, SD, and 95 % confidence intervals of the output PDF are given as results of the uncertainty analysis.

2.4 Experimental Methods

The main test materials of interest in this LCA were WBF provided by Greenlight Products Ltd (plus cardboard box from Hydropac Ltd); and the additional potato/maize starch-based foams produced in Greenlight Ltd for comparison with WBF.

2.4.1 Experimental Set-Up

2.4.1.1 AD Inocula

The inocula were collected from a mesophilic (30–40 °C), wet (<15 % dry solid), continuous-feeding and multiple stage (hydrolysis step and methanogenesis stage) digestion system operated by a UK commercial AD plant. The operation temperature for the anaerobic digesters was 37 °C and OLR to digesters was variable due to the varying BFMSW composition; based on laboratory results by this UK commercial AD plant, the average OLR over 3 months (Jan 2009–March 2009) is 2.393 g COD/L/day with a coefficient of variation (CV) of 0.184.

2.4.1.2 BMP

The BMP assay was conducted according to the techniques developed by Owen et al. [75]. The media contain nutrients and vitamins for mixed anaerobic cultures [75] and Resazurin was added as an indicator to detect oxygen contamination (turns pink when oxidized). The BMP assay was run in 165 or 39 ml serum bottles fitted with leak proof Teflon seals and with controls of inoculum without substrate.

In each bottle, the total liquid volume of 100 or 20 ml was added (volumes for 165 and 39 ml serum bottle respectively), including media, inoculum and substrates. Anaerobic conditions were maintained during media and inoculum transfers by flushing the media flasks and assay bottles with a 70 %/30 % v/v mix of N_2/CO_2 at a flow rate of approx 0.5 L/min. Each serum bottle was then immediately capped with Teflon seals when the gas flushing needle was removed.

The inocula were taken from active BFMSW anaerobic digesters operated by a UK commercial AD plant (see 2.4.1.1). To deplete the residual biodegradable organic material present in inocula before the BMP test, they were pre-incubated in a 1 L batch reactor under anaerobic conditions at 30 $^{\circ}$ C until no significant CH₄ was produced. Then the pre-incubated inocula were used in the BMP assays to give a final concentration of 2 gVSS/L in the serum bottles.

To determine the inoculum activity, the protocol proposed by Angelidaki et al. [2] was applied. Model substrates chosen to determine hydrolytic, acidogenic, acetogenic and methanogenic activities were amorphous cellulose (1 g/L), glucose

(1 g/L), a mixture of propionic and butyric acid (0.5 g/L for each acid), and acetic acid (1 g/L) respectively.

The BMP assays for different substrates including foams and cardboards were conducted at an approximate 1:1 ratio of inoculum VSS to substrate COD [82]. All the serum bottles were incubated at 37 °C and shaken at 200 rpm in Gallenkamp Orbital Incubator.

Gas and liquid samples were collected to determine the composition of biogas and the concentration of VFAs. All controls and substrates were assayed in triplicate for gas composition analysis and the CVs for the three replicates were within 0.08; where VFA analysis was undertaken, four identical bottles were set up for each feeding, and one was used for VFAs measurements.

2.4.2 Analytical Methods

2.4.2.1 Gas Composition Analysis

In the BMP test, the volume of biogas produced in the serum bottle was determined by a glass syringe. A glass syringe lubricated with diH_2O and preflushed with the CO_2/N_2 (30 %/70 % v/v) gas mixture was used to determine the gas volumes produced in the serum bottle headspace. The volume reading was taken by allowing the syringe plunger to gently move and equilibrate between the bottle and room air pressure. After determining the volume, the syringe with biogas was removed.

To determine the composition of biogas, a 1 ml headspace gas sample was collected using a 1 ml plastic syringe (Terumo) and assayed in a gas chromatograph (Shimadzu GC-14A) equipped with thermal conductivity detector (TCD); a Porapak N column (1500 \times 6.35 mm) was used for analysis. The carrier gas for GC analysis was helium set at a flow rate of 50 ml/min. The temperature of the column, detector and injection port were set at 28, 38 and 128 °C respectively. The peak areas and gas concentration readings were calculated and collected on a Shimazdu Chromatopac C-R6A integrator. Calibration gases were accurate to 5 % and the CV for 10 identical samples was 0.02. Ultimate CH₄ potential was expressed as the amount of yielded CH₄ (converted to standard temperature and pressure) divided by the quantity of VS and COD added.

2.4.2.2 Volatile Fatty Acids

After mixing samples well by inverting the serum bottles, 2 ml liquid samples were collected from the bottles using plastic syringes (through Teflon seals). These were then centrifuged at 13,000 rpm for 2 min and the supernatant was filtered through a

 $0.22~\mu m$ filter (VWR Labshop). 1 ml of the filtered sample was then transferred to GC vials, acidified by adding one drop of 98 % sulphuric acid and analyzed on the gas chromatograph (Shimadzu GC-2014) fitted with a flame-ionised detector (FID) and a SGE capillary column (BP21, 12 m \times 53 mm ID with film thickness 0.5 μ m). The carrier gas was helium at a flow rate of 102.5 ml/min; the temperature for injector and detector were constant at 200 and 250 °C respectively; the initial temperature for the column was 80 °C, then increasing by 10 °C/min to 160 °C after which the temperature was held for 1 min. The concentration for acetic, propionic, n-butyric, iso-butyric, n-valeric, iso-valeric and n-caproic acids were analyzed and the CV for ten identical samples was 0.066.

2.4.2.3 Element Sulphur Analysis

A three-step sequential microwave digestion by HNO₃, H₂O₂, and HCl and Inductive coupled Plasma (ICP) measurement developed by Kalra et al. [57] for multiple-element analysis of plant materials was used for S elemental determination. Unlike the HNO₃-HClO₄ wet digestion which has been reported as a method with low recovery of S due to S-containing gases or incomplete oxidation of certain compounds [35, 108], this microwave digestion method in closed vessel could minimize S loss [93]. Furthermore, ICP is applicable to all soluble form of S.

1 g fresh foam/cardboard sample (with moisture content determined) was transferred into a digestion vessel to which 10 ml HNO₃ was added, the vessel was swirled gently to ensure all sample came into contact with HNO₃. All vessels were loosely capped and placed in the microwave oven (Anton Paar Multiwave 3000). Samples were digested for 30 min at 540 W setting. After completion of the heating cycle, the vessels were cooled for 5 min, then a 1 ml H₂O₂ was added to each sample solution. Mixtures were kept at room temperature for over 5 min until the bubbling ceased. Then the digestion vessels were placed back into the oven and a second heating cycle at 540 W was run for 15 min. The digestion solutions were cooled down for 5 min before adding 2 ml HCl and returned back to oven. At the end of the final heating cycle (180 W 10 min), a clear solution was obtained. The sample solutions were filtered through filter paper (Whatman Grade No. 42) into a 50 ml volumetric flask. The vessels were rinsed with 1 M HCl for three times to ensure the materials were quantitatively transferred into the funnels. The filtration volume was made up to 50 ml. The sample was analyzed on ICP-OES (Inductive Coupled Plasma-Optical Emission Spectrometer) (Perkin Elmer Optima 7300DV). Argon was used as both carrier gas and purging gas (to remove interfering oxygen from the system). The detection limits for S is $30 \,\mu \,g/L$ and the three emission lines used for sulphur were S I 180.669, 181.975, 182.563 nm.

A NaSO₄ standard was used for calibration and the recovery rates for S and the matrix interferences were tested by spiking the samples and blanks with NaSO₄.

2.4.3 Physical-Chemical Methods

2.4.3.1 Total solid (TS), volatile solid (VS)

Total solid (TS) and volatile solid (VS) were assayed according to standard methods [3, 70, 88, 89]. The empty aluminium dishes were placed in a furnace at 550 °C for 1 h. After cooling in a desiccator, the sample was transferred into the pre-weighed dish, and placed in an oven at 103-105 °C for 24 h until achieving constant weight (constant weight is defined as less than ± 0.3 mg change in the weight upon one hour of re-heating). The resulting weight was recorded for the measurement of TS and then the dish was placed in a muffle furnace at 575 ± 25 °C for approximately 24 h. After cooling in a dessicator, the sample was weighed and then placed back in the muffle furnace at 575 \pm 25 °C, and ashed to constant weight. VS content refers to the difference between the weight of a sample before and after ashing. The calculation was performed according to the following equations

$$\%TS = \frac{WEIGHT_{ovendrysample+dish} - WEIGHT_{dish}}{WEIGHT_{recivedsample}} \times 100$$
 (2.7)

%VS of TS =
$$\frac{WEIGHT_{ovendrysample+dish} - WEIGHT_{ash+dish}}{WEIGHT_{receivedsample} \times \%TS/100} \times 100$$
 (2.8)

where

WEIGHT_{dish} WEIGHT_{recivedsample} $WEIGHT_{ovendrysample+dish}$ WEIGHT_{ash+dish}

the weight of empty aluminium dish the weight of sample as received

the weight of sample plus dish after oven drying the weight of sample plus dish after ashing in muffle

furnace.

2.4.3.2 Total Suspended Solid, Volatile Suspended Solids

Total Suspended Solid (TSS) and Volatile Suspended Solids (VSS) were assayed according to standard methods [3]. Glass fibre filters were prepared for the assay by inserting them onto the base and clamping these into funnels. Under vacuum, the filters were washed with three successive 20 ml volumes of deionised water (diH₂O). All traces of water were removed by continuing to apply vacuum. The glass fibre filters were then placed in aluminum dishes and held in the muffle furnace at 575 \pm 25 °C for 1 h. The filters were rewashed with three additional successive 20 ml deionised water aliquots, and dried in an oven at 103-105 °C for one hour. Then the dishes and filters were removed directly to the desiccator and cooled for use in VSS/TSS assays.

A prepared filter was placed on the base and clamped on a funnel. The filter was wetted with a small volume of deionised water to seal it against the base. Then a small amount of sample (0.1–0.25 ml) was transferred to the filter by pipette and the filter (with sample on it) was rinsed with diH $_2$ O three times. All traces of water were removed under vacuum. The filter with sample was removed to the prepared aluminium dish and oven dried at 103–105 °C for 24 h. The mass of the sample was then determined and then was placed back to the oven until constant weight was achieved. Afterwards, the dish and filter were placed in the muffle furnace at 575 \pm 25 °C overnight and directly removed to desiccator. After cooling, the sample mass was recorded and it was then returned to the furnace to ash to constant weight. VSS and TSS were calculated according to the following equations

$$TSS(g/L) = \frac{WEIGHT_{ovendry} - WEIGHT_{dish+filter}}{Inoculum}$$
(2.9)

$$VSS(g/L) = \frac{WEIGHT_{ovendry} - WEIGHT_{ash}}{Inoculum}$$
(2.10)

where

WEIGHT_{dish+filter} the weight of empty aluminium dish and filter after oven

drying

WEIGHT_{ovendry} the weight of oven dried dish, filter plus residue

WEIGHT_{ash} the weight of residue, dish and filter after ignition in muffle

furnace

Inoculum (mL) the volume of inoculum filtered.

2.4.3.3 COD Measurements

The measurement of COD was based on the Standard Closed Reflux Colorimetric Method [3]. Digestion solutions were prepared by adding 10.216~g of $K_2Cr_2O_7$ (dried overnight at $103~^{\circ}C$), 167~ml of concentrated H_2SO_4 and 33.3~g of $HgSO_4$ into 500~ml of diH_2O . The mixture was then cooled at room temperature before diluting to 1,000~ml with diH_2O . 1~ml of the prepared sample was added to a Hatch reflux tube, followed by 0.6~ml of digestion solution. Then 1.4~ml of acidified silver sulphate reagent (2.5~%~m/m $M_2SO_4~ml$ in $M_2SO_4~ml$ was carefully added to the tube so that an acid layer was formed under the digestion solution layer. After the tubes were sealed and inverted three times (to mix properly) they were refluxed in a Hach COD reflux reactor (Model 45600) at $150~^{\circ}C~ml$ for 2~ml After cooling to room temperature, the samples were analysed on a UV/VIS scanning spectrophotometer (Shimadzu Model UV-2101PC) at 600~ml wavelength. Solutions of potassium hydrogen phthalate (KHP with theoretical COD of 1.176~ml O_2/ml .) were used as standards for calibration.

Total COD (TCOD) was obtained by taking 50 mg of sample and diluting it to 50 ml with diH_2O . The presence of particles in suspension makes it difficult to take representative samples. All COD assays were performed in ten replicates. The CV for the replicate samples was within 0.12.

The calculation of theoretical CH_4 potential (COD equivalence of CH_4) was based on the following equation

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
 (2.11)

Each mole of CH_4 consumes two moles of oxygen. Therefore, 1 g COD destruction is equivalent to 0.35L CH_4 at 0 °C and 760 mm Hg pressure (STP) or 0.395L CH_4 at 35 °C and one atmosphere [96].

2.4.3.4 Total N Measurements

The measurement of total nitrogen was conducted based on the Hach TN kit protocol (Hach Lange GmbH). A 5 mg sample was added to digestion tube and diluted with 0.5 ml diH2O. An alkaline persulfate digestion converted all forms of nitrogen to nitrate. Sodium metabisulfite was added after the digestion to eliminate halogen oxide interferences. Nitrate reacts with chromotropic acid under strongly acidic conditions to form a yellow complex with an absorbance maximum at 410 nm. The total N was measured on a Shimadzu UV/VIS scanning spectrophotometer (Model UV-2101PC) against blank. Ammonium chloride was used as a standard. The detection limits are 10–150 mgN/L, and the CV for ten identical samples was 0.11.

2.4.3.5 PVOH Measurement

This method was used to determine the PVOH residue left in the serum bottles after the BMP assay. The PVOH sample provided by Greenlight Ltd was used as a standard; a standard PVOH calibration solution (0–20 mg/L) was prepared.

PVOH was determined by a colorimetric method based on formation of a PVOH-iodine-boric acid blue complex. The PVOH-iodine complex is a helix structure formed by the vinyl alcohol groups and iodine; this helix is further stabilized by boric acid through its linkage of OH groups [26, 54]. Only the concentration range from 0 to 20 mg PVOH/L falls within Beer's law behaviour and so all samples were prepared within this range [6, 26].

4 % Boric acid solution was prepared by dissolving 4 g boric acid crystals in 90 ml water, at approx 80 °C and then diluting solution to 100 ml (after cooling to room temperature). Iodine solution was prepared by adding 1.27 g iodine and 2.5 g of potassium iodide in 100 ml diH2O to give final concentrations of 0.05 M I2 and 0.15 M KI. 0.15 ml of sample was treated with 0. 75 ml of 4 % boric acid solution and 0.15 ml of iodine solution in turn and mixed well after each addition.

The final solution was diluted to 2.5 ml and kept at 25 °C for 15 min and then its absorbance was measured at 690 nm on a UV/VIS scanning spectrophotometer (Shimadzu UV-2101PC) against a blank solution containing the same amounts of boric acid and iodine solution.

2.4.3.6 Total Protein Measurements

Total protein content was measured by using a total protein kit (Sigma, product codes TP0300 and L3540) which was based on the modified Lowry assay developed by Peterson [78]. 5–10 mg foam samples were added to a test tube and diluted to 1 ml with diH2O and 1 ml of Lowry reagent was added to each tube and mixed well. After maintaining at room temperature for 20 min, 0.5 ml Folin and Clocalteu's phenol reagent was added to the tubes with rapid and immediate mixing, and then the samples were left at room temperature for a further 30 min to develop a purple colour. The samples were transferred from tubes to cuvettes and analyzed on a Shimadzu UV/VIS scanning spectrophotometer (Model UV-2101 PC) against a blank at wavelength 750 nm [78]. All the absorption readings were finished within 30 min to avoid inaccuracy caused by the gradual loss of colour (colour loss is approx 1 % per hour at 20 °C).

Bovine serum albumin (BSA) was used as a standard to determine calibration curves. The detection limit was 5 mg/L and the CV for ten identical samples was within 0.166.

Besides the determination of total protein present in WBF, this method was also applied to estimate the wheat protein residue left in the serum bottles after the BMP test. After mixing the samples, over 1 ml liquid samples were collected from bottles by using a 5 ml plastic syringe (through Teflon seals) and filtered through a 0.22 μm filter (VWR Labshop) to remove cellular proteins. Then 1 ml filtered samples were analyzed by using method describe above. Wheat protein degradation was estimated by the difference in total protein content in bottle fed with WBF (extracellular protein + wheat protein residue) and in PSBF/MSBF/blank bottles, where only secreted extracellular protein but no wheat protein were present.

2.4.3.7 Determination of Structural Carbohydrates and Lignin Content

The carbohydrates and lignin content in cardboard was analyzed according to NREL standard methods [45, 90]. Before the assay the filtering crucibles were prepared by placing them in a muffle furnace at 575 + 25 °C for at least 4 h to ash to constant weight.

TS in the sample was determined by the method in Sect. 2.4.3.1; at the same time 300 mg air-dried samples were transferred to pressure tubes, then 3 ml 72 % $\rm H_2SO_4$ was added to each and mixed. Then pressure tubes were incubated in water bath at 30 \pm 3 °C for 60 min; every 10–15 min, samples were stirred to ensure a

uniform hydrolysis. After this, the H_2SO_4 was diluted to 4 % by adding 84 ml di H_2O ; the tubes were capped with Teflon screw caps and placed in an autoclave at 121 °C for 1 h. After cooling, the hydrolysis solution was vacuum-filtered through the pre-weighed filtering crucible; filtrates were collected for analysis of the acid-soluble lignin and the carbohydrates contents.

All remaining solids were transferred into filtering crucibles and rinsed with more than 50 ml diH₂O. The crucible and acid-insoluble residues were dried at 105 ± 3 °C for 24 h until a constant weight and after recording the weight, the crucible and residue were transferred into the muffle furnace at 575 + 25 °C for 48 h until achieving constant weight; then crucible and residue were removed to a dessicator to cool down, and the weights were recorded.

Approx 20 mls of the filtrates were transferred into a flask and neutralized by adding CaCO₃. Then samples were then centrifuged twice at 13,000 rpm for 15 min. Approx 1 ml of supernants was transferred to vials and analyzed by HPLC (Agilent Technologies 1,200 series) with a Bio-Rad Aminex HPX-87H column at 50 °C with water as the mobile phase and a flow rate of 0.6 ml/min. Carbohydrate compositions were determined by running against standards for glucose, xylose, galactose, arabinose, and mannose.

Approx 2.5 ml of filtrate was also transferred into a cuvette and acid-soluble lignin was determined by running against a blank sample of diH₂O on the UV–Visible Spectrophotometer (LightwaveII, Biochrom Ltd) at a wavelength of 330 nm. This wavelength and absorptivity constant ϵ (9.1642 L/g-cm) for acid-soluble lignin contained in cardboard were derived from another PhD study at our laboratories [101]. If necessary, the samples were diluted to bring absorbance within the absorbance range 0.7–1.0.

All the samples were performed in five replicates; filter paper (>98 % of cellulose) was used as an internal standard to control for the sugar recovery rate in the hydrolysis; standard sugars were also running through the autoclave hydrolysis procedure with 4 % $\rm H_2SO_4$ to correct for losses due to degradation during dilute acid hydrolysis.

The carbohydrates and lignin content were calculated based on the following equations

$$ASL = \frac{UV_{abs} \times V_{filterate} \times Dilution}{\varepsilon \times ODW_{sample}}$$
(2.12)

$$ODW_{sample} = \frac{Weight_{airdrysample} \times TS\%}{100}$$
 (2.13)

$$AIL\% = \frac{(Weight_{crucible plusair} - Weight_{crucible}) - (Weight_{crucible plusash} - Weight_{crucible})}{ODW_{sample}} \times 100\%$$

$$(2.14)$$

$$C_{corsample} = \frac{C_{HLPLC}}{\% R_{avesugar} / 100}$$
 (2.15)

$$\%sugar = \frac{C_{corsample} \times Anhydrocorrection \times V_{filtrate} \times \frac{1g}{1000mg}}{ODW_{sample}} \times 100$$
 (2.16)

where: Eq. 2.12 is for calculation of acid-soluble lignin (ASL); UV_{abs} is the average UV–Vis absorbance for the sample; V_{filtrate} is the volume of filtrate 87 ml; ε is the absorptivity constant of acid-soluble lignin contained in cardboard 9.1462 L/g-cm [101]; dilution = (Volume sample + Volume diluting solven)/Volume sample, here equals to 1; ODW_{sample} refers to as the dry weight of sample which is calculated from Eq. 2.13. Equation 2.14 is for estimation of acid-insoluble lignin percentage (AIL %); weight crucible plus air is the oven-dried weight of crucible and acid-insoluble residue; Weight crucible plus ash is the ignited weight of crucible and ash.

Equations 2.15 and 2.16 were applied to calculate polymeric sugar content in cardboard. C_{corsample and} C_{HPLC} refer to corrected sugar concentration and sugar content obtained from HPLC respectively; %R_{avesugar} is the average recovery rate for a specified sugar standard, which is obtained by the ratio of HPLC-detected sugar concentration to the known sugar concentration. %sugar is the percentage of each sugar as received based; Anhydro-correction is to convert to the concentration of polymeric sugars from the corresponding sugar monomer, anhydro corrections for C-5 sugars (xylose, arabinose) are 0.88 (132/150) and for C-6 sugars (glucose, galactose, and mannose) are 0.90 (162/180).

2.4.4 Statistical Methods

A non-parametric test method—one-tailed Mann–Whitney test was performed on each set of BMP results for different substrates to determine the substrate(s) with greatest biodegradability in AD over the digestion period. All the data were analyzed in Matlab (Matlab R2007b) at significance level $\alpha = 0.05$.

2.5 Composition and Properties of Materials Studied

Data on composition and properties of the products modelled especially the novel materials was not available. Therefore, it was necessary to characterize the composition of modelled products by laboratory research to ensure the important components present in the materials studied were accounted for in LCA model.

As defined in Sect. 2.1.2.2, the raw materials concerned in the modelled product systems (coolbox, display board, and construction concept products) were mainly WBF, potato/maize starch-based foams and cardboard. Their physical-chemical parameters were analyzed using the methods indicated in Sect. 2.4, and are presented below.

2.5.1 Composition of Product Systems

WBF, potato and maize starch based foam were collected from different batches of production representing the foams produced at Greenlight Ltd over the period of Aug 2006–Feb 2009. The cardboard box produced in The Box Factory Ltd in 2007 was used to simulate the cardboard component of coolbox (Hydropac Ltd, product code: CUIB001). The composition of different materials reported by manufacturers and their applications is given in Table 2.2. Moisture and protein contents in wheat flour and moisture contained in starch were derived from manufacturers (Heygates Ltd, Roquete France and Novidon), whereas the moisture content of PVOH feedstock was determined in the laboratory.

2.5.2 Characterisation of Materials

The foams and cardboard collected was kept at 4 °C to be prepared for experimental work. The properties of these materials were analyzed according to the methodology described in Sect. 2.4. Before analysis, the test material was kept spread out at room temperature for 2–3 days and turned once per day to ensure even air-drying until the change in weight was less than 1 % in 24 h. Then the samples were fed into a cutter mill until the entire sample was milled and passed a 10-mesh sieve. All the milled and sieved samples were homogenized and analyzed immediately.

The physico-chemical properties of WBF, cardboard and two additional starch-based foams including the TS, VS, total protein, total N and COD etc., are presented in Table 2.3.

2.5.2.1 TS/VS

VS/TS ratios for all three foams are over 99 %, which indicates a trace amount of inorganic material present in the foams; whereas the cardboard contain higher levels of inorganic material (lower VS/TS). The VS/TS results for cardboard (0.895) in this study are close to the data revealed by a study [94] (0.847) and the Phyllis database [24] (VS/TS = 0.932) but differred from the results reported by Owens and Chynoweth [76] (VS/TS = 0.977) and by Jokela et al. [53] (VS/TS = 0.77).

2.5.2.2 Total N and Total Protein Content

Normally wheat flour contains 10–15 % of protein (based on dry weight); approximately 80 % of the endorsperm protein is comprised of gluten including monomeric gliadins and polymeric glutenin (both soluble in SDS) [23, 43]. The

Table 2.2 Composition of materials

	Composition (% w/w)	Data source	LCA case studies			
			Cool	Display board	Trough mould	Void former
WBF	86.26 % wheat flour (9.5 % protein; moisture 14 %) 13.32 % PVOH (moisture 3.78 %) 0.29 % soy oil Trace amount soy flour	Greenlight Products Ltd Heygates	V	V	V	V
PSBF	87.23 % potato starch (Moisture 20 %) 12.35 % PVOH (moisture 3.78 %) 0.02 % talc 0.4 % soy oil Trace amount soy flour	Greenlight Products Ltd Roquete Ltd Novidon Ltd.	•	•	•	•
MSBF	89.64 % maize starch (Moisture 13 %) 9.73 % PVOH (moisture 3.78 %) 0.09 % talc 0.54 % soy oil Trace amount soy flour	Greenlight Products Ltd Roquete Ltd	•	•	•	~
Cardboard	34.8 % kraftliner (virgin paper based) 30.4 % Wellenstoff (recycled paper based) 34.8 % testliner (recycled paper based)	The Box Factory Ltd Hydropac Ltd	~			

remaining 20 % is albumins (soluble in water or dilute salty solution) and globulins (soluble in dilute salty solution but not water) [23, 43]. The protein contents were determined with two methods—the Lowry microassay [78] and the TN/ protein conversion method i.e. the protein concentration is obtained by multiplying its total N by a nitrogen to protein conversion factor which is calculated from the amino acids composition [72].

In this study the method to determine total N was persulphate digestion, which was developed as an alternative to the Kjeldahl method [19]. The main difference between Kjeldahl and persulphate digestion is that the former can determine organic N and NH₄⁺-N (not N from NO₂⁻ and NO₃⁻) whereas the latter can convert all forms of N (organic N, and NH₄⁺/NO₂⁻/NO₃⁻-N) to NO₃⁻-N [19, 92]. Persulphate digestion has been widely applied to water and plant material [81, 91, 92]. The results from previous studies indicate that persulphate digestion is an accurate and precise method for analyzing plant material—N recovery was complete and agreed with Kjeldahl and the results showed lower variability than Kjeldahl [81, 91]. Therefore, results obtained from persulphate digestion (within

Table 2.3 Physical and chemical properties of materials (SD is indicated in brackets)

	WBF	PSBF	MSBF	Cardboard
Gravimetric tests				
TS (%)	93.30 (0.766)	92.72 (0.264)	93.18 (0.188)	95.79 (0.321)
VS (% of TS)	99.10 (0.238)	99.55 (0.057)	99.87 (0.122)	89.46 (0.037)
Ash (% of TS)	0.90	0.45	0.13	10.54
COD test				
COD (mgO2/g TS)	1187.96 (172.67)	1167.26 (251.573)	1252.62 (448.674)	1133.47 (137.117)
COD (mgO2/g VS)	1198.75 (174.245)	1172.5 (252.703)	1254.20 (449.214)	1267.01 (153.273)
Total protein				
mg/g TS	42.55 (6.831)	3.30 (0.551)	4.23 (0.588)	0.00
% of COD	5.37	0.43	0.51	0.00
Total N				
mg/g TS	13.72 (1.519)	0.00	0.00	2.23 (0.0474)
Total S				
SI 181.975 (mg/g TS)	0.90 (0.032)	0.00	0.00	0.76 (0.011)
SI 180.669 (mg/g TS)	0.94 (0.033)	0.00	0.00	0.93 (0.019)
SI 182.563 (mg/g TS)	0.88 (0.031)	0.00	0.00	0.59 (0.009)
Structural carbohydr	ates and lignin o	content (% of dry	weight)	
Glucose	_	_	_	65.84 (0.963)
Xylose	_	_	_	10.04 (0.329)
Galactose	_	_	_	2.34 (0.099)
Arabinose	_	_	_	0.385 (0.048)
Mannose	_	_	_	6.09 (0.163)
Acid-soluble lignin	_	_	_	1.74 (0.223)
Acid-insoluble lignin	_	-	_	11.26 (0.835)

detection limits) in this study were considered as representative of total N contained in the material for N balance calculations in the LCA model.

The total N results for WBF obtained in this study, 1.37 % of WBF (equivalent to 1.59 % of wheat flour), were close to the results reported in previous studies for wheat grain (1.92 % of TS) [95] and wheat flour (1.63–2.07 % of TS) [4]. Total N contained in the cardboard was determined as 0.223 % of TS, which is higher than the 0.04 % TS found by Jokela et al. [53] but close to other values reported in the literature [30, 94] and the value of 0.25 % of TS cited in the Phyllis database [24].

When converting total N content of WBF to total protein, two Nitrogen Factor (NF) recommended in previous studies were compared—5.7, a recommended NF for wheat grain [4, 36, 72, 95] and 5.52, a proposed NF for wheat flour [69, 86]. In this research, NF 5.52 was applied to WBF due to wheat flour being the main component of WBF. Using this NF, the converted protein from Eq. 2.17 is 75.7 mg/g TS, which gives a higher value than the Lowry microassay result (42.55 mg protein/g TS). This can be partly explained by a non-protein N fraction

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present in the total N results [69], such as free amino acids, amides, and other non-polymeric N constituents [47]. However, the non-protein N fraction in wheat is reported to be negligible, only accounting for 1.5 % of total N [47]. Therefore, another factor may be the main reason for the difference between two results. Starch contained in the WBF is a potential interfering substance in the Folin phenol method [77]. Technically, the limitations in methodology could be rectified. For instance, in the persulphate digestion method, inaccuracy caused by non-protein N could be overcome either by determining non-protein N content or extracting protein before N determination [55, 58]; eliminating interfering substances in the protein assay, DOC-TCA precipitation sep suggested by Peterson [77] could be modified (DOC-TCA precipitation may not applicable to wheat proteins). However, considering that the main objective is to determine the total N content in foam/cardboard for N balance in the LCA model, the methodological modifications for protein content determinations were beyond the current scope of this work and were not explored further.

$$\%Protein = \%Nitrogen \times NF$$
 (2.17)

where: NF = nitrogen factor.

The trace amount of protein content in the MSBF or PSBF could be explained by the protein contained in soy flour—a previous study reported the protein content in soy flour as typically 50 % (within the range of 51–53 % over an 8-year study period) [79]. The soy protein might be introduced into foams via the trace amount of soy flour used as material to lubricate equipment during the foam production process. But the total N content did not confirm the protein assay results. The detection limit for persulphate digestion (detection range 10–150 mgN/L) and Peterson's modified Lowry assay (detection range above 5 mg/L) could cause this error. Converting protein to total N based on Eq. 2.17 (the NF of soybean or meal 5.5 was applied) [69], 0.6 and 0.77 mg N/g TS for PSBF and MSBF were obtained and thus these trace amounts of N were considered as negligible in the N balance calculation for the LCA model.

2.5.2.3 Total COD

In addition to total nitrogen and protein measurement, a total COD test was carried out to analyze the stoichiometric CH_4 potential. The measured COD/TS ratio for foams is between 1.16 and 1.25 g O_2 /g TS, which is close to the calculated theoretical COD value converted from the starch $(C_6H_{10}O_5)_n$ and PVOH $(C_2H_4O)_n$ components in the foams. Here WBF is given as an example to illustrate the calculation carried out based on Eq. 2.18 [96]. Equivalent COD for starch and PVOH are 1.185 and 1.818 g COD/g respectively. As the formula of the protein detected in WBF was not determined, the percentage of COD represented by protein was estimated by assuming a stoichiometric conversion factor of 1.5 which was derived from the protein formula $C_{16}H_{24}O_5N_4$ presented by Rittmann and McCarty [84] and

used to represent solid protein of kitchen waste in a previous study [68]. Therefore, based on the compositions listed in Table 2.2 the calculated equivalent COD for WBF is 1.3 g/g TS, which is consistent with the experimental results.

For the formula $C_nH_aO_bN_c$ (1 mol)

$$COD = \frac{2 \times n + (a - 3 \times c)/2 - b}{2} \times 32 \text{ g O}_2$$
 (2.18)

The COD results for WBF and PSBF are quite close whereas MSBF is slightly higher than other two foams. The COD of cardboard is slightly higher than foams on a total VS basis; but, on the basis of fresh sample, COD value of cardboard is very close to or lower than foams. This suggests that similar potential CH₄ yields could be expected from the same amount of dried/fresh cardboard and foams.

2.5.2.4 Total Sulphur Content

Sulphur is taken by the plant from soil and transferred into amino acids and other organic compounds in plant tissue in the form of sulphate [61]. It is component part of amino acids therefore a component of most proteins, taking a part in initiating protein synthesis. In the case of wheat protein, sulphur plays a role in forming wheat protein determining the baking quality of winter wheat. The sulphur sequestered in wheat protein/wood tissue is present in the final products (WBF/cardboard). The S content in bio-based foams and cardboard was analysed according to the methodology described in Sect. 2.4.2.3.

To test the reliability of the S-measurement technique applied, the blank and additional samples were spiked with NaSO4 standard (final concentrations of standard is 50 ppm S). The recovery rate for three emission lines and different samples are shown in Table 2.4. On three emission lines, the recovery rate for NaSO₄ varied between 100.6 and 105.36 %, depending on the samples. This range is confirmed by Kalra et al. [57], they tested S recovery rate by using the same microwave digestion plus ICP-OES method, and found the recovery for different sulphur sources ranged from 95.5 to 112.9 %; particularly for Na₂SO₄, recovery rate was 104.8 ± 3.2 – 112.9 ± 1.9 % depending on the amounts added. Soon et al. [93] also tested this method, they indicated that the S value obtained was higher than the certified limits in the case of some plant tissue (the recovery rate varies between 100.41 and 110.62 %). The recovery rate calculated in this study together with the previous studies are good indications of the high accuracy of the technique used for S element determination.

The S content determined by three emission lines of ICP-OES varied between 0.88 and 0.94 mg/g TS for WBF and between 0.55 and 0.86 mg/g TS for cardboard (see Table 2.3). The result measured by emission line S I 180.669 nm was preferred as it was recommended as more sensitive line [33, 60] and it showed no interference from calcium (SI 181.979 nm has spectral overlap of S and Ca).

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NaSO ₄ added a	s spike			
Emission lines	Amount added (mg/L)	Blank + spike (recovery %)	WBF + spike (recovery %)	Cardboard + spike (recovery %)
SI 181.975	50	100.82	101.79	101.60
(mg/g TS)		(6.92)	(0.36)	(2.90)
SI 180.669	50	105.36	104.06	102.31
(mg/g TS)		(6.23)	(4.53)	(2.59)
SI 182.563	50	100.60	102.33	102.64
(mg/g TS)		(7.48)	(0.47)	(3.04)

Table 2.4 Recovery of S element (SD is indicated in bracket)

Comparing the reading from S I 180.669 emission line with the sulphur content observed in other studies, 0.094 % of WBF is lower than the data reported by Soon et al. [93], Kalra et al. [57]. According to these two previous studies, S accounts for 0.235 % [93] and 0.186 % [57] of wheat flour (oven dry basis), which is equivalent to 0.203 and 0.160 % of WBF respectively (calculation based on 86.26 % of wheat flour component in WBF). For S content in cardboard, the result revealed here (0.093 % of oven dry basis) is slightly lower than the results recorded in Phyllis database (0.12 % of dry wt) [24].

Based on the discussion above, 0.94 mg S/g WBF and 0.93 mg S/g cardboard (dry basis) were used in the LCA to calculate the downstream release of this S during subsequent processing, product use and final disposal stages of the life cycle.

2.5.2.5 Structural Carbohydrates and Lignin Content of Cardboard

As presented in Table 2.3, approx 84.7 % of oven-dried weight corresponded to polysaccharides, this result is higher than the carbohydrate content of cardboard reported by Yáñez et al. [106] (75 % polysaccharides).

Amongst all the polymeric sugar contained in cardboard, glucan was main component, accounting for 65.8 % of the mass. This result is consistent with studies by Shi et al. [87] that 64.1 % of the dry weight of mixed paper and 48.8 % of cardboard was glucan, and Yáñez et al. [106], who reported 59.7 % of cellulose content in cardboard.

Hemicelluloses are the second most abundant polysaccharide types in the plant cell wall, usually constituting about 20–35 % of the mass [87]. Hemicellulose (including xylan, galactan, mannan, araban) accounted for 18.86 % of the mass of oven-dried cardboard in the present study. Xylan was the major monomer (10 % of oven-dry basis), close to the 8.5 % reported by Shi et al. [87]. Conversely, in the current study other sugars contained in hemicellulose were not negligible with 6 % mannan and 2.3 % galactan. Yáñez et al. [106] and Barlaz et al. [5] reported 13.8 and 9.9 % hemicellulose content respectively- somewhat lower than the hemicellulose content in the cardboard in the present study.

After dilute acid hydrolysis, part of the lignin was soluble in H₂SO₄ but most was acid-insoluble accounting for over 11 % of the oven-dry mass of cardboard,

which is consistent with previous studies [87, 106], their results fell into the range 14–15 % of acid-insoluble lignin content (oven-dry basis).

All the test results presented here were corrected for the recovery rate of standard sugars or filter paper. If the recovery rate of glucose is disregarded then the average conversion efficiency of cellulose contained in filter paper was 99.2 %; if the recovery rate was included then the efficiency was quantified as 104 %. This indicated that the two-step acid hydrolysis was thorough and efficient. Therefore, it could be assumed that nearly 100 % of the polymeric sugars contained in cardboard were hydrolyzed to sugar monomer.

Based on the compositional analysis, it was estimated that C component sequestered from atmosphere during wood growing and present in cardboard was 45.84 % on oven-dry basis, which is equivalent to 1.68 kg CO₂/kg oven-dried cardboard. Where the C content in polymeric sugar was calculated from their molar mass; C contained in lignin fraction was estimated as 62.2 % oven dry basis, which was derived from the softwood composition in the Phyllis database [24]. The reason for choosing softwood data is the raw wood logs/saw mill residues used for paper making are primarily derived from softwood, accounting for 71 %, especially for kraftliner which is the main component of facing for the cardboard under analysis and 81.5 % of the feedstocks are softwood [25]. This C content obtained from laboratory test was used in the LCA model to track the fate of C over the life cycle of the cardboard component contained in coolbox.

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Chapter 3 LCA of Wheat Agro-Eco-System

3.1 Introduction

As indicated in previous LCAs, the agricultural system is one of main contributors to environmental burdens caused by crop-based products (including bio-polymers and bio-energy) [26, 64]. Several environmental issues are involved e.g. GWP, acidification and eutrophication, where trace gas emissions/leaching from agricultural land such as N_2O , CH_4 , NO_3^- are the main concerns.

Global and UK statistics give a good picture of emissions/leaching from agriculture. In 2005, 10–12 % of global anthropogenic total GHGs and, especially, 50 % of CH₄ and 60 % of N₂O were attributable to agriculture [60]; whereas, in the UK an even higher percentage (75 %) of N₂O emission was caused by agriculture [19, 18] and soil N₂O emission accounts for 92 % of this [18]. In addition, approx 10 % of NH₃ emission in the UK [18] and 60 % of nitrate and 25 % of phosphate emissions to water in England originate from agricultural land [17].

In most LCA studies on crop-based products, factors such as soil type, atmospheric deposition, changes in the soil quality and quantity etc. were not considered in the system boundary [3, 66]. But these factors are not negligible and can be sensitive parameters for the LCA model e.g. soil emissions which are highly variable depending on inter-related factors like soil type and farming practice [3]. To incorporate these factors into the LCA system boundary, process-oriented models can be considered. Compared with empirical models, process-based models simulate more of the factors involved in the agricultural C/N cycle [45] and thus the output is more site-specific and allows LCA system boundary expansion.

Amongst process-oriented models, DNDC is one of the most well-established. It has been validated worldwide and verified by field measurements [65, 7, 59, 6, 9, 8, 32, 4, 5, 1]. Furthermore, it has been applied to develop regional GHGs inventories in the USA [44], New Zealand, UK [6], China [55] and the EU [41]. But for modelling N₂O pathways, DNDC differs from the IPCC approach: the former concerns direct N₂O emissions whereas the latter includes both direct and indirect

 N_2O emissions (indirect N_2O via two pathways: NH_3/NO_x deposition and N leaching) [45, 36, 37]. Efforts have been made to compare both methods [29, 45, 35, 6]. Li et al. [45] and Hutchinson et al. [36] concluded that the IPCC approach and DNDC gave similar estimations of annual national inventories of direct N_2O fluxes from arable lands but that geographical patterns differed. However, the comparisons of different modeling approach at the field-specific scale need further exploration.

Actually, empirical models or 'default' factors such as the IPCC Tier 1 default factors have been applied in the majority of LCA or LCA-like studies, for calculation of soil N_2O emissions e.g. EBAMM [26], BESS model [48, 47]. However, the IPCC methodology is intended to be general and broadly applicable, but not for particular sites [35]. Moreover, it introduces a large degree of uncertainty in the estimations of direct/indirect N_2O emissions because of (1) uncertainty in the EFs themselves [37], (2) spatial and temporal variability of N_2O emissions, especially uncertainty in indirect emissions, and (3) regional differences in climatic and environmental conditions [35]. On the contrary, only a few studies concern integration of process-oriented models (RothC Daycent) with LCA study [2, 39, 34]. Neither discussion on LCA system boundary expansion by incorporating process-oriented models nor comparisons of different modeling approaches within the LCA context have been found.

In the current LCA, both DNDC and IPCC approaches were applied to simulate the field emissions from the specific wheat agro-eco-system under examination and the sensitivities of the LCA results to different modeling approaches were examined.

3.2 Product System and System Boundary

3.2.1 Function and Functional Unit

This chapter mainly focuses on one phase of life cycle for WBF products, i.e. Soisson wheat farming which is the principal feedstock for WBF. Therefore, in this chapter, LCIA results are presented on the basis of 1 kg Soisson wheat grain.

3.2.2 Product System and System Boundary

The Soisson wheat investigated was produced on Heygates Farms Swaffham Ltd. The crop year 2006 for Soisson was selected to represent the average technology and farm practice at the Swaffham farm. The boundary for this unit process was specified as "to farm gate", which includes the following field operations:

- Plough-based cultivation and drilling.
- Crop protection—spraying of herbicides, insecticides, fungicides, trace elements, growth regulators, and adjuvant.

- Fertilization—application of granular fertilizers to fields.
- Combine harvesting—100 % of straw is incorporated in the soil.

As defined in Fig. 3.1 the main inputs involved are farm machinery and fossil fuel consumed during field operations, wheat seed, and CO₂ sequestration into wheat grain. Besides the wheat grain and straw produced, environmentally relevant outputs are considered such as emissions from the field to the atmosphere and water (e.g. NO₃⁻, NH₃, N₂O, NO) and emissions due to the combustion of fossil fuel (N₂O, CO₂, CH₄).

The following factors were included in the system boundary, the deposits onto land from the atmosphere, the changes in soil quality and quantity over time (period between cultivation of Soisson and the subsequent crop), soil type, climate and farming practice. In addition, crop rotation over the period 2003–2007 was also taken into account; as indicated by Audsley et al. [3], although a specific crop is studied, it interacts with other crops in rotation, which influences soil quality. For instance, the residual nutrient in soil carried over from the previous crop or the previous field operations could lead to an unsteady state of soil fertility over time. These factors are included in the present study. However, the general representation of land use (apart from the factors described above) as an impact category and labour factors are excluded from the system boundary.

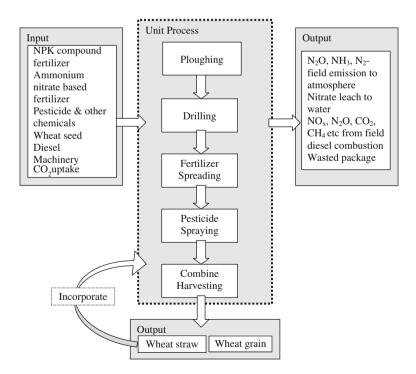


Fig. 3.1 Unit process of the specific wheat grain production for WBFs

3.3 Life Cycle Inventory Analysis

The inventory data for Soisson were based on the crop years 2003–2007 developed in collaboration with Heygates Farms Swaffham Ltd, chemical and fertilizer manufacturers, Rothamsted Research and NSRI of Cranfield University. The database covered six intensively managed fields with a total area of 73.29 ha. The LCI calculation procedure is outlined below.

3.3.1 Inventory for Soil Properties

The six fields studied are located in a nitrate vulnerable zone, with approximate soil composition sandy loam 44.84 %, loamy sand 13.69 %, sandy clay loam 21.91 % and light sandy loam 19.57 %. This soil composition was assessed by the Swaffham farm according to the RB209 method [49]; it was quite similar to the soil textures determined by using the USDA soil texture triangle method, in which soil is divided into 12 major textural classes, as determined by soil physical composition in terms of mineral particles (total sand/silt/clay content) [62].

Soil physical composition and other soil parameters were derived from an arable land database provided by NSRI of Cranfield University. Two soil associations and eight soil series (soil type) are involved [52] in the studied area—association A and B covers 253 and 301 km² accounting for 0.17 and 0.2 % of lands in England and Wales, respectively. The hydraulic properties and texture of the soils vary between different horizons/layers though only topsoil is used as an input in the DNDC model [25] (top soil is referred to as surface layer of soil down to plough depth, containing partly decomposed organic debris) [53]. Therefore, only the properties of the upper 30 cm soil are presented in Table 3.1, where top soil was determined as sandy and loamy texture (according to USDA textural triangle, soil texture is 20–34 % sand; 36–60 % sandy loam; 20–30 % loamy sand).

As indicated in Table 3.1, the mean values of associations A and B were calculated to represent the average properties of soils in the studied area. Ranges given in Table 3.1 were obtained from the difference between associations A and B for each parameter. The proportion of this range to the average value was used to define the uncertainty of soil parameters in the DNDC model. Other soil properties such as hydrological characteristics were also taken into account in the crop model. According to the NSRI database, no water retention between 0 and 120 cm soil layers is identified [52]; this area shows low run-off potential but high leaching capacity with little ability to attenuate non-absorbed pesticide leaching, which indicates groundwater vulnerable to pesticide contamination. In terms of natural soil fertility, mixed soil is found in this area varying from high fertility, lime-rich (containing excessive chalk and limestone) to low fertility [52].

Table 3.1 Hydraulic properties and texture of top soil

Soil association	Series	Soil Series Fraction of association name total area	Lower depth	Upper depth	Bulk density	Particle density	Porosity	Field capacity	Field Field capacity capacity in sandy soil	Wiling point	Hydro conductivity	Sand Total	Silt content	Clay content Organic carbon	Organic carbon	ЫН	Soil texture
		%	cm	cm	g/cm ³	g/cm ³	0-1	0-1	0-1	0-1	m/hr	% by weight	% by weight	% by weight	% by weight		
А	A-1	36.0	0.0	30.0	1.18	2.59	0.544	0.364	0.335	0.153	0.10	59.0	25.0	16.0	3.40	7.80	sandy loam
	A-2	34.0	0.0	30.0	1.54	2.63	0.414	0.188	0.15	0.056	0.12	88.0	7.0	5.0	1.00	8.10	sand
	A-3	30.0	0.0	25.0	1.39	2.62	0.469	0.286	0.254	0.10	0.07	85.0	0.6	0.9	1.80	7.70	loamy sand
	Average	0	0.0	28.5	1.37	2.61	0.48	0.28	0.25	0.11	0.10	77	14	6	2	7.87	
В	B-1	40.0	0.0	30.0	1.57	2.64	0.405	0.294	0.275	0.136	0.03	61.0	25.0	14.0	0.80	7.70	sand loam
	B-2	20.0	0.0	30.0	1.47	2.63	0.441	0.276	0.247	0.102	0.05	83.0	10.0	7.0	1.30	7.0	loamy sand
	B-3	20.0	0.0	25.0	1.50	2.63	0.43	0.283	0.258	0.111	90.0	73.0	19.0	8.0	1.10	7.0	sandy loam
	B-4	10.0	0.0	25.0	1.22	2.59	0.529	0.31	0.271	0.097	0.11	88.0	8.0	4.0	3.50	09.7	sand
	B-5	10.0	0.0	30.0	4.1	2.63	0.452	0.19	0.149	0.054	0.17	0.68	7.0	4.0	1.50	0.9	sand
	Average	•	0.0	28.5	1.49	2.63	0.43	0.28	0.25	0.11	90.0	73	17	6	1	7.24	
Average for A B	A B			28.5	1.43	2.62	0.46	0.28	0.25	0.11	0.08	75	16	6	2	7.56	
Range of each parameter	ch paran	neter			0.123	0.017	0.043	0.001	0.005	0.008	0.034	3.4	3.2	0.1	8.0	0.632	

3.3.2 Inventory for Climate

Daily meteorological data collected from a weather station (Broom's Barn) were used to represent daily maximum and minimum temperature (°C), precipitation (cm) and wind speed (m/second) of the studied area. As shown in Table 3.2, over the period 2003–2007 the annual average precipitation fluctuated whereas average temperature and wind speed were relatively stable. From the data range (the max and min data over a year), it is clear that extreme values i.e. highest and lowest temperature as well as lowest daily precipitation occurred in 2003. As for the year 2006, the annual max/min average temperature was slightly higher than other years (except 2003), in addition the greatest daily precipitation and lowest daily max temperature over five years (2003–2007) were observed on Julian day 208 and Julian day 33, respectively, in 2006.

Other important parameters including atmospheric NH_3/CO_2 concentration and rainfall NH_4^+ concentration were also taken into account. Based on 2006 UK map for NH_4^+ ion content of rain [10], rainfall NH_4^+ concentration for Swaffham farm area was estimated as 44 μ eq/l, which equals to 0.616mg N/l. Atmospheric NH_3 concentration was calculated according to the measurement-based data from Stoke Ferry site within NAMN network, which is 9.2 miles away from the farm [12]. NH_3 concentration shown for Stoke Ferry database fluctuated every year, generally a higher concentration was observed from early March to early November; if comparing annual average data for 2003–2007, maximum and minimum NH_3 concentration occurred in 2003 and 2004, respectively (2.55 NH_3 μ g/m³ and 2.15 NH_3 μ g/m³). The mean value for 5 years (2003–2007) approx 2.35 NH_3 μ g/m³ was used in the DNDC model.

CO₂ concentration and its annual increase rate were derived from several sources. According to the CO₂ records on the CDIAC website (Carbon Dioxide Information Analysis Centre), the CO₂ concentration in 2006 varied between 379 and 383 ppm and its annual increase rate during the period 2000–2007 ranged

Table	3.2	Daily	climate	data
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		Temperature maximum °C	Temperature minimum °C	Daily Precipitation cm	Wind speed m/second
2003	Average	15.13	6.53	0.151	1.764
	Range	$0.10 \sim 36.70$	$-5.90 \sim 19.70$	$0.000 \sim 2.160$	$0.162 \sim 4.942$
2004	Average	14.59	7.10	0.205	1.686
	Range	$1.50 \sim 29.70$	$-4.20 \sim 20.10$	$0.000 \sim 3.460$	$0.405 \sim 5.637$
2005	Average	14.47	6.80	0.148	1.709
	Range	$0.50 \sim 30.50$	$-4.40 \sim 17.40$	$0.000 \sim 2.710$	$0.023 \sim 6.979$
2006	Average	14.66	7.01	0.193	1.822
	Range	$-1.60 \sim 33.50$	$-5.70 \sim 19.30$	$0.000 \sim 3.730$	$0.081 \sim 5.694$
2007	Average	14.43	6.73	0.198	1.922
	Range	$0.40 \sim 28.30$	$-5.20 \sim 15.80$	$0.000 \sim 3.220$	$0.255 \sim 5.694$

between 1.5 and 2.5 ppm/year depending on sites and year. In the case of DNDC input data, the average increase rate 1.93 ppm/year reported by Reay et al. [56] and a background CO_2 concentration 380 ppm indicated by IPCC [38] and suggested by Goulding [31] were applied.

3.3.3 Inventory for Fertilizer and Chemicals

3.3.3.1 Specification of Fertilizer Chemical Products

In the six fields studied over 2003–2007, 24 different chemical fertilizers including NPK compound fertilizers and NH₄NO₃ fertilizers were applied. Based on the data provided by four fertilizer manufacturers, the fertilizer grades are specified in Table 3.3.

Besides fertilizers, pesticides, adjuvant, trace elements applied in Swaffham farm from 2003 to 2007 were also analyzed. These crop protection products varied between years and fields, depending on the crops grown and soil type, also relying on the commercial availability, as some products were withdrawn for commercial reasons. Based on the data provided by the farm and the Chemicals Regulation Directorate on-line database (2009) and the adjuvant supplier (De Sangosse Ltd), active substances for each crop protection product were quantified. Table 3.4 is given as an example which lists active substances for protection products used in 2006 for Soisson (data on Opte-Man is missing), of which 90 % were no longer used for the following crop in 2007.

The database established here for fertilizers and pesticides were applied in further inventory data analysis and are presented in the next sections.

3.3.3.2 Unit Processes for Fertilizer/Chemicals Manufacturing

The production processes for fertilizers and pesticides were built up based on the Eco-invent database [63], BAT data released by EFMA [23] and other studies [24].

The process for producing the NH_4NO_3 fertilizer Axan and Extran was modified. The production systems for producing NH_4NO_3 involve three processes: ammonia production, nitric acid production and ammonium nitrate production (Fig. 3.2).

There are two main types of process for ammonia synthesis gas in operation in Europe [23]: steam reforming of natural gas or other light hydrocarbons and partial oxidation of heavy fuel oil. The former process is more efficient and natural gas is the dominant feedstock accounting for nearly 80 % of world NH₃ capacity. Thus, the EU average for NH₃ manufacturing was used (85 % steam reforming of natural gas and 15 % partial oxidation). The intermediate product NH₃ is further oxidized to give NO, and then NO₂ from oxidation of NO is absorbed in water to form HNO₃. During this process, abatement methods for N₂O and NO_x emissions are

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Fertilizer grade	Compounds	Chemical Composition (%)
Axan	Ammonium as N	13.50
	Nitrate as N	13.50
	SO_3	6
Extran	Ammonium as N	16.90
	Nitrate as N	16.60
0.11.20 + 5mgo	Muriate of potash(60.5 % K ₂ O)	33.05
	Triple Super Phosphat (46 % P_2O_5)	23.91
	Granular Kieserite(25.6 % MgO 51.2 %SO ₃)	19.53
	Limestone	23.51
5.11.20 + 5mgo	Muriate of potash(60.5 % K ₂ O)	33.05
	Ammonium nitrate (34.5 % N)	2.01
	Di-ammonium phosphate (18 % N, 46 % P2O5)	23.91
	Granular Kieserite(25.6 % MgO 51.2 %SO ₃)	19.53
	Limestone	21.50
0.15.30 + 3.7mgo	Muriate of potash($60.5 \% \text{ K}_2\text{O}$)	50.00
	Triple Super Phosphat (46 % P ₂ O ₅)	32.60
	Granular Kieserite(25.6 % MgO 51.2 %SO ₃)	14.80
	Limestone	2.60
15.15.15	Muriate of potash(60.5 % K ₂ O)	25.00
	Ammonium nitrate (34.5 % N)	26.46
	Di-ammonium phosphate (18 % N, 46 % P ₂ O ₅)	32.60
	Limestone	15.94
Oxide 60	Calcined magnesite (80 %MgO)	9.93
	Salt (97–99 % NaCl as 50 % NaO)	18.06
	Triple Super Phosphat (46 % P ₂ O ₅)	7.93
	Sylvinite (16 % $K_2O + 31 \text{ %Na}_2O + 0.5 \text{ % Boron}$)	63.01
	Limestone	1.07
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Fertilizer grade	Compounds	Chemical Composition (%)
Frontier $26N + 35SO_3$	Ammonium sulphate (21 % N 60 % SO_3)	58.30
	Ammonium nitrate (34.5 % N)	39.80
	Limestone	1.90
0.14.25 + 6MgO $+ 12.5$ SO ₃	Kornkali (40 %k2o 6 %MgO 12 % SO ₃)	62.50
	Granular Kieserite(25.6 % MgO 51.2 %SO ₃)	7.50
	Triple Super Phosphat (46 % P ₂ O ₅)	30.00
Omex 16-0-8	Urea (46.6 % N)	35.00
	KCI (60.5 %K ₂ O)	15.50
Nitrofio 30 %N	Urea (46.6 % N)	33.00
	Ammonium Nitrate (35 % N)	44.00
Omex 4:10:23	Ammonium nitrate (34.5 % N)	1
	Mono-ammonium phosphate (11 % N, 52 % P_2O_5)	4.50
	Di-ammonium phosphate (20.5 % N, 52 % P_2O_5)	15.00
	KCI (60.5 % K ₂ O)	38.50
	Mg(OH)2 as 26 % MgO	9.50
Omex 0:2:7.5	Phosphate rock (34 % P_2O_5)	9
	$KC1 (60.5 \% K_2 O)$	12.50
	Mg(OH)2 as 26 % MgO	17.50
	NaCl (50 %NaO)	31
Omex 4:12.5:25	Mono-ammonium phosphate (11 % N, 52 % P2O5)	S
	Di-ammonium phosphate (20.5 % N, 52 % P2O5)	19
	KCI (60.5 % K ₂ O)	40.50
Omex 3:11.5:18	Mono-ammonium phosphate (11 % N, 52 % P2O5)	5
	Di-ammonium phosphate (20.5 % N, 52 % P2O5)	17
	KCI (60.5 % K ₂ O)	31
	Mg(OH) ₂ as 26 % MgO	13.50

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Table 3.	

Fertilizer grade	Compounds	Chemical Composition (%)
Omex 4:8:24	Mono-ammonium phosphate (11 % N, 52 % P_2O_5)	3
	Di-ammonium phosphate (20.5 % N, 52 % P_2O_5)	12.50
	Ammonium nitrate (34.5 % N)	2.50
	KCl (60.5 % K ₂ O)	40.00
	Mg(OH)2 as 26 % MgO	12.00
Omex 0:4.5:5.5	Phosphate rock $(34 \% P_2O_5)$	13.50
	KCI (60.5 % K ₂ O)	6
	Mg(OH)2 as 26 % MgO	21.00
	NaCl (50 %NaO)	31
Omex 3.5:10.5:1	Mono-ammonium phosphate (11 % N, 52 % P ₂ O ₅)	'n
	Di-ammonium phosphate (20.5 % N, 52 % P2O5)	15
	KCl (60.5 % K ₂ O)	20
	$Mg(OH)_2$ as 26 % MgO	17.50
Omex 0:4:5.5	Phosphate rock (34 % P_2O_5)	12
	KCl (60.5 % K ₂ O)	6
	$Mg(OH)_2$ as 26 % MgO	19
	NaCl (50 %NaO)	31
Omex 0:4:8	Phosphate rock $(34 \% P_2O_5)$	12.00
	KCl (60.5 % K ₂ O)	13.50
	Mg(OH)2 as 26 % MgO	19
	NaCl (50 %NaO)	24
AN 34.5 %	Ammonium nitrate (35 %N)	09.86
Double Top AN	Ammonium nitrate35 % N	0.475
	Ammonium sulphate (21 % N 60 % SO ₃)	0.495

Products	Field of use	Active ingredients	Concentration of ingredients
Herbicide	Ally Max Sx	Metsulfuron-methyl	143 g/kg
		Tribenuron methyl	143 g/kg
	Diflufenica	Diflufenican	500 g/L
	Stomp	Pendimethalin	400 g/L
	Axial	Pinoxaden	100 g/L
	Gf-184	Florasulam	2.5 g/L
		Fluroxypyr	100 g/L
	Roundup ace	Glyphosate	450 g/L
Insecticide	Hallmark with Zeon	Lamda-cyhalothrin	100 g/L
Fungicides	Joules	Chlorothalonil	500 g/L
	Opus	Epoxiconazole	125 g/L
	Bas 500 06	Pyraclostrobin	200 g/L
	Proline	Prothioconazole	250 g/L
	Amistar	Azoxystrobin	250 g/L
Adjuvant	Adigor	Methylated rapeseed oil	470 g/kg
	Activator-90	Natural fatty acids	150 g/kg
		Polyoxyethylene (5-8 EO) C10-C15 primary alcohol	750 g/kg
Growth	Stabilan	Chlormequat	700 g/L
Regulator	'S		

Table 3.4 Specifications of pesticide for crop year 2006

introduced into plants [61]. NH₃ and HNO₃ are further neutralized to form granular NH₄NO₃ via Neutralisation, Evaporation and Solidification steps.

 N_2O emissions from the HNO₃ process are a potentially important GHG emission. This is estimated as 8.39 kg N_2O/t HNO₃ in the Eco-invent database but it is not indicated whether N_2O abatement technology is included. By collaboration with the fertilizer manufacturer Yara UK Ltd, a site-specific dataset for NH_4NO_3 was built: the inventory for NH_4NO_3 manufacture from the Ecoinvent database was reviewed by Yara UK Ltd and the N_2O emissions during HNO_3 production process were adjusted based on the assumption that a 70 % reduction is achievable by introducing N_2O abatement technology (catalytic destruction technology) [67].

3.3.4 Inventory for Wheat Grain Farming

In the six fields, the average yields of wheat grain and straw in 2006 were 8.57 and 4 t/ha, respectively. At harvest, 100 % of wheat straw was incorporated into the field. No wheat grain was retained and used as seed, and no unsuitable quality grain was rejected by the flour mill. Therefore, no co-products were involved, wheat straw does not take any allocation and 100 % of the environmental burdens related to the inputs were allocated to wheat grain.

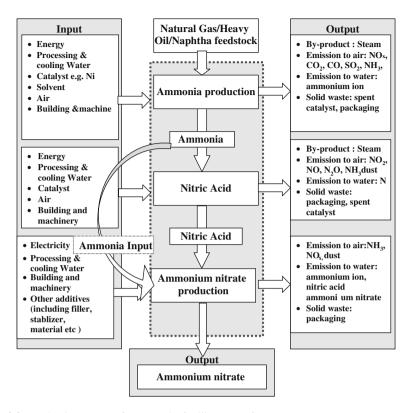


Fig. 3.2 Production process for NH₄NO₃ fertilizer manufacture

3.3.4.1 Fertilizer Application

In the crop year 2006, only chemical fertilizers were applied for wheat production, no organic fertilizers were used. N fertilizer was mainly applied at the beginning of the crop-rapid-growth and N-uptake period, i.e. from March to June as in this period wheat was N-demanding; whereas, in winter/autumn, the N requirement of wheat was low thus all N was supplied by soil reserves.

In the six fields, all fertilizers were applied according to RB209 guidelines [49]. Specifically, before fertilization, N application rate was calculated by determining SNS index and referring to the appropriate crop table (Soil Nitrogen Supply (SNS) index system). The SNS index is determined by a field assessment method based on information about previous cropping, fertilizer use, soil type and winter rainfall [49]. In another words, the SNS index method is highly site-specific taking into account soil texture, N uptake by previous crop, N loss via leaching and, crop nitrogen requirement. For example, in Field 1 and 2 (Table 3.5), soil type is classified as deep clay soils and light sandy soils according to RB209; annual precipitation varied between 550 and 750 mm during 2003–2007 (706 mm for 2006), and winter rainfall fell into the range of 150–250 mm. Thus, these data

Fields	Field 1	Field 2	Field 3	Field 4	Filed 5	Field 6
Soil type	Sandy clay loam	Sandy loam	Sandy loam	Sandy Clay loam	Light sandy loam	Loamy sand
Previous	Set aside	Potato	Sugar	Set aside	Potato	Sugar
crop			beet			beet
N	187.67	218.15	217.88	167.62	218.15	218.22
P2O5	27.17	0.00	0.00	19.47	0.00	0.00
K2O	49.39	0.00	0.00	35.39	0.00	0.00
SO3	48.73	24.03	23.94	32.10	24.03	23.94
MgO	12.35	0.00	0.00	8.85	0.00	0.00
Limestone	58.07	0.00	0.00	38.06	0.00	0.00

Table 3.5 Effects of soil type and previous crops on fertilizer input (kg/ha)

together with previous cropping determined the SNS index and the N recommendation was 100 and 160 kg N/ha for Fields 1 and 2 respectively.

As for P/K fertilizer, the application rate in the six fields was determined by previous crop and target soil index levels. For winter wheat, target levels are 16-25 mg P/L and 120-180 mg K/L which is maintained to ensure crop yield [49]. Nutrients removed by the previous crop was estimated from the typical potash/phosphate content in crops [49]. For instance, in Field 1, no crop was grown in the previous year and thus there was no nutrient off-take but the movement of K/P in soil, and leaching loss lowered the soil nutrient content, which required K/P compound fertilizer supply; whereas, in Field 2, no K/P compound fertilizers were applied due to the excess K/P nutrients left from the previous crop: nutrients applied in $2005 (390.9 \text{ kg } \text{K}_2\text{O/ha}, 238.4 \text{ kg } \text{P}_2\text{O}_5\text{/ha})$ were higher than nutrient off-take by the potato crop $(336.4 \text{ kg } \text{K}_2\text{O/ha}, 58 \text{ kg } \text{P}_2\text{O}_5\text{/ha})$.

In addition, sulfur and limestone were also applied. Limestone is used to reduce soil acidity and improve plant growth [37]. In the farm studied, lime was applied for the purpose of adjusting pH (only applied to sandy clay loam soil). Sulfur is another important plant nutrient. According to RB209, a similar amount of sulfur as phosphorus is required by the crop and extra sulfur nutrient input is normally needed for cereal grown in England due to sulfur deficiency [49]. There is a high risk of sulfur deficiency in the six fields due to the current low atmospheric sulfur deposition and sandy textured soil. Specifically, annual sulfur deposition in this area decreased from 13 kg S/ha/yr to below 7 kg S/ha/yr during the period of 1996–2006 [49, 11], ranking as one of the regions with lowest sulfur deposition in the UK; moreover, the sandy soil texture results in a high potential for sulphate-S leaching. This explains the higher application rates of SO_3 in the six fields than P_2O_5/K_2O and all the application rates fall into a range 25–50 kg SO_3 /ha which is similar to the range recommended in RB209 (25–40 kg SO_3 /ha) [49].

As indicated in Table 3.5, the fertilizer application rates varied from one field to another due to many factors including soil type and the residual soil fertility carried over from previous cropping [15]. These factors were accounted for within the system boundary for each individual field: the effects of soil, allocations of

Fertilizer	Average field rate (t/ha)	Overall application rate (t/ha)
NPK fertilizer 00:11:20 + 5 MgO	0.247	0.018
NPK fertilizer 5:11:20 + 5MgO	0.177	0.026
Axan (27 %N-9 %SO ₃)	0.251	0.251
Extran (33.5 %N)	0.416	0.416
Compounds	Average application rate (kg/kg wheat grain)	Overall application rate (kg/kg wheat grain)
Muriate of Potash	0.01636	0.00170
Triple 46	0.00689	0.00051
Granular kieserite	0.00967	0.00100
Limestone	0.01122	0.00115
Di-ammonium phosphate	0.00494	0.00071
Ammonium Nitrate as N	0.02434	0.02421
SO_3	0.00264	0.00264

Table 3.6 Inventory data for fertilizer input

fertilizer-related environmental burdens to the following crop in the rotation or the residual soil nutrient taken by wheat from previous crops. However, to represent the 'typical' fertilizer input for Soisson wheat at Swaffham farm, an average value for the six fields was used as the inventory.

Application of NPK compound fertilizers (0:11:20 + 5 % MgO and 5:11:20 + 5 % MgO) and N straight fertilizers (Axan and Extran) for the six fields are shown in Table 3.6. The average field application rates and overall application rates are as defined in the British survey of fertilizers: the former is "the sum of nutrient applied divided by the total area of those fields which received dressings of nutrient"; the latter is "calculated as the total quantity of nutrient divided by the total extent of area (including any areas without application of the fertilizer)" [16]. NPK compound fertilizers were not applied to every field while straight N fertilizers were used in all six fields. This practice is confirmed by results reported in a previous study [66] and the 2006 fertilizer survey [16]—the majority of N fertilizer applied on winter wheat was the "straight" forms (in 2006, the crop area receiving straight N and compound N fertilizer dressings were 79 and 32 %, respectively).

Based on the data shown in Table 3.3, application rates of compounds and nutrient to the wheat grain are illustrated in Table 3.6. These site-specific nutrient input data were compared with the results reported for UK generic wheat produced in intensive farms in 2006 [16] and in other studies (Table 3.7). The difference in N inputs between the specific wheat production in the present study and generic wheat production mainly results from the different end uses for wheat grain (milling or non-milling wheat) and other factors such as different treatment of straw. Studies 1 and 4 are based on the assumption that all straw is incorporated; whereas studies 3 [33] and 4 [54] are based on non-milling wheat, thus these latter data show slightly lower amounts of fertilizer input. The GB average fertilizer input data in Table 3.7 represent both non-milling and milling winter wheat [16]. If only including GB milling wheat, its overall application rate is 218 kg/ha, which is very close to that for

	2006 GB [15]	Study 1 [66]	Study 2 [3]	Study 3 [33]	Study 4 [54]
208.548	192.00	224.00	240.00	197.00	185.00
4.841	34.00	43.52	59.55	48.00	93.90
8.800	41.00	37.24	60.26	68.00	55.40
2.200	0.00	12.83	10.00	NA	NA
27.015	21.93	6.00	NA	NA	NA
9.833	286.70	241.50	NA	363.40	NA
	4.841 8.800 2.200 27.015	4.841 34.00 8.800 41.00 2.200 0.00 27.015 21.93	4.841 34.00 43.52 8.800 41.00 37.24 2.200 0.00 12.83 27.015 21.93 6.00	4.841 34.00 43.52 59.55 8.800 41.00 37.24 60.26 2.200 0.00 12.83 10.00 27.015 21.93 6.00 NA	4.841 34.00 43.52 59.55 48.00 8.800 41.00 37.24 60.26 68.00 2.200 0.00 12.83 10.00 NA 27.015 21.93 6.00 NA NA

Table 3.7 Comparison for nutrient input data Overall application rate Units = kg/ha

Notes NA = information not available

Soisson wheat. However, the applications of P/K fertilizer and limestone are much lower for Soisson wheat grain in the present study than for the wheat varieties indicated in the other studies. This relates to the site-specific conditions.

From the above analysis, it is concluded that the data collected from the Swaffham farm and the overall application rate for the six fields of Soisson wheat are consistent with generic farming practices for UK winter wheat.

3.3.4.2 Biocides, Growth Regulators and Adjuvant Applications

All the active substances contained in protection products and applied for Soisson are quantified in Table 3.8 and compared with UK pesticide application for generic wheat (2006) [30]. Here average application rate and overall application rate are defined as for fertilizer—the former is referred to as the sum of active substances applied divided by the total area of those fields which received dressing of substances; the latter is calculated as the total quantity of active compounds divided by the total extent of area (including any areas without application).

The Soisson wheat received on average three herbicide applications, one insecticide and three fungicide applications and two growth regulator sprays, which is very close to the GB average pesticide application for generic wheat [30].

All of the fungicides were applied between April and June and chlorothalonil was the dominant product (it was applied twice in all fields). This is consistent with generic farm practice for GB wheat [30]—most fungicide for GB wheat are applied during the same period to control a broad spectrum of diseases and chlorothalonil was the most commonly—used fungicide and more than one application was recorded in most farms.

Herbicides were applied for Soisson between autumn (November) and early spring (April) for the purpose of weed control. But the active compound applied for Soisson was different from UK generic wheat. Isoproturon was the most common active substance for weed-control for generic wheat, but this was not the case for Soisson.

In all six fields, growth regulators were applied twice in the middle of March and the end of April. Soisson was treated with insecticide in Nov 2005. GB Pesticide survey reported a similar practice for generic wheat—growth regulator

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Product	Name	Active substances [14]	Proportion of treated	Average application rate (kg/ha)	e (kg/ha)
			area for Soisson (%)	GB wheat (2006)	Soisson (2006)
Herbicide	Diflufenican	Diffufenican	100.00	0.522	0.503
	Stomp	Pendimethalin	100.00	0.997	0.601
	Axial	Pinoxaden	20.22	0.038	0.030
	Gf-184	Florasulam/Fluroxypyr	7.46	0.105	0.094
	Ally Max Sx	Metsulfuron-methyl/tribenuron methyl	92.54	0.009	0.004
	Roundup ace	Glyphosate	33.25	0.764	1.503
Insecticide	Hallmark with Zeon	Lamda-cyhalothrin	100.00	0.005	0.003
Fungicide	Joules	Chlorothalonil	100.00	0.471	1.000
	Opus	Epoxiconazole	100.00	0.067	0.125
	Bas 500 06	Pyraclostrobin	100.00	0.092	0.080
	Proline	Prothioconazole	100.00	0.101	0.100
	Amistar	Azoxystrobin	100.00	0.089	0.163
Growth Regulator	Stabilan	Chlormequat	100.00	1.036	1.610
Adjuvant	Adigor	Methylated Rapeseed Oil	20.22	NA	0.218
	Activator-90	Natural fatty acids	100.00	NA	90000
		Polyoxyethylene (5-8 EO)	100.00	NA	0.030
		C10-C15 primary alcohol			
Summary					
Product				GB wheat (2006)	Soisson (2006)
Herbicide	Number of	Number of spray round applied to crops		2.80	2.86
	Number of products	products		4.10	3.53
	Number of	Number of active substances		5.80	4.53
Insecticide	Number of	Number of spray round applied to crops		1.40	1.00
	Number of products	products		1.40	1.00
	Number of	Number of active substances		1.40	1.00

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ed to crops ed to crops ed to crops	(namumaa) ara aram				
Aurea for Solsson (%) Number of spray round applied to crops Number of active substances Number of spray round applied to crops Number of products Number of active substances Number of spray round applied to crops Number of active substances Number of active substances Number of active substances Number of active substances			Proportion of treated	Average application	rate (kg/ha)
gulator			area 10f 301880fi (%)	GB wheat (2006)	Soisson (2006)
gulator	Fungicide	Number of spray round applied to crops		3.00	3.00
		Number of products		5.40	5.00
		Number of active substances		7.50	5.00
	Growth Regulator	Number of spray round applied to crops		1.60	2.00
		Number of products		2.00	1.00
		Number of active substances		2.50	1.00
Number of products Number of active substances	Adjuvant	Number of spray round applied to crops		NA	1.20
Number of active substances		Number of products		NA	1.20
		Number of active substances		NA	2.20

Notes NA = data not available

application was made during March–May, and the majority of insecticides were applied in autumn for aphid control. Only one insecticide and one growth regulator product were used for Soisson, which is consistent with other GB farms [30]; Moreover, both products used for Soisson were the most commonly-applied ones for UK generic wheat.

As indicated above, the pesticide applications for six fields were consistent with UK average data. The overall application rate was applied in the LCA model to represent Soisson farm practice. However, there is a data gap in accessible databases for producing, packaging, and delivering the specific chemical products; instead, a general inventory for pesticide production from the Eco-invent dataset was applied to represent herbicides, insecticides and fungicides. Unit processes relating to adjuvant and growth regulator were derived from Eco-invent and the study of Audsley et al. [3].

3.3.4.3 Energy Consumption and Machinery for Field Operations

Table 3.9 shows data obtained from 6 fields on fuel consumption, tractor horse-power and average number of passes required for the field operations during the 2006 crop season at Swaffham farm. Chemicals and fertilizers were applied on average 5.86 and 3.22 times per hectare respectively. These data together with cultivation and harvesting passes were consistent with general UK practice [66].

Fuel used in field operations was diesel oil, which has a net calorific value of 43.4 MJ/kg [20] and a density of 0.85 kg/L. The process energy data indicate that cultivation and harvesting are the main energy consumers, this is consistent with previous studies [66]. The calculation of machinery input i.e. proportion of tractor used per hectare was based on total service life and work rate as shown in Table 3.9, and the weight of machinery obtained from the Eco-invent database (V2.0). The inventory used for producing and delivering of diesel fuel and manufacturing machinery was derived from the Eco-invent database (V2.0).

3.3.4.4 Carbon Dioxide Input

The C content of the wheat grain was estimated based on Eqs. 3.1, 3.2 and 3.3:

$$C_{WHEATGRAIN} = C_{FLOUR} \times F_{FLOUR} + C_{FEED} \times F_{FEED}$$
 (3.1)

$$C_{FLOUR} = \frac{C_{FLOURS} \times P_{FLOURS} + C_{FLOURP} \times P_{FLOURP}}{(1 - M_{FLOUR})} \times 100\%$$
 (3.2)

$$C_{FFED} = \frac{C_{FEEDS} \times P_{FEEDS} + C_{FEEDFI} \times P_{FEEDFI} + C_{FEEDFAT} \times P_{FEEDFAT} + C_{FEEDP} \times P_{FEEDP}}{1 - M_{FEED}} \times 100\%$$
(3.3)

Field operations	Activities	Tractor (kW)	Diesel (L/ha)	Passes per crop season (per ha)	Machinery service life (year)	Capacity (ha/hr)	Proportion of tractor life used per ha (%)
Cultivation	Plough	160	37	1	5	2	0.00228
	Drill	160	37	1	10	1.6	0.00143
Pesticide Spraying	Spray	120	15	5.856	10	16	0.00014
Fertilizer Application	Fertilizer Spreading	160	12	3.219	10	16	0.00014
Harvesting	Combine harvesting with straw chopping	300	40	1	10	4	0.00057

Table 3.9 Inventory for field operation in wheat production

where $C_{WHEATGRAIN}$ C_{FLOUR} C_{FFED} are the C content in dry wheat grain, flour and wheat feed; F_{FLOUR} and F_{FEED} represent the proportion of wheat flour and wheat feed in final products derived from wheat grain; M_{FEED} and M_{FLOUR} are the moisture content of wheat feed and wheat flour; whereas, C_{FLOURS} and C_{FLOURP} are the C content in starch and protein component in wheat flour respectively; P_{FLOURS} and P_{FLOURP} represent the fraction of starch and protein component in wheat flour; $C_{FEEDS}P_{FEEDS}$, $C_{FEEDFAT}P_{FEEDFAI}$, $C_{FEEDP}P_{FEEDP}$, $C_{FEEDFI}P_{FEEDFI}$ represent the carbon content and fraction of different components contained in wheat feed (starch, fat, protein, and fibre in order).

Harvested wheat grains were further processed in the flour mill to two products—wheat flour and wheat feed. Data obtained from Heygates Ltd. UK including the proportions of wheat flour/feed and the compositions of these two products are given in Table 3.10. The theoretical carbon content in starch (formula $(C_6H_{10}O_5)_n$) was calculated from molar mass as 44.4 %; C contained in protein was estimated as 54.55 % based on the formula $C_{16}H_{24}O_5N_4$ [57]. The composition of oil was derived from Phyllis database (76 % C content dry basis). C content presented in fibre was estimated on the basis of typical composition of wheat fibre (Table 3.11) [40]; C component in each anhydrous sugar monomer was calculated from its formula; lignin was estimated to contain 60 % C [21]. Therefore, C contents of wheat flour/feed and wheat grain were calculated as 45.56, 47.09 and 45.91 % on dry basis respectively. CO_2 sequestered in the wheat grain was therefore estimated as 1.47 kg CO_2 /kg fresh grain (moisture content 14.5 %), which is slightly higher than the data presented in the Eco-invent database (V2.0).

3.3.4.5 Other Inputs

In addition to the inputs above, 0.025 kg wheat seed sown/kg wheat grain produced was also taken into account [66]. The seed production process in Eco-invent

	Wheat flour	Wheat feed	Wheat grain
Proportion of products(% harvested grain)	77.00	23.00	100.00
Moisture content (%)	14.00	12.77	14.50
Starch (% of dry basis)	88.95	63.47	83.09
Protein(% of dry basis) ^b	11.05	17.16	12.45
Oil (% of dry basis)	NI^a	7.76	1.78
Fibre (% of dry basis)	NI^a	7.72	1.78
Ash (% of dry basis)	NI^a	3.90	0.90
C content (% of dry basis)	45.56	47.09	45.91

Table 3.10 C-content for wheat grain

Notes a. NI = No information; b. In Heygate lab tests, total N was analyzed, then protein content was estimated from equation %Protein = % Nitrogen \times NF. Where NF = Nitrogen Factor; NF $_{\text{FLOUR}} = 5.75$; NF $_{\text{FEED}} = 6.25$

Table 3.11 Composition of fibre contained in wheat grain

% Fibre									
Composition	Arabinan	Xylan	Galactan	Glucan	Mannan	Uronic acid	Cellulose	Lignin	C (%)
Soluble NCP ^a	5.07 %	6.52 %	1.45 %	2.90 %	1.45 %	0.72 %	-	_	8.14
Insoluble NCP ^a	15.94 %	27.54 %	1.45 %	5.07 %	0.72 %	2.90 %	-	-	24.16
Cellulose	-	-	-	-	-	-	14.49 %		6.44
Lignin	-	-	-	-	-	-		13.77 %	8.26
Total fibre	21.01 %	34.06 %	2.90 %	7.97 %	2.17 %	3.62 %	14.49 %	13.77 %	47.00

Notes a. NCP = Non-cellulosic polysaccharides

database v2.0 was adopted but the CO₂ sequestered in seed was excluded to avoid C double counting.

Data for the delivery of wheat seed, fertilizers and other agrochemicals were collected from Heygates Farms Swaffham Ltd and fertilizer manufacturers and suppliers (J & H Bunn Ltd. UK, Yara UK Ltd and Frontier Ltd). The inventories as well as the assumptions made for the truck capacity are shown in Table 3.12; all the transportation processes were based on Eco-invent v2.0 datasets.

3.3.4.6 Atmospheric Emissions From Field Operation

Atmospheric emissions from the agricultural system involve $N_2O/NH_3/CH_4$ from soils and GHGs as well as other pollutants (CO, VOCs etc.) from field operations. Here the emissions from fuel combustion estimated based on methods recommended in the 2006 IPCC Guidance [37] and 2009 EMEP-EEA Guidebook (previously referred to as EMEP-CORINAIR Guidebook) [22] are presented.

The equation applied for calculation of three GHGs ($CO_2/CH_4/N_2O$) from offroad transportation is:

	Transport mode assumptions	Distance×weight(kg km)
Wheat seed	16 t lorry	0.422
Axan and Extran	16t lorry	18.845
	Ferry	28.125
NPK fertilizer	16t lorry	0.489
Pesticides	Lorry with 7.5 t capacity	4.311E-03

Table 3.12 Transportation of inputs for 1 kg wheat grain

$$Emissions = \sum_{I} (Fuel_j \times EF_j)$$
 (3.4)

where Fuel_i is fuel consumed, EF_i is GHG emission factors, j is fuel type.

Other emissions from diesel combustion including CO, NH₃, NMVOC, NO_x, PM10, PM2.5 (particulate matter with aerodynamic diameter less than $10/2.5 \mu m$) and/or TSP (total suspended particulate), were estimated based on the Tier 1 approach in EMEP-EEA Guidebook [22].

$$E_{pollu \tan t} = \sum_{fueltype} FC_{fueltype} \times EF_{pollu \tan t, fueltype}$$
 (3.5)

where $E_{pollutant}$ is the emission of the specified pollutant; FC _{fuel type} is the fuel consumption for each field operation; $EF_{pollutant, fuel type}$ is the emission factor for specific pollutant for each fuel type.

The default EFs recommended in the by 2006 IPCC Guideline and EMEP-EEA guidebook were used and compared with factors derived from previous studies [3, 51] and the Eco-invent v2.0 database (combine harvest process). Higher GHG emission factors were found in the IPCC approach (Table 3.13). Based on Eqs. 3.4 and 3.5, the obtained results are illustrated in Table 3.14, which are very close to the Eco-invent dataset.

3.3.4.7 Direct and Indirect Field Emissions

N₂O Emissions From Soil

Besides field operation-related pollutants, direct and indirect N_2O emissions from soil are also important atmospheric GHGs. As described in the methodology (Sect. 2.2), N_2O was estimated by two approaches. Here only the results derived from IPCC empirical method are analyzed, the process-oriented model is discussed in Sect. 3.3.4.

N₂O produced in soils is a gaseous intermediate in the sequence of denitrification and a by-product of nitrification, highly related to the availability of inorganic nitrogen in soil. In total three pathways were considered in the IPCC approach [37]:

 Direct N₂O field emission resulting from addition of N (synthetic fertilizers and crop residues)

	IPCC Default (2006)	Eco-invent database	EMEP- CORINAIR [22] ^a	Study 1 [51]	Study 2 [3]
CO ₂ (kg/MJ)	7.410E-02	7.127E-02	7.281E-02	6.860E-02	7.005E-05
CH ₄ (kg/MJ)	4.150E-06	2.975E-06	1.267E-06	6.000E - 07	NA ^c
$N_2O(kg/MJ)$	2.860E-05	2.768E-06	3.134E-06	5.640E-07	NA ^c
GHGs ^b (kg CO ₂ eq/MJ)	8.270E-02	7.217E-02	7.378E-02	6.880E-02	NA ^c
CO(kg/MJ)	NA ^c	2.214E-04	2.521E-04	NA ^c	6.705E - 07
NH3(kg/MJ)	NA ^c	4.608E - 07	1.843E-07	NA ^c	
NMVOC(kg/MJ)	NA ^c	1.003E-04	7.756E-05	NA ^c	2.111E-07
NOx(kg/MJ)	NA ^c	1.176E-03	8.074E - 04	NA ^c	1.316E-06
PM10(kg/MJ)	NA ^c	NA	4.005E - 05	NA ^c	NA ^c
PM2.5(kg/MJ)	NA ^c	1.031E-04	4.005E - 05	NA ^c	NA ^c
TSP(kg/MJ)	NA ^c	NA ^c	4.005E - 05	NA ^c	NA ^c
SO2(kg/MJ)	NA ^c	2.325E-05	$9.22E - 05^{d}$	NA ^c	9.562E-08

Table 3.13 Emission factors for diesel combustion in agricultural machinery

Notes

^d All S in the diesel is assumed to be transformed completely into SO_2 [22]; S content in diesel was assumed as 0.2 % (wt) [21]

Table 3.14 Gases emitted from field operations	Table 3.14	Gases	emitted	from	field	operations
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Emission/Activities (kg/ha)	Plough	Drill	Pesticide spraying	Fertilizer application	Combine harvesting
CH ₄	5.664E-03	5.664E-03	2.296E-03	1.837E-03	6.124E-03
CO_2	1.011E + 02	1.011E + 02	4.100E + 01	3.280E + 01	1.093E + 02
N_2O	3.904E-02	3.904E-02	1.583E-02	1.266E-02	4.220E - 02
CO	3.440E-01	3.440E-01	1.395E-01	1.116E-01	3.719E-01
NH_3	2.516E-04	2.516E-04	1.020E - 04	8.160E-05	2.720E - 04
NMVOC	1.059E-01	1.059E-01	4.292E - 02	3.433E-02	1.144E-01
NO_x	1.102E + 00	1.102E + 00	4.468E-01	3.574E-01	1.191E + 00
PM_{10}	5.466E - 02	5.466E - 02	2.216E-02	1.773E-02	5.909E - 02
$PM_{2.5}$	5.466E-02	5.466E - 02	2.216E-02	1.773E-02	5.909E - 02
TSP	5.466E-02	5.466E - 02	2.216E-02	1.773E-02	5.909E - 02
SO ₂	1.26E-01	1.26E-01	5.10E-02	4.08E-02	0.136

Notes

 Indirect N₂O emission resulting from deposition of ammonia and NO_x. Here, only the ammonia volatilized and nitrogen oxidized due to addition of N (synthetic fertilizer) were considered

^a Diesel net calorific value used 43.4 MJ/kg [20]

^b GWP 100 yr for CH₄ and nitrous oxide: $CH_4 = 25 kgCO2$ eq/kg, $N_2O = 298$ kg CO_2 eq/kg [from IPCC Fourth Assessment Report (AR4)] [27]

^c NA = Not available

^{1.} The emission factors for CO_2 , N_2O and CH_4 from diesel combustion are 74100 kg/TJ, 28.6 kg/TJ and 4.15 kg/TJ respectively(assumption: full oxidation of diesel)

^{2.} Diesel density and net calorific value used are 0.85 kg/L and 43.4 MJ/kg [20]

 Indirect N₂O emissions caused by leaching/runoff from land due to fertilizer N and crop residue N inputs

Based on the IPCC Tier 1 approach (2006), equations for the estimation of direct/indirect N₂O emissions are as follows

• Direct emission (kg N₂O-N/kg wheat grain):

$$N_2 O_{DIRECT} - N = [(F_{SN} + F_{CR}) \times EF_1]$$
 (3.6)

• Indirect emission caused by atmospheric deposition (kg N₂O-N/kg wheat grain):

$$N_2 O_{(ATD)} - N = F_{SN} \times FR_{GASF} \times EF_4 \tag{3.7}$$

• Indirect emission caused by leaching (kg N₂O-N/kg wheat grain):

$$N_2 O_{(L)} - N = (F_{SN} + F_{CR}) \times FR_{LEACH} \times EF_5$$
(3.8)

• Amount of N in crop residues (above-ground and below-ground) for 1 kg wheat grain (kg N/kg wheat grain)

$$F_{CR} = Crop_{(T)} \times Area_{(T)} \times (R_{AG(T)} \times N_{AG(T)} + R_{BG(T)} \times N_{BG(T)})$$
(3.9)

EFs and uncertainty range given in Table 3.15 were derived from IPCC methodology [37]; the grain moisture content reported by Swaffham farm (14.5 %) which is consistent with 2006 national statistics [19] was used to estimate the dry matter of wheat grain.

Based on Eqs. 3.7–3.9, and the uncertainty ranges given in Table 3.15, direct and indirect N_2O for the six fields were calculated (uncertainty range was calculated by using min and max values of EF). As shown in Table 3.16, a large degree of uncertainty is introduced into the estimated N_2O field emission due to the uncertainties in the EFs. Generally over 75 % of N_2O emissions were produced via the direct pathway (nitrification, denitrification) and indirect emission caused by leaching was higher than indirect N_2O caused by atmospheric deposition. N_2O emissions for the six fields fall into a range of 0.00066—0.00079 kg N_2O/kg grain, which is slightly lower than the data in Eco-invent v2.0 database. Two fields (1 and 3) with sandy clay loam soil showed the lowest N_2O emissions, which can be explained by the lower N fertilizer input but higher wheat grain yield compared with other fields (see Table 3.5 N input). This result was used in the LCA model and compared with DNDC-simulated results for sensitivity and uncertainty analyses.

CO₂ Emissions From Liming

CO₂ emitted from liming or urea application is included as an important soil emission in IPCC Guidelines. No urea was applied for Soisson in 2006, only two

Table 3.15 EFs to estimate N₂O field emission from soil

Factors		Value	Data source and uncertainty range
F_{SN}	Annual amount of synthetic fertilizer N applied to soil	0.0243 kg N/kg wheat grain	Farm data range for six fields: 0.0197– 0.263 kg N/kg grain
EF ₁	EFs for N_2O emitted due to N input	N input	IPCC default value Range 0.003–0.03
FR_{GASF}	Fraction of synthetic fertilizer N that volatilizes as NH ₃ and NO _x	0.1 kg N volatilized/kg N applied	IPCC default value Range 0.03–0.3
EF ₄	EFs for N ₂ O from atmospheric deposition of N on soil and water surfaces	0.01 kgN ₂ O–N/kg N volatilized	IPCC default value Range 0.002-0.05
FR_{LEACH}	Fraction of N added to soil lost through leaching and runoff	0.3 kg N/kg N addition	IPCC default value Range 0.1–0.8
EF ₅	EFs for N ₂ O from N leaching and runoff	$0.0075~\rm kg~N_2O-N/kg~N$ leached	IPCC default value range 0.0005–0.025
$Crop_{(T)}$	Annual yield of crop on dry matter basis	Average for six fields 7.325 t dry matter/ha	Farm data (Yield for each field see Table 3.18- Range: 7.097-7.524 t dry/ha)
Area (T)	Area harvested for 1 kg crop	0.000117 ha/kg wheat grain (yield of Soisson = 8.567t wheat grain/ha)	Farm data range for six fields: 0.000114– 0.00012 ha/kg wheat grain
$R_{AG(T)} \\$	Ratio of above-ground residue dry matter to $Crop_{(T)}$	1.61 kg residue (dry basis)/kg crop (dry basis)	Calculated from IPCC Tier 1 range: 1.658–1.562
$N_{AG\left(T\right)}$	N content of above ground residue for crop	0.006 kg N/kg residue (dry basis)	IPCC default value
$R_{BG(T)} \\$	Ratio of below-ground residue to Crop _(T)	0.6 kg residue (dry basis)/ kg crop (dry basis)	Calculated from IPCC Tier 1 range 0.862–0.348
$N_{BG(T)}$	N content of below-ground residue for crop	0.009 kg N/kg residue (dry basis)	IPCC default value

fields with sandy clay loam soil were treated with limestone to adjust pH and improve wheat growth; overall application rate of limestone for Soisson is much lower compared with the 2006 UK average wheat (see Table 3.7), only 0.001148 kg limestone/kg grain was applied.

Liming practice is not taken into account in the DNDC model, therefore, only the IPCC Tier 1 Approach [37] was adopted to estimate liming-induced CO_2 emissions:

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Table 3.16	

	Crop _(T)	$Area_{(T)}$	Fcr kg N/kg fresh	$ m N_2O_{DIRECT}$ ko N/ko fresh	$ m N_2O_{(ATD)}$ ko N R o fresh	$ m N_2O_{(L)}$ kg N/kg fresh	$ m N_2O_{total}$ k $ m oN_2O/k\sigma$ fresh
	natter/ha	grain	grain	grain/yr	grain/yr	grain/yr	grain/yr
Field 1	7524	0.000114	$0.0129(0.0107)$ $\sim 0.0152)$	0.000342(9.614E-05) $\sim 0.0011)$	2.13E-05(1.28E-06) $\sim 3.20E-04)$	7.705E-05(1.60E-06 $\sim 7.30E-04)$	$0.000693 \\ (0.000156 \\ \sim 0.00337)$
Field 2	7353	0.000116	$0.0128(0.0107 \\ \sim 0.0151)$	$0.000382(0.000108$ $\sim 0.00121)$	2.54E-05(1.52E-06) $\sim 3.80E-04)$	8.60E - 05(1.80E - 06 $\sim 8.09E - 04)$	0.000775 0.000175 0.000175
Field 3	7524	0.000114	$0.0129(0.0107)$ ~ 0.0152	$0.000377(0.000106$ $\sim 0.00120)$	2.48E - 05(1.49E - 06 $\sim 3.71E - 04)$	8.48E-05(1.77E-06 $\sim 7.99E-04)$	0.000764 $(0.000172$ $\sim 0.00372)$
Field 4	7267.5	0.000118	$0.0129(0.0107)$ ~ 0.0152	0.000326(9.13E-05) $\sim 0.00105)$	1.97E - 05(1.18E - 06) $\sim 2.96E - 04)$	7.34E-05(1.52E-06) $\sim 6.98E-04)$	$0.000659 \\ (0.000148 \\ \sim 0.00321)$
Field 5	7096.5	0.00012	$0.0128(0.0106$ $\sim 0.0151)$	$0.000391(0.000111) \sim 0.00124)$	2.63E-05(1.58E-06 $\sim 3.94E-04)$	8.80E - 05(1.85E - 06) $\sim 8.27E - 04)$	$0.000794 \\ (0.000179 \\ \sim 0.000387)$
Field 6	7353	0.000116	$0.0128(0.0107)$ $\sim 0.0151)$	$0.000382(0.000108$ $\sim 0.00121)$	2.54E-05(1.52E-06) $\sim 3.81E-04)$	8.60E - 05(1.80E - 06) $\sim 8.10E - 04)$	$0.000776 (0.000175 \sim 0.00378)$
Average 7325	7325	0.000117	$0.0129(0.0107)$ $\sim 0.0152)$	0.000373(0.000105) $\sim 0.00118)$	2.43E-5(1.46E-6 $\sim 3.65E-04)$	8.38E-05(1.75E-06 ~ 7.90E-04)	0.000755 $(0.00017$ $\sim 0.00367)$

Notes Moisture content of grain = 14.5 % [16]

$$CO_2 - C = M_{Limestone} \times EF_{Limestone} + M_{Dolomite} \times EF_{Dolomite}$$
 (3.10)

where, CO₂-C is the annual CO₂ emission from lime application (kg C/kg grain); M is annual amount of limestone or dolomite applied (kg/kg grain); EF is emission factors (0.12 and 0.13 for limestone and dolomite). As no dolomite was applied, from Eq. 3.10, the total CO₂ emission from liming was estimated as 0.000505 kgCO₂/kg wheat grain, which bring much lower GWP impacts than N₂O field emissions [27]. Whether liming-induced CO₂ emission makes a negligible contribution to GWP profile of WBF products is tested later in sensitivity analysis.

3.3.4.8 PK Leaching and Run-Off

As N leaching was estimated using DNDC model (see Sect. 3.4), only P/K losses are discussed here. The P leaching loss was estimated based on previous research carried out on a range of UK soils by Fortune et al. [28] who reported annual cumulative total P loss in drainage waters from four sites ranged between 0.03 and 5 kg/ha. One of the sites they studied (13 % clay, 75 % sand, pH = 7.14) which is very similar to the soil texture in the current study, gave 0.24–0.73 kg P leaching/ ha. The potential P leaching loss in Swaffham farm was assumed to fall into this range, which is equivalent to 2.801E-05-8.521E-05 kg P/kg fresh wheat grain. The mean value was used in the LCA inventory (5.661E-05 kg P leaching per kg wheat grain) and the data range was applied in sensitivity analysis. Total P loss via either run-off or leaching was estimated as 1.5 kg P/ha in the UK wheat model by Williams et al. [66], which is much lower than the average annual P run-off estimated for tilled land in England and Wales (14.6 kg P/ha) [13]. However, 1.5 kg P/ha is preferred as it is more specified to winter wheat and gives similar estimation to the Eco-invent database; thus the P run-off loss in the 6 fields in this study was assumed as 1.185 E-04 kg P loss per kg fresh wheat grain. As for K loss, a leaching factor suggested in the UK wheat model 2 kg/ha [66] was applied in this study, which is equivalent to 2.334 E-04 kg K loss per kg wheat grain.

3.3.5 Inventory for Crop Rotation

The interaction between Soisson and previous/subsequent crops within the crop rotation was included in the system boundary. The inventories for crop rotation, fertilizer application rates and field operations on the six fields during the five-year period are given in Appendix B.

3.4 Agricultural Eco-System Modeling

This section presents inventory analysis of gases flux and leaching from the wheat agro-eco-system; results derived from this process-based modeling approach (DNDC) were incorporated into the LCA model.

3.4.1 DNDC-Simulated Results from 2003 to 2007

The average daily precipitation and air temperatures for 2003-2007 and the DNDC simulation results over the same period are given in Figs. 3.3, 3.4 and 3.5. Generally an increased trend in predicted CO_2 fluxes occurred over the period. This can be attributed to change in SOC storage and C transfer between the different SOC pools simulated.

A large amount of N was modelled to be lost as either NH_3 or NO_3^- leaching, which implied a low soil buffering effects. Specifically, buffering effects are referred to as the mechanisms by which NH_4^+ ions introduced into soil through fertilisation are fixed either via microbial assimilation or via absorption by soil absorbance such as clay minerals [46]. In the fields studied, sandy texture soils with low organic matter and low clay content dominate; this texture does not favour N fixation via absorption. Free NH_4^+ ions together with the released NH_4^+ during organic carbon decomposition or microbial death, are either transferred to NH_3 (existing in liquid or gas phase) or nitrified to NO_3^- which has no affinity for soil absorbance and easily moves to water leaching flow. As indicated in previous studies [42, 46] except for the soil buffering effect, the release of NH_3 gas or NO_3^- leaching are also influenced by factors such as climate and soil pH, clay content

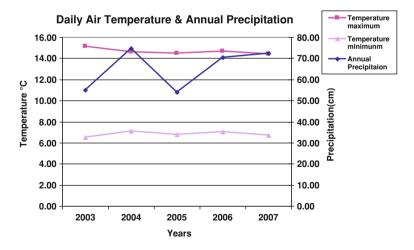


Fig. 3.3 Climatic conditions during 2003–2007

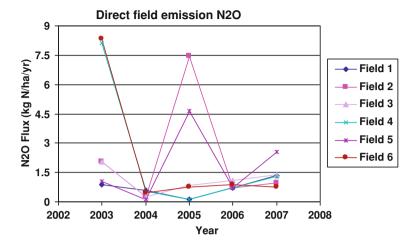


Fig. 3.4 N₂O emissions from six fields

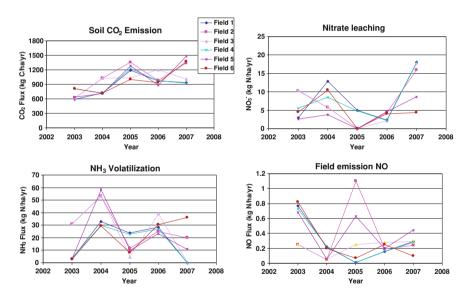


Fig. 3.5 NH₃/NO/CO₂ emissions and NO₃⁻ leaching from six fields

(pH and clay content regulate $\mathrm{NH_3/NH_4}^+$ equilibrium and gas diffusion, respectively). This confirmed the modelled results: as shown in Figs. 3.3 and 3.5, high leaching paralleled with high annual precipitation, whereas $\mathrm{NH_3}$ fluxes estimated roughly matched average maximum air temperature curves and high $\mathrm{NH_3}$ flux could be partly explained by the low soil clay content (9.33 %) and high soil pH (7.56), which favoured $\mathrm{NH_3}$ release and $\mathrm{NH_3}$ diffusion, respectively.

Strong NH₃ volatilization and NO₃⁻ leaching effects, as well as demands of plants limited the inorganic N availability which could be further converted to N₂O/NO via nitrification/denitrification. Thus, in contrast to NH₃ and NO₃⁻, small amounts of N were estimated to be lost as N₂O/NO and their patterns are the inverse of the NH₃ and NO₃⁻ losses. Comparing different fields, various flux curves were found due to different farm management. As shown in Fig. 3.4, N₂O emissions for Field 1 and 3 were quite constant over the whole crop rotation, only showing slightly higher emissions in 2007, which was partly due to a high N-input for oilseed rape. Fields 2 and 5 showed similar trends in N₂O flux: emissions kept relatively stable from 2003 to 2004, increased sharply in 2005 and declined in 2006 followed by a slightly increase in 2007, which reflected the sharp increase in synthetic N fertilizer used for potatoes grown on both fields in 2005 and on Field 5 in 2007. While for Field 4 and 6 a high N₂O flux was found in 2003, N₂O emissions decreased in 2004 and remained low from 2005 to 2007, which could be attributable to high N input for the potato crop on both fields in 2003. Compared with N₂O, only small amounts of NO emission were estimated; NO flux curves gave similar trends to N₂O except for Field 1 and 5 where a sharp decline was found from 2003 to 2004.

A high variation in gas flux/leaching from six fields were found in the DNDC results. Comparing with other years simulated, the 6 fields of wheat showed relatively small variability in 2006 when the same crop was grown on all fields, but still gave a range: NO_3^- leaching varied between 2.2 and 4.6 kg N/ha/yr; NH₃, N₂O, and NO fluxes fell in the range of 23.1–39.2, 0.71–1.08 and 0.16–0.28 kg N/ha/yr respectively. Thus to represent the overall wheat management at the Swaffham farm, average values were used for the LCA inventory. However, the levels of variation observed in the emissions and leaching from the six fields were explored further in sensitivity analysis.

3.4.2 Gas Emissions/Leaching Inventory for Soisson

The gas emissions and leaching from the six fields during the period between Soisson-cultivation and the following crop are presented in Table 3.17. Various interactions occurred between successive crops in the rotation and the change in soil quality was included in the system boundary by accounting for their effects on N and C losses. Only a proportion of the residual nutrients carried over from previous crop benefited the Soisson crop, thus only associated soil fertility changes and gas emissions and leaching over the Soisson crop cycle (from Soisson cultivation to the subsequent crop cultivation) were allocated to Soisson. As for surplus nutrients from the Soisson wheat crop that were left on the land, the induced emissions and leaching was allocated between Soisson and the subsequent crops according to time boundary (Soisson were only responsible for those occurring before the beginning of the subsequent crop-cultivation).

Unit:kg emissions	Field 1	Field 2	Field 3	Field 4	Field 5	Field 6
per kg grain						
Total N ₂ O flux	1.056E-04	1.557E-04	1.628E-04	1.075E-04	1.571E-04	1.697E-04
Total NO flux	3.629E-05	5.750E-05	6.253E-05	3.525E-05	5.911E-05	6.438E - 05
Total NH ₃ flux	6.047E - 03	4.366E-03	4.369E-03	5.974E-03	4.213E-03	4.329E-03
Total CO ₂ flux	3.190E-01	6.933E-01	2.365E-01	3.342E-01	6.456E - 01	4.867E - 01
Total NO ₃ ⁻ leaching	1.912E-04	2.559E-03	1.862E-04	2.032E-04	2.812E-03	2.065E-03

Table 3.17 DNDC-simulated emissions/leaching over the Soisson wheat crop cycle

As seen in Table 3.17, relatively higher CO₂ emissions/N leaching were found in Field 2, 5, 6, where a longer crop cycle for Soisson was considered (the following crops in these three fields were cultivated at the beginning of 2007, whereas the following crop in Field 1, 3, 4 was oilseed rape which was cultivated in August 2006). 90–95 % of N leaching and over 50 % of CO₂ flux was estimated to occur after Aug 2006 in field 2, 5 and 6. Differences in NH₃/NO/N₂O fluxes between fields were not primarily attributable to different crop cycle, but to the previous crops. In Fields 1 and 4, no previous crop was grown (no fresh residue added) so organic matter in the plant residue SOC pool dropped significantly, a lower decomposition rate and soluble carbon concentration was estimated in 2005; as a consequence, microbial biomass depleted and, a decline was estimated in humans SOC for Field 1 and 4 in 2006. In other words, in both fields, the rate of microbial biomass decomposition and humans decomposition increased in 2006, which was also indicated by the soluble C pool indicator (higher dissolved SOC was estimated in both fields). In the DNDC model, decomposed C was simulated to partially convert to soluble C and partially to CO₂, which could explain the CO₂ emission difference between Fields 1 and 4 and Field 3. During C decomposition, fixed N was transformed to NH₄⁺, which could be either lost via volatilisation or nitrified to NO₃⁻. Due to low concentrations of C and N substrates (low soluble C and no N fertilizer input in 2005), low denitrifiers/nitrifiers growth rate than in the other fields were estimated in Fields 1 and 4. Consequently the N₂O/NO fluxes during the Soisson crop cycle estimated in Fields 1 and 4 were lower than the other fields. On the contrary enhanced NH₃ flux from Fields 1 and 4 was estimated as DNDC output, due to low nitrification/denitirfication rates in these two fields.

By analysing daily gas/leaching trends in different fields over the Soisson crop cycle (see Figs. 3.6 and 3.7), it was found that: trends of emissions/leaching did not differ significantly in the six fields across the crop cycle, i.e. high peaks in different fields occurred within the same period; the peaks in N_2O and N leaching were highly related to the N fertilizer inputs and were also influenced by rainfall events; the timing of NH_3 emissions peaks roughly matched the trends of daily maximum temperature.

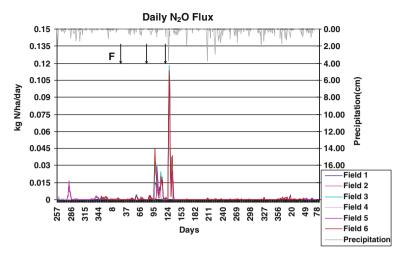


Fig. 3.6 N₂O flux over Soisson crop cycle

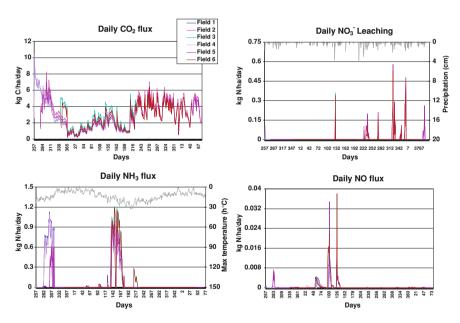


Fig. 3.7 Daily NO/NH₃/CO₂ flux and N leaching over Soisson crop cycle *Notes Grey curve* indicate daily precipitation (cm) or daily max temperature (°C)

3.4.3 Comparison of DNDC and IPCC Model Outputs

The comparison between two approaches for N_2O emission simulation is summarized in Table 3.18.

The IPCC Tier 1 approach does not directly account for interaction between various components of the N cycle, nor are the potential impacts of agricultural management other than N addition assessed although it can be argued that it to an extent reflects climatic/soil conditions via crop production [35], and farm management could be indicated through N fertilization. As an alternative, DNDC directly accounts for regional agro-eco-system difference and site-specific agriculture management.

IPCC gave a much higher estimation of direct N_2O emissions than DNDC. This finding is confirmed by a study conducted by Brown et al. [6]: N_2O emission from UK agricultural system estimated by the DNDC approach was lower than obtained by IPCC method. According to the UK N_2O emissions map developed by Brown et al. [6], the farm under analysis in the present study is within a relatively low N_2O emission region.

In order to identify the main contributor of N sources to N_2O emissions, different scenarios were run with DNDC. Specifically, fertiliser-induced N_2O emission was estimated by the difference in fluxes between a zero-fertiliser run and the 'baseline' scenario run in the DNDC simulation. As shown in Table 3.19, DNDC estimated that fertilizer-induced N_2O accounts for 75–95 % of the direct N_2O fluxes with between 0.28 and 0.39 % of N fertilizer applied released as N_2O . This finding is consistent with the IPCC approach: the EFs obtained here via DNDC are within the IPCC uncertainty range of EF of 0.3–3 %. The IPCC approach also estimated that most of direct N_2O emissions were caused by fertilizer (approx 65 %).

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Table 3	ıx	$N_{\alpha}()$	tield	emissions	simulation

	IPCC Tier 1	DNDC
Approach classification	Empirical model	Process-based model
Application	National GHGs inventory	Site specific and national GHGs inventory
N ₂ O emission pathway	Direct emissions Indirect emissions(air decomposition and leaching)	Direct field emissions
Factors considered	(1) Fertilizer input. (2) Crop residue	(1) Fertilizer type/input. (2) Crop rotation.3) Daily climate. (4) Soil property/texture.5) Farm management
Uncertainty	Large degree of uncertainty	Uncertainties caused by variability of input data
Simulated results (average of 6 fields) kg N ₂ O/kg wet grain	Direct N ₂ O 5.86 E-04.Total emissions 7.55 E-04	Direct N ₂ O 1.430E-04

Table 3.19 Fertilizer-induced N₂O emissions

	Field 1	Field 2	Field 3	Field 4	Field 5	Field 6
N ₂ O-baseline (kg N/ha)	0.591	0.852	0.911	0.581	0.830	0.929
N ₂ O Zero-fertilizer (kg N/ha)	0.065	0.198	0.057	0.065	0.187	0.108
Fertilizer-induced N ₂ O (kg N/ha)	0.526	0.654	0.855	0.517	0.642	0.820
Fertilizer input (kg N/ha)	187.665	218.150	217.880	167.620	218.150	218.215
Emission factor (kg N ₂ O-N/kg N input)	2.802E-03	2.997E-03	3.922E-03	3.083E-03	2.945E - 03	3.758E-03

However, both approaches have limitations. A degree of uncertainty is introduced in the IPCC Tier 1 approach due to the uncertainties in EFs and indirect N_2O emission estimations [37, 35]; furthermore, IPCC was developed for national GHGs inventory reporting, not taking into account regional differences in agroecosystem characteristics. On the contrary, DNDC modelling approach is more site-specific, simulating N_2O under the expanded LCA system boundary; although uncertainties are also introduced into DNDC results due to the variability of input parameters, the derived N_2O fluxes from DNDC have been well validated in previous studies and verified to match with field-measured results [58, 50].

DNDC was preferred and applied in the LCA model as the 'default' modelling method. But the sensitivity of the LCIA results to different modelling approach and to uncertainties in both the IPCC and DNDC approaches were analysed.

3.5 LCIA Results for Wheat Farming System

The results for the LCIA of the Soisson wheat grain production process are presented below. Contribution analyses of cradle-to-farm gate LCIA for Soisson grain with average agricultural practice scenario are presented first then the LCIA comparisons of wheat grains produced in six fields are given.

3.5.1 Contribution Analysis for Soisson Grain

The characterised LCIA profiles for wheat grain agricultural system are given in Table 3.20 and Fig. 3.8. The N fertilizer production and field emissions were found to be the main cause of impacts in most of the impact categories except ODP.

Straight N fertilizers including Axan and Extran are the main contributors to abiotic depletion, accounting for nearly 50 % of impacts, as $\mathrm{NH_4NO_3}$ production is a fuel-demanding process, especially natural gas and heavy fuel oil used as feedstock. Additionally, 41.3 % of impacts on abiotic depletion were attributable to the field operations due to the diesel fuel consumed, especially the chemical application which caused 15 % of impacts.

On GWP100, the effect of CO₂ component sequestered in wheat grain was indicated by the 'below-the-line' scores, which balanced the burdens caused by other processes thus giving wheat grain with a net negative GWP score. Analysing only the GWP100 burdens (i.e. positive emissions causing GWP), GHG fluxes from soil were the main contributor (68.4 % of the GWP100 positive value), not due to direct N₂O field emission, which only accounted for 4.8 % of GWP100 burdens but mainly caused by CO₂ emitted from soil. CO₂ dominated the GWP100 burdens (62.6 %) and CO₂ emission profile over the whole wheat grain product system (99.5 %) mainly resulting from the decomposition of crop residues and SOM and partly induced by liming (see Appendix F). 76 % of N₂O profiles

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Impact category	Abiotic depletion	Acidification	Acidification Eutrophication	GWP100	ODP	Human toxicity	Fresh water Eco-tox	Marine Eco-tox	Terrestrial Eco-tox	POCP
Unit	kg Sb eq	kg SO2 eq	kg PO4— eq	kg CO2 eq	kg CFC-11 eq		kg 1,4-DB eq			kg C2H4
Total	1.40E - 03	9.295E-03	2.727E-03		2.57E-08	8.46-02	1.13E-02			1.53-05
C02	0.00E + 00	7.85E-03	2.39E-03	-9.75E-01	0.00E + 00	4.88E-04	0.00E + 00	0.00E + 00	0.00E + 00	-2.24E-05
absorb + Field										
emission										
Wheat seed	3.89E - 05	9.45E - 05	7.82E-05	1.19E - 02	7.25E-10	1.22E-02	1.29-03	9.24E - 01	4.13-05	1.24-06
0:11:20(N:P:K)	6.86E - 06	1.04E - 05	1.03E-05	9.27E - 04	8.48E-11	6.23-04	1.31E - 04	2.57-01	6.25-06	4.46-07
5:11:20 (N:P:K)	8.82E - 06	3.98E - 06	5.36E - 07	1.05E-03	1.18E - 10	7.27-04	1.21E - 04	2.26E - 01	7.11–06	1.90E - 07
Axan	2.23E - 04	1.95E - 04	3.84E - 05	3.36E - 02	3.27E-09	1.94-02	2.72E-03	7.208E + 00	2.63E - 04	4.43E - 06
Extran	4.58E - 04	3.99E - 04	7.88E-05	6.91E - 02	6.71E-09	3.98-02	5.59E-03	1.48E + 01	5.40E-04	9.11E-06
Pesticide	3.36E - 05	1.74E - 05	1.09E - 06	2.78E - 03	4.72E-10	1.43-03	2.41E-04	9.63E - 01	4.71E-05	7.85E - 07
Plough	8.90E - 05	9.96E - 05	1.87E - 05	1.54E - 02	2.10E - 09	1.29E-03	1.37E - 04	7.25E-01	8.38E-06	2.91-06
Drill	8.80E - 05	1.04E - 04	1.89E - 05	1.51E - 02	1.70E - 09	1.5003	1.41E - 04	9.952E - 01	8.38E-06	3.08-06
Pesticide spraying	2.10E - 04	2.36E - 04	4.45E - 05	3.66E - 02	4.97E - 09	2.93E - 03	3.06E - 04	1.70E + 00	1.93E - 05	6.87E - 06
Fertilizer spreading	9.25E - 05	1.04E - 04	1.95E - 05	1.61E - 02	2.19-09	1.29E-03	1.35E - 04	7.47E - 01	8.51E-06	3.02E - 06
Harvesting	9.58E - 05	1.08E - 04	2.02E - 05	1.66E - 02	2.27-09	1.34E - 03	1.40E - 04	7.73E-01	8.82E-06	3.13-06
Transport, road	4.58E - 05	3.54E - 05	7.66E-06	6.55E - 03	1.02E - 09	1.12-03	2.25E-04	4.89E - 01	1.27E-05	1.18E - 06
Transport,	2.01E - 06	6.63E - 06	5.62E-07	3.02E - 04	3.4011	1.91E - 04	8.63E - 06	3.50E - 02	7.46E-07	2.11-07
transoceanic										
Growth regulator	4.89E - 06	2.78E - 05	7.64E-07	2.28E-03 1.88-11	1.88-11	3.37-04	7.04E-05	5.93E - 01	2.76E-05	1.06E - 06
Adinyant	5.51E-08	9.11E-08	6.90E-08	-2.73E-07	8.65-13	6.82E-06	4.96E-05	1.38E - 03	2.19E-05	9.07E-09

Notes Main contributors in each impact categories

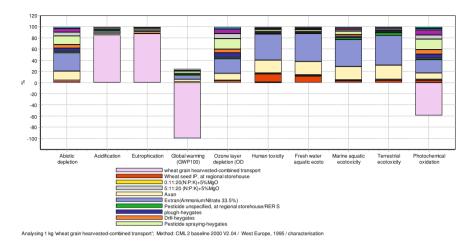


Fig. 3.8 Characterised LCIA profiles of harvested wheat grain (unit: per kg harvested grain)

occurring from cradle to farm gate came from direct N_2O field emission or N_2O emitted from nitric acid production process (48.5 and 33.4 % respectively). Field operation only shared a small proportion of burdens in GWP100, approximately 13.8 %, caused by the GHGs emissions from diesel combustion.

Another impact category with negative environmental scores was POCP where NO field emissions contributed to negative values. In fact, NO can react with ozone (O_3) to form NO_2 and O_2 under certain conditions [43, 42], which is beneficial for destroying O_3 formed and further reducing impacts in POCP. However, the beneficial NO effect was overridden by the burdens induced by field operations and N fertilizers production. Due to SO_2 and CO emissions from NH_3 production process together with other emissions, N fertilizer making occupied 36 % of the positive scores on POCP; in addition, 50 % of positive score were attributable to diesel consumed in field operations or transportation due to SO_2 emitted from the diesel refining and SO_2 and CO released from diesel combustion.

As shown in Fig. 3.8, both acidification and eutrophication profiles were dominated by gas flux/leaching from soil, especially NH₃. 96 % of total NH₃ emission for wheat grain system came from NH₃ soil emission, which accounted for 84 and 63 % of acidification and eutrophication burdens respectively. Thus, in total the field emission of NH₃ and NO accounted for 84.5 % of acidification burden; NH₃ and NO together with NO₃ $^-$ and P leaching from field contributed to 87.6 % of the impact on eutrophication. Only 6.5 % of the acidification burden and 4.3 % of the eutrophication scores were caused by fertilizer manufacturing (NPK together with straight N fertilizers); whereas field operation only occupied 7.4 and 4.5 % of the acidification and eutrophication profiles, respectively.

On toxicity impact categories, NH_4NO_3 based straight N fertilizers were the main contributors, causing over 70 % of the impact, where the NH_3 production process and the infrastructure (chemical plant/machinery) were the main causes. Nearly 60 % of impacts on human toxicity were attributable to atmospheric

chromium, nickel, and arsenic and PAH emissions, 80 % of which were related to straight N fertilizer production process (NH₃ production, and manufacturing ferrochromium/copper components of chemical plants). As for fresh water eco-toxicity, it was dominated by nickel vanadium and cobalt emissions (nearly 80 % of the impacts). Over 80 % of these were either for NH3 making or facility constructions, such as nickel ion released from the disposal of residues during ferronickel manufacture and Ni catalyst production (Ni catalyst is used in NH₃ steam reforming), vanadium and nickel released to water during the production of steel material used for facility construction (reinforcing steel and chromium steel), and atmospheric vanadium emission from NH3 steam reforming. These substances together with barium and barite were also responsible for over 90 % of the burdens in marine eco-toxicity. Both barium and barite are mainly released from the production chain of diesel (either diesel refinery or crude oil production), 72 % and 16 % of the burdens on marine eco-toxicity were therefore shared by N fertilizer and field operation. Terrestrial eco-toxic impacts were mainly caused by vanadium mercury arsenic air emissions and chromium released to soil from steel production or NH₃ manufacturing.

As for the ODP impact category, almost 90 % of the impacts were related to either field operations or N fertilizer production (about 50 % and 40 % respectively) due to the production of diesel needed for field work and feedstock (natural gas and heavy fuel oil) required for making NH₃. Specifically, CBrF₃ released from crude oil production (raw material either for diesel or heavy fuel oil) and CBrClF₂ released from transport of natural gas were the main contributors.

3.5.2 LCIA Comparison of the Six Fields

The wheat grains harvested from the 6 fields along with average Soisson grain production are compared in Fig. 3.9 and Table 3.21. The characterized scores showed little difference from each other on most impact categories, except for GWP100, POCP, where there were differences between individual fields.

Generally, Fields 2 3 5 and 6 showed very close environmental profiles to average Soisson grain, in most impact categories except GWP100 where average grains gave better scores than Field 2 and 5. Fields 1 and 4 brought higher burdens than average Soisson in acidification, eutrophication, POCP; but in other impact categories, they represented better or similar profiles in comparison with average.

On abiotic depletion, diesel and natural gas consumed (for field operation and N fertilizer making process respectively) are the main contributors in all fields. But Field 5 presented slightly higher resource depletion compared with the other fields mainly due to the low wheat grain yield. In both Fields 1 and 4 lower levels of straight N nutrients were applied than other four fields instead extra NPK fertilizers were introduced, and therefore, less natural gas resource was consumed. Extra diesel energy input for NPK fertilizer application partly overrode the beneficial effects of low N input; whereas the small difference between Field 1 and 4

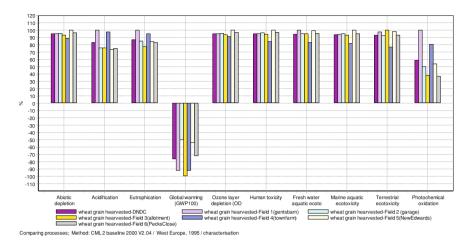


Fig. 3.9 Comparison of characterisation results for 6 fields (unit: per kg harvested grain)

on abiotic depletion was resulted from different N application rates (167 and 187 kgN/ha, respectively).

Analyzing ODP and toxicity impact categories, similar profiles to the average Soisson grain were found in each individual field, ODP scores were highly related to field operation and N fertilizers; scores on human toxicity and eco-toxicity were dominated by production of NH₃ and chemical plant components required for fertilizer manufacture; whereas, the main driver for the difference in environmental scores between six fields were the differing application rates for N fertilizer and P, K nutrients and other crop protection products, as well as different wheat grain yield. Comparing six fields, relatively low efficiency of energy/fertilizer usage (low grain yields) in Field 5 resulted in its slightly higher environmental scores than the other fields on ODP, human toxicity and eco-toxicity; Field 4 benefited from the low N fertilizer application rate, presenting the best profiles on all these five impact categories. Although N fertilizer input was also relatively low in Field 1, other wheat protection products and nutrients increased its environmental burdens: P and K fertilizer as well as limestone input to Field 1 caused 3-13.5 % of environmental burdens on these 5 impact categories; the adjuvant (Methylated Rapeseed Oil active substances) which was only applied in Fields 1 and 3 also contributed nearly 10 % of impacts for both fields in the terrestrial ecotoxicity impact category.

In the case of GWP100, acidification, eutrophication and POCP impact categories, different environmental profiles of six fields were mainly driven by the difference in their gas fluxes and leaching. The same amount of C was sequestered per unit of wheat grain produced in each field, but the varying burdens caused by $\rm CO_2$ emission from soil drove the different GWP100 scores: $\rm CO_2$ emission accounted for approx 55–72 % of GWP positive burdens in the 6 fields (see Appendix F); whereas, another important field emission $\rm N_2O$ (direct) only contributed to 5–9.5 % of GWP positive scores. As indicated in Table 3.17, ranking

Table 3.21 Characterised LCIA profiles for 6 fields (Unit: per kg wheat grain harvested)

*			,				
Impact category	Average	Field 1	Field 2	Field 3	Field 4	Field 5	Field 6
Abiotic depletion (kg Sb eq)	1.40E - 03	1.40E - 03	1.41E - 03	1.38E - 03	1.31E - 03	1.47E - 03	1.42E-03
Acidification (kg SO ₂ eq)	9.30E - 03	1.12E - 02	8.48E - 03	8.46E - 03	1.09E - 02	8.30E - 03	8.41E - 03
Eutrophi-cation (kg PO_4^{3-} eq)	2.73E - 03	3.13E - 03	2.66E - 03	2.42E - 03	2.96E - 03	2.65E - 03	2.60E - 03
GWP100 (kg CO ₂ eq)	-0.75	-0.89	-0.50	-0.96	-0.89	-0.54	-0.70
ODP	2.57E - 08	2.56E - 08	2.58E - 08	2.53E - 08	2.46E - 08	2.70E - 08	2.61E - 08
(kg CFC-11 eq)							
Human toxicity (kg 1,4-DB eq)	8.46E - 02	8.44E - 02	8.58E - 02	8.41E - 02	7.50E - 02	8.91E - 02	8.63E - 02
Fresh water ecotoxicity (kg 1,4-DB eq)	1.13E - 02	1.19E - 02	1.14E - 02	1.14E - 02	9.92E - 03	1.19E - 02	1.14E - 02
Marine Ecotoxicity (kg 1,4-DB eq)	3.05E + 01	3.07E + 01	3.09E + 01	3.02E + 01	2.66E + 01	3.24E + 01	3.00E + 01
Terrestrial ecotoxicity (kg 1,4-DB eq)	1.02E - 03	1.07E - 03	1.02E - 03	1.10E - 03	8.46E - 04	1.08E - 03	1.02E - 03
POCP (kg C_2H_4 eq)	1.53E - 05	2.60E - 05	1.29E - 05	9.97E - 06	2.09E - 05	1.39E - 05	9.57E - 06

for C loss via field emissions was Field 3 < Field 1 < Field 4 < Field 6 < Field 5 < Field 2 and this matched well with the ranks of characterised total GWP of 6 fields. Both acidification and eutrophication profiles were dominated by the NH₃ flux from soil, which contributed to 81-88 % of acidification burdens and 56-70 % of eutrohpication scores. Both Fields 1 and 4, where the highest DNDCsimulated NH₃ flux occurred, showed above-average characterised score on both impact categories. Another N loss route via leaching also caused between 2.1 and 12.4 % of eutrophication burdens, in the six fields; therefore, Fields 2 and 5 with higher N leaching had higher eutrophication burdens than Field 3. Another factor—difference in PK nutrient inputs between six fields (only applied in Fields 1 and 4) also played a minor part in the eutrophication profile, accounting for 0.06-4.2 % of eutrophication score. Another field emission-driven impact category is POCP. As indicated in Table 3.17, the highest NO flux was estimated in Fields 3 and 6, therefore, the beneficial effect of NO was reflected via the POCP scores, where Fields 3 and 6 presented the best environmental performance. The lowest NO flux was simulated in Fields 1, and 4; this along with the diesel consumed for extra fertilization (NPK) in Fields 1 and 4 resulted in their higher POCP scores compared with other fields.

3.5.3 Normalized LCIA Profiles for Wheat Grain

The normalized indicator results for average Soisson grain and comparison of six fields are given in Figs. 3.10, 3.11 and Table 3.22, where the reference system West Europe 95 was applied.

As indicated in Figs. 3.10 and 3.11, normalization causes a shift in significance of the impact category results. For all the wheat grain product system studied,

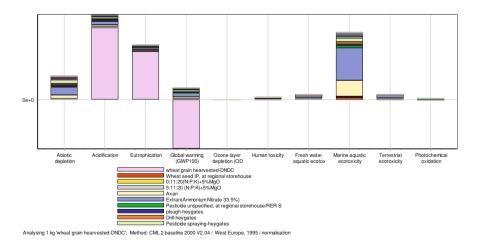


Fig. 3.10 Normalized LCIA profile of average wheat grain (unit: per kg harvested grain)

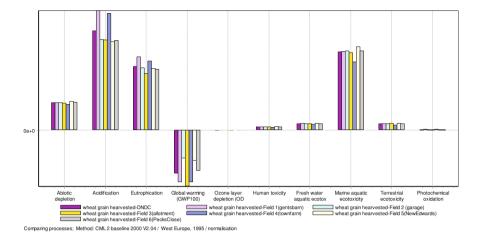


Fig. 3.11 Normalized LCIA comparisons of 6 fields (unit: per kg harvested grain)

acidification impacts is shifted to first place, appearing as the most significant. Indicator results for four other impact categories are also of relative significance (from high to low significance), i.e. marine eco-toxicity, eutrophication, abiotic depletion. Other toxic impacts and ODP impacts are of relatively low significance; whereas GWP100 shows significant negative beneficial impacts.

Amongst all the components over life cycle of Soisson grain, field emissions/ leaching appear as relatively significant sources of acidification and eutrophication burdens; N fertilizers are shown as important sources of both marine eco-toxic impacts and abiotic resources depletion. These represent the major option for improvement of agricultural management.

These normalized LCIA profiles offered a good insight in the relative contribution of wheat grain product to environmental problems in relation to the reference region (West Europe). However, the normalized indicator results only provided reference information to specific time and spatial scales; different reference systems could change the outcomes.

3.6 Sensitivity Analysis

3.6.1 Sensitivity Analysis on N₂O Modelling Approach

Sensitivity analysis was conducted to test the influence of different crop modelling approaches to GWP100 profiles. The results are presented in Fig. 3.12.

As indicated in Sects. 3.4.3 and 3.3.4.7, the IPCC Tier 1 approach gave higher estimations of N_2O field emission than the DNDC modelling approach; by using the IPCC approach, approximately 77 % of total N_2O flux was estimated as direct

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Impact category	Abiotic	Acidification	Acidification Eutrophication GWP100		ODP	Human	Fresh water	Marine Eco- Terrestrial	Terrestrial	POCP
	depletion					toxicity	Eco-tox	tox	Eco-tox	
Total	9.41E-14	3.40E-13	2.19E-13	-1.55E-13	3.08E-16 1.12E-14	1.12E-14	2.24E-14	2.68E-13	2.16E - 14	1.85E-15
CO ₂	0.00E + 00	2.87E - 13	1.92E-13	-2.03E-13 0.00E + 00 6.45E-17	0.00E + 00	6.45E-17	0.00E + 00	0.00E + 00	0.00E + 00 0.00E + 00	-2.71E-15
absorb + Field										
emission										
Wheat seed	2.62E - 15	3.46E - 15	6.27E-15	2.48E-15	8.70E - 18	1.61E-15	2.55E-15	8.14E - 15	8.75E - 16	1.50E - 16
0:11:20 (N:P:K)	4.62E - 16	3.79E - 16	8.22E-16	1.93E-16 1.02E-18	1.02E-18	8.22E-17	2.60E - 16	2.26E-15	1.32E-16	5.40E - 17
5:11:20 (N:P:K)	5.95E - 16	1.46E - 16	4.30E-17	2.19E-16 1.42E-18	1.42E-18	9.59E-17	2.39E-16	1.99E-15	1.51E - 16	2.30E - 17
Axan	1.50E - 14	7.12E-15	3.08E-15	7.00E-15	3.92E-17	2.55E-15	5.38E-15	6.35E - 14	5.57E-15	5.37E - 16
Extran	3.08E - 14	1.46E - 14	6.32E-15	1.44E-14 8	8.06E-17	5.25E-15	1.11E-14	1.31E-13	1.15E - 14	1.10E - 15
Pesticide	2.26E - 15	6.38E - 16	8.76E-17	5.79E-16 ±	5.67E-18	1.89E - 16	4.77E-16	8.48E - 15	9.98E - 16	9.50E - 17
Plough	5.99E - 15	3.65E-15	1.50E - 15	3.21E-15	2.52E-17	1.71E-16	2.72E-16	6.38E - 15	1.78E - 16	3.52E - 16
Drill	5.93E - 15	3.82E-15	1.52E-15	3.14E-15	2.04E-17	1.97E - 16	2.79E-16	8.77E-15	1.78E - 16	3.72E - 16
Pesticide spraying	1.42E-14	8.65E - 15	3.57E-15	7.61E-15	5.97E-17	3.87E-16	6.06E - 16	1.49E - 14	4.10E - 16	8.32E - 16
Fertilizer spreading	6.24E - 15	3.80E - 15	1.57E-15	3.35E-15	2.63E-17	1.71E-16	2.67E - 16	6.58E - 15	1.80E - 16	3.66E - 16
Harvesting	6.46E - 15	3.94E - 15	1.62E-15	3.46E-15	2.72E-17	1.77E-16	2.78E-16	6.81E - 15	1.87E - 16	3.78E - 16
Transport, road	3.09E - 15	1.30E - 15	6.14E - 16	1.36E-15	1.23E-17	1.47E - 16	4.46E - 16	4.31E-15	2.70E - 16	1.43E - 16
Transport,	1.35E-16	2.43E-16	4.51E-17	6.28E-17	4.08E-19	2.52E-17	1.71E-17	3.09E - 16	1.58E - 17	2.55E-17
transoceanic										
Growth regulator	3.29E - 16	1.02E - 15	6.13E - 17	4.73E-16 2.25E-19	2.25E-19	4.44E-17	1.39E-16	5.23E-15	5.85E-16	1.28E - 16
Adjuvant	3.71E-18	3.33E-18	5.53E-18	-5.67E-20	1.04E-20	9.00E - 19	9.83E-17	1.22E-17	4.65E-16	1.10E - 18

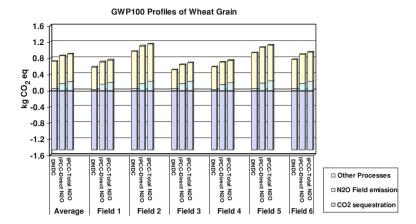


Fig. 3.12 Comparison of DNDC and IPCC (unit: kg wheat grain harvested)

emission. GWP100 profiles of wheat grain varied significantly with the different models. Compared with DNDC results, IPCC-estimated N_2O (including both direct and indirect) showed increases in GWP100 burdens for wheat grain (approx 18.4–36.7 % varying between fields). For the average Soisson grain studied, GWP100 dropped down from -0.746 to -0.565 kg $\rm CO_2$ eq/kg grain harvested when the IPCC Tier 1 approach was applied.

Disregarding the negative beneficial GWP100 scores and analyzing only the GWP100 positive burdens caused by the wheat grain, in six fields, DNDC-simulated $\rm N_2O$ only contributed to 4.8–9.5 % of the GWP100 positive scores; whereas, 20–33 % of GWP100 positive burdens was attributable to IPCC-simulated total $\rm N_2O$ emission. In the case of average wheat grain, DNDC-derived $\rm N_2O$ only caused 5.9 % of GWP positive scores, but IPCC-derived direct and total $\rm N_2O$ were responsible for 20.3 and 24.7 % of GWP positive burdens respectively.

Although the GWP100 profile for wheat grain is very sensitive to the modelling approaches adopted, the ranking of GWP100 profiles for the 6 fields remained relatively stable—only ranking of Fields 1 and 4 reversed when IPCC approach was adopted. The sensitivity of GWP100 scores for WBF products as well as their comparison with petrochemical polymers to different modelling approaches were further examined and are presented in following chapters.

3.6.2 Liming-Induced CO₂ and P Loss

To test the sensitivity of LCIA results to liming induced CO_2 and P loss, different scenarios were run against base-line: in scenario 1 it was assumed that no liming-induced CO_2 was emitted; min value in P leaching (2.801E-05 kg P/kg fresh wheat grain) was assumed as scenario 2. Scenario 3 assumed that all P nutrient

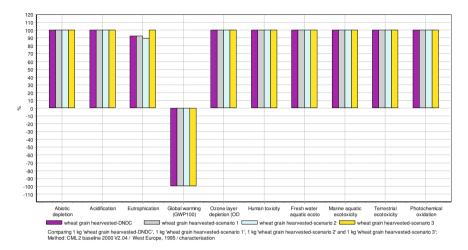


Fig. 3.13 Sensitivity analysis for liming-induced CO_2 and P loss (unit: kg wheat grain harvested)

applied to Soisson was released either via leaching or run-off. Their comparison results are shown in Fig. 3.13.

Characterised GWP100 scores show a negligible change (0.001 kg CO_2 eq/kg fresh grain) due to liming-induced CO_2 emissions. In the case of P loss, reduction in P leaching only decreased the eutrophication score by 3.2 %; although scenario 3 brought approximately 10 % increase in eutrophication impact compared with the baseline scenario, the P-loss assumption was extreme. Therefore, according to the threshold (10 %) defined in Sect. 2.3.1.2, liming-induced CO_2 was concluded to be a negligible parameter, however, the LCIA profiles of wheat grain were sensitive to P loss assumptions.

3.7 Discussion

In summary, an expanded system boundary was included in this LCA study through DNDC modelling, incorporating climate, soil, and crop rotation. The timeframe was defined as wheat crop cycle. The climatic factors including daily temperature and precipitation as well as atmospheric C/N deposition, soil texture and soil quality change over time boundary were taken into account and their effects were directly reflected via effects on the modelled field emissions and leaching. Interactions between successive crops in rotation were included in the LCA by assessing the effects of field management on soil quality and the influences of residual nutrients left on lands by previous crop on the subsequent crop cycle.

3.7 Discussion 147

Climatic conditions, soil and agricultural managements are ecological drivers that can have substantial effects on field emissions/leaching. However, the empirical model approach and EFs adopted in most LCA studies do not adequately reflect regional agro-ecosystem characteristics and thereby introduce a large degree of uncertainty or accuracy into LCI. In the present LCA study, LCIA results showed, for this site-specific winter wheat (from cradle to farm gate) that the C/N loss via either leaching or gaseous emissions were one of the main contributors to environmental impacts on GWP100, POCP, acidification and eutrophication impact categories. In comparison with DNDC-derived N_2O emission, IPCC gave much higher estimation of N_2O field emission, which led to a higher GWP100 positive score for the wheat grain system.

Other major contributors to environmental burdens include N fertilizer manufacture and field operation, especially on the ODP, abiotic depletion, eco-toxicity and human toxicity impact categories. CO₂ sequestered from atmosphere during wheat growth led to a beneficial negative GWP100 score for wheat grain. Normalized LCIA profiles indicated that impacts on acidification, eutrophication, and marine eco-toxicity and GWP100 appear as relatively significant.

The LCIA results for wheat grain produced in different fields varied, depending on farm practices. Generally, in the six fields, N fertilizer inputs as well as diesel consumed in the field operations produced higher influences on ODP, abiotic depletion, and human/eco-toxicity impact categories; K/P fertilizer as well as crop protection products only shared a small proportion of the toxic impacts and ODP burdens; while the remaining impact categories were more affected by field emissions/leaching. For this site-specific wheat grain analysis, shorter crop cycle and less N input brought better GWP100 profiles; whereas, crop rotation appeared to influence impacts on acidification and eutrophication: set-aside before wheat crop cycle (no previous crop) induced higher NH₃ flux further brought higher burdens on both impact categories.

As shown in Sect. 3.6, liming-induced CO_2 is not a sensitive parameter, but the characterised eutrophication profile was sensitive to assumed P losses. In future research, process-oriented models could be explored to give more site-specific estimation of P runoff/leaching. However, it was beyond the scope of this study to explore further.

Sensitivity analysis was carried out on N_2O estimation, to test the effects of different modelling approach on GWP100 scores and also to examine the sensitivity of GWP100 profiles to the different system boundary definition. Although IPCC Tier 1 could reflect climate/soil conditions via crop production, it does not directly consider these inputs in N cycle nor are the impacts caused by farm management assessed. In other words, LCA study using IPCC-estimated N_2O emissions does not include the climate/soil/crop rotation into the system boundary. Through the sensitivity analysis, it was concluded that GWP100 scores of wheat grain were very sensitive to different modelling approaches as well as the system boundary definition.

Both the IPCC and DNDC approaches have limitations, as both approaches introduce uncertainties to the LCIA results. As discussed before, uncertainties over

the range of EFs introduce uncertainties in IPCC-estimated GHG emissions; a potential solution could be country or region specific EFs rather than globally applicable ones. In the case of DNDC method, variability of input parameters brings uncertainty to the simulated results. Because of apparent importance, inventory data quality and uncertainties in LCIA results were analysed and the results are presented in Chap. 7.

3.7.1 Key Findings

The process-oriented model DNDC was successfully incorporated into the LCA approach by integrating DNDC-generated results into LCA inventory. This was considered to deliver an improved, site-specific inventory than the use of the commonly used IPCC Tier 1 approach to GHG emissions from agricultural systems.

Major contributors to cradle-to-farm gate environmental impacts of Soisson wheat emerged: the C and N gaseous emissions from agricultural land, N fertilizer manufacturing and field operations.

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Chapter 4 LCA Case Studies of Starch-Based Foam

4.1 Introduction

Research on starch-PVOH composites has been carried out since 1980s [2, 14], but limited LCAs on this topic were found via a thorough search of publicly available studies in English and they were mainly focused on packaging applications. Literature review also suggested limitations occurring in previous LCA studies: except one study [8] which covered a range of environmental aspects and modelled both aerobic and anaerobic degradation, LCA studies mainly focused on selective impact categories (GWP, abiotic depletion, acidification and eutrophication) and limited coverage of biological treatments. Moreover, the data quality especially the uncertainties, at both LCI and LCIA levels were not interpreted in any of the studies reviewed.

In contrast to most synthetic polymers for which complete datasets were developed by Plastic Europe [4] there is a serious data gap for PVOH production although it is a widely applied polymer [22]. Consequently in previous LCA studies, either the surrogate database (e.g. polyethylene) for PVOH was used [16] or PVOH was declared as missing data [27]. Although one LCA inventory for PVOH was developed based on German producers and patent specifications [8, 28], it is not disclosed and furthermore, this dataset was considered to have a large degree of uncertainties [8, 22]. Thus in the current study, a PVOH dataset was developed based on both published patents and theoretical estimations. But in future research, reliable LCA inventories for PVOH needs to be developed.

Besides, in the current LCA study, not only WBF packaging application was modelled but also concept construction products were covered; a range of aspects of natural environment, human health or resources were taken into account. In addition, data quality analyses were also carried out to investigate the sensitivity and uncertainties of LCIA indicator results.

4.2 Product System and System Boundary

As shown in Fig. 2.3, wheat grains were delivered to the mill (Heygates Ltd) and then further processed in foam manufacture (Greenlight Products Ltd).WBF produced then entered different WBF product systems, including coolbox, thorough mould, refractory former and display board. In addition to WBF, other two foams derived from starches (PSBF/MSBF) have been manufactured based on the same technology since 2008; they were launched to the market as main products supplied by Greenlight instead of WBF as potato/maize starch offered more comparative price than wheat flour. Thus PSBF and MSBF were explored in current LCA study and compared with WBF.

The system boundaries for main unit processes are presented below.

4.2.1 Flour Milling

The milling process for the 'Temple flour' (brand name) is indicated in Fig. 4.1. On arriving at the mill and being accepted by the quality control section, wheat grains enter the water conditioning treatment to permit separation of the bran and endosperm. The impurities such as straw, paper, metal and stone are then removed in the cleaning stage and cleaned and conditioned wheat grains are fed into milling stage. Experiencing repetitive grinding operations (break, scratch and reduction systems) and separations (scalping, grading, dressing, and purification), wheat grain is opened and the endosperm is removed from the bran and ground into flour. A simplified description for grinding and separation is as follows [21]:

- Break system—removal of endosperm from bran in large pieces,
- Scalping and grinding—removal of large branny particles and grading of released endosperm according to size
- Scratch—removal of small pieces of bran sticking to endosperm
- Purification—removal of branny particles from oversized endosperm released from scratch and grading
- Reduction and dressing—grinding of endosperm into flour and sieving out of flour before the next grinding stage

The inputs are electricity, water, wheat grain, polypropylene packaging and infrastructure. No inputs to machinery maintenance are included—such 'consumables' have been determined to be insignificant in consultation with the millers in relation to the bulk grain throughput at the mill. The outputs include flour (75.46 % of wheat grain input), co-product 'wheat feed' (for animal husbandry—22.54 % of wheat grain input), rejects, and dust; the flour dust is sent back to the product system, the rejects leave the process (approx 2 % of wheat grain inputs), including straw, which is included with the wheat feed, and other rejects (metal and stone) which are disposed of by land filling.

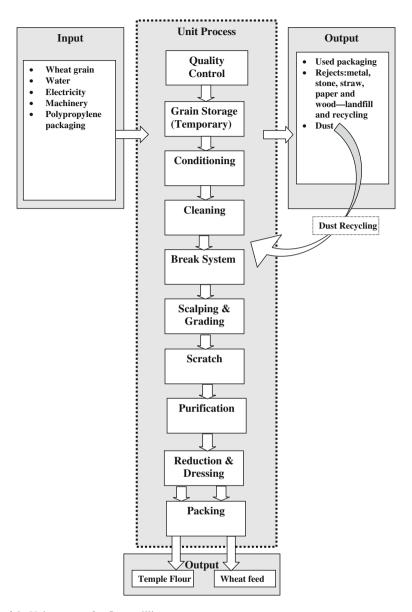


Fig. 4.1 Unit process for flour milling

4.2.2 Foam Production

The manufacturing process for WBFs is illustrated in Fig. 4.2. During the process, 6 foam tubes extruded from the extruder are fed in parallel into the RPS (Rapid Packing and Stacking) machine. Here, the 6 foam extrusions are converted to

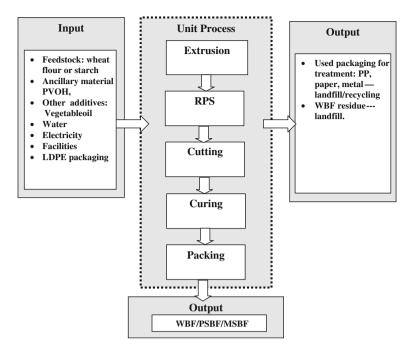


Fig. 4.2 Unit process of WBF production. *Note* This process flowchart is developed based on the existing production process for 'Greenfill' (starch-based loosefill, which is produced by using the same inputs and machinery as WBF/PSBF/MSBF)

square-cross sections and bonded together to form a plank; in the cutting and curing process, planks are cut to specified lengths and conveyed to the packing process.

Because the WBF is currently being developed comprehensive production data are not available and so several input–output data are based on the loosefill ('Greenfill') production process. The main waste output from loosefill production is wasted foam (about 5 % of WBF extruded) and the packaging used (paper, polypropylene (PP), PE packaging for raw material)—WBF waste and PE packaging were land filled; PP and paper packaging was recycled. The inputs are mainly feedstock wheat flour, ancillary material PVOH and other additives, electricity and water consumed and packaging. It was assumed that WBF are packed prior to dispatch from Greenlight to the foam converters or other users and the same LDPE packaging (currently for loosefill) was assumed as a surrogate for packaging requirements for WBF. Another input was soy flour which was only used for lubricating machinery when starting up/shutting down the system, therefore, it was also taken into account as input.

In addition to WBF, other two types of starch-based foams derived from different feedstock but based on same technology and process, were also produced in Greenlight i.e. PSBF and MSBF. Their system boundary is defined as the same as WBF (Fig. 4.2).

4.2.3 PVOH

There are many routes for PVOH production, but commercial manufacturing of PVOH is only carried out from VAC. The PVAc derived from VAC is further hydrolyzed to PVOH [11, 20].

Different methods are applied in industry to polymerize VAC to PVAc, such as suspension, solution or emulsion polymerization, amongst which, solution polymerization is one of the most commonly used technologies due to its advantages such as easy control and high-quality PVAc derived. Therefore, in the current study, the methanol solution polymerization with azobisiso-butyronitrile (AIBN) as the initiator was modelled. An efficient recycling/recovery system was assumed: waste monomer VAC and methanol were separated, purified and recycled back into reactor [20].

The obtained PVAc from solution polymerization requires alcoholysis process (in alcohol) to convert to PVOH; generally alkaline alcoholysis is applied on an industrial scale [11]. Therefore, a continuous alkaline alcoholysis process with sodium hydroxide as the catalyst in methanol medium was modelled. As shown in Fig. 4.3, hydrolysis was followed by a drying process to separate the PVOH gel from the methanol/methyl acetate solution. The solvent output from alcoholysis mainly including methanol, methyl acetate sodium acetate was assumed to be separated and recovered internally [11, 20]. Methyl acetate is hydrolyzed into methanol and acetic acid through a cation exchange resin column [11, 20]. Therefore, PVOH was the only product from this process.

During the whole process, electricity and natural gas were assumed to be the only energy sources for heat and mechanical work. AIBN catalyst and chemicals added for solvent recovery were omitted from system boundary due to no data available.

4.2.4 Corrugated Board Box Production

Figure 4.4 describes the corrugated board box production process, which is based on a specific case study from The Box Factory Ltd., and the generic base-paper making processes derived from the EU database [10]. The external dimensions of box studied are $405 \times 270 \times 140$ mm (L \times W \times H) and corrugated board under study was manufactured from 2 layers of linerboard basepaper and one fluting medium basepaper glued to two facings. Outer and inner linerboard papers were made from Kraftliner (wood-based virgin paper) and Testliner (recycled paper-based), respectively; the fluting was produced from a recycled-paper based paper known as Wellenstoff.

For Kraftliner, pulpwood logs delivered to the paper mill were passed through a debarking drum and chipper. The wood chips obtained then enter Kraftliner cooking, in which the chips are digested in an alkaline environment (Na₂CO₃ and

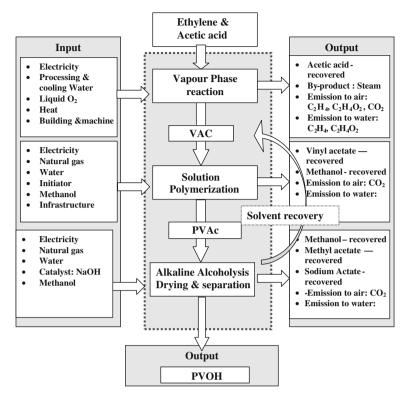


Fig. 4.3 Unit process for PVOH production

Na₂SO₄ added) at 150–170 °C. The resulting pulp is refined, screened, washed and then delivered to paper machine for paper production. The spent chemicals from Kraftliner cooking are recovered. In the paper machine, the paper produced from pulp is dewatered in several steps; waste water is collected and recycled. The energy consumed in Kraftliner production (in total around 15 GJ/t) mainly comes from internal burning of the black liquor and wood bark, which can be considered as avoided energy in LCA. The inputs primarily include wood, additives (e.g. starch), paper, PE packaging and fuel consumed in heat generation and transport. The airborne emissions from fuel combustion, waterborne emissions after effluent treatment and solid waste produced during wood processing and pulping (e.g. ash, wood bark) are also included.

During production of Testliner and Wellenstoff components, recovered paper is pre-selected and conveyed to the pulper, where paper is submerged in water and converted to a pulp. The pulps are passed through a screening, and cleaning treatment to eliminate undesirable rejects, and then enter the paper machine. The paper production is similar to that of the Kraftliner process, but a surface treatment procedure is added, involving starch input. In Testliner and Wellenstoff production, CHP generation from natural gas provides steams and the excess

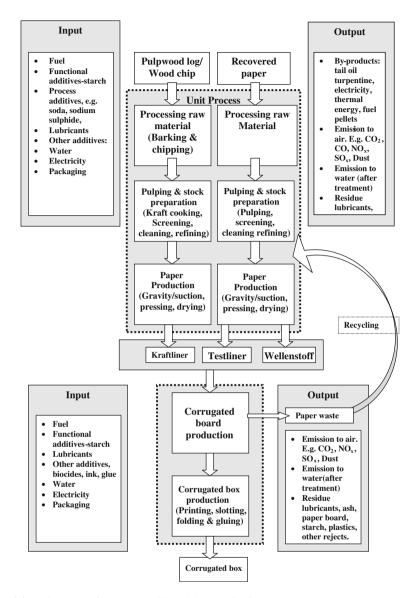


Fig. 4.4 Unit process for corrugated board box production

electricity generated is sold to the public grid, which is allocated an avoided production 'credit' against national grid electricity. So the inputs include various grades of recycled paper, additives, water, natural gas and other fossil fuel used in internal transports. Outputs include emissions from fuel combustion, residues produced in pulping (lubricant, paper, plastic, treated sludge are recycled) and waterborne emission after water treatment.

Linerboard (Kraftliner and Testliner) and fluting medium (Wellenstoff) are fed into the corrugators machine. Wellenstoff paper is conditioned with heat and steam and forms a fluted shape and glue is applied to the tips of flutes. Two linerboards are attached to the fluting medium to form the corrugated board. After printing, slotting, folding and gluing, the corrugated board box is manufactured. For this process, the main inputs are starch glue, ink, stitch, packaging, water, and energy used for steam production; outputs include paper waste, emissions from fuel combustion.

4.2.5 WBF/LDPE Foam Conversion and Insulated Coolbox Production

Conventional PE (polyethylene) is petroleum-derived material polymerized from ethylene. Different production technology is applied in industry [4]; in this LCA study the average EU polymerization data for LDPE which is derived from Eco-profile of European Plastics Industry [4] was used and the transformation process of LDPE pellets into LDPE foam was estimated based on EPS transformation due to the lack of data. The same aliphatic hydrocarbon blowing agent as EPS was assumed for LDPE transformation i.e. pentane.

The LDPE block/WBF was delivered to the company specialising in foam conversion (Foam Engineers Ltd., UK). Here the LDPE block/WBF is cut and converted to the shaped pieces of insulation for the final manufacture of the coolbox. Conversion efficiency is approximately 80 %, i.e. 20 % LDPE waste was produced and recycled, and the 20 % of WBF waste was assumed to be composted. The LDPE/WBF insulation material and the corrugated board box are assembled by the coolbox manufacturer (Hydropac Ltd, UK).

4.2.6 The Production of EPS/WBF Trough Mould and Concrete Formwork

The unit processes and system boundary for conventional EPS production, manufacture of trough mould and concrete formwork are shown in Fig. 4.5. The process for making expandable PS was derived from European database [4], which represents the average EU PS production process; the transformation process of PS into EPS foam was based on a LCA study conducted by EUMEPS (European Manufacturers of Expanded Polystyrene) [9]. The case studies of trough mould and refractory lining/concrete former for Doha Villa were developed from site-specific information supplied by the manufacturer (Cordek Ltd, UK).

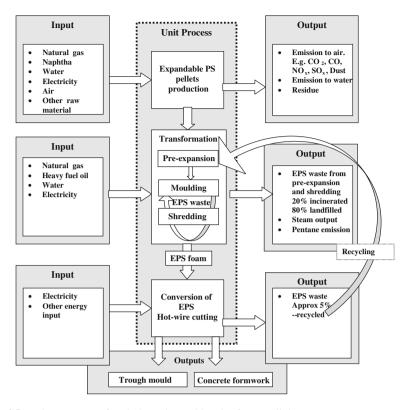


Fig. 4.5 Unit processes of EPS through mould and refractory lining

In the transformation process, the EPS waste from moulding (10.7 kg waste/t final EPS foam) is shredded and sent back to the moulding step; EPS waste from pre-expansion and shredding steps (3.76 kg/t final EPS foam) was assumed to be disposed of as a ratio of 20 % to incineration and 80 % to landfilling [9]. In the conversion process (Cordek Ltd), EPS block was converted by hot-wire cutting system to the specified shapes; the conversion efficiency is approximately 95 %, i.e. 5 % of EPS was rejected as residue to be sent to the recycling system. In the case of WBF, residue (5 % of WBF) produced during conversion was assumed to be composted. The electricity consumed and infrastructure input during conversion was missing data due to unavailability.

4.2.7 Production of Display Board

The basis for this process was developed with Caledonian Industries Ltd; but it is limited in aspect to a comparison of the quantities of the backing foams needed for display board manufacturer. It excludes the bonding and the rolling film

components and any fixtures and fittings. The service life is estimated as 3 months and a foam thickness of 10 mm and display area of 2 m² is assumed.

The display board contained 20 % recycled content and 80 % virgin HDPE (manufacturer's information). The unit processes were concerned in HDPE display board production, i.e. HDPE production, HDPE conversion. The average EU production process was used to represent the extruded HDPE used in display board [4]; during conversion of HDPE to display board, approximately 20 % of the HDPE residue was produced, it was assumed that residues were shredded and reconverted back into PE pellets, which were then sent to a specialized company, entering another display-board life cycle. In the case of WBF conversion, the residue generated (20 % of WBF) was assumed to be disposed via active home composting (well managed aerobic composting system). The electricity and infrastructure inputs to the conversion process were omitted from current LCA study due to data being unavailable.

4.3 Inventory Analysis

This section mainly presents the data collection and calculation procedures.

4.3.1 Data Collection and Data Sources

The inventory developed for four case studies includes primary data collected from industry through questionnaires, site visits, and the secondary data derived from publicly available sources and from Ecoinvent databases (version 2.0) (Pre Consultants, NL). The data sources are presented in Table 4.1.

4.3.2 Flour Milling

The input–output inventory for temple flour is given in Table 4.2. For all inputs in this unit process, except the CO_2 sequestered during wheat grain growth, the allocation between flour, wheat feed and waste is based on economic value: 93.55, 6.45 and 0 % respectively (flour price: £260/t; wheat feed price: £60/t). Carbon counting was applied to sequestered C component presented in wheat flour; according to the calculation presented in Sect. 3.3.4.4, the C contained in wheat flour was estimated as 45.56 % of dry weight which was equivalent to 1.47 kg CO_2/kg wet wheat flour (with 14 % moisture).

Table 4.1 Source of data for LCA case study

Unit processes	Data sources
Foam production	
Wheat flour milling	Heygates Ltd
WBF/PSBF/MSBF production	Greenlight Product Ltd
Soy flour production	[6]
PVOH production	[11, 12, 23]
Transportation	Greenlight product Ltd and feedstock suppliers
Coolbox case study	
Cardboard production	Box factory EU average data [10]
LDPE resin production	EU average data [4]
Transformation of LDPE into foam	Assumed same as EPS transformation [9]
Conversion of LDPE/WBF	Foam Engineers Ltd
LDPE Coolbox production	Hydropac Ltd
WBF coolbox production	Based on Hydropac Ltd in-house testing data
Use stage of coolbox and transport	Hydropac Ltd
Display board case study	
Extruded HDPE production	EU average data [4]
HDPE display board	Caledonian Industries Ltd
WBF concept product	Caledonian Industries Ltd and assumptions
Use stage of display board	Assumptions
Construction products	
Expandable PS production	EU average data [4]
Transformation of PS into EPS	EU average data [9]
EPS refractory lining/trough mould	Case studies from Cordek Ltd
EPS formwork for Doha Villa	Cordek Ltd, Buro Happold
WBF concept construction products	Research data from Brunel university
	Case studies from Cordek Ltd
Distribution and transportation	Cordek Ltd and assumptions
Other processes	
Other processes	Eco-invent databases

Table 4.2 Inventory for flour milling (unit per kg wheat flour)

Input-output	Inputs	Outputs (Kg)
Wheat grain	1.325 kg	-
Process water	0.087 kg	_
Electricity from national grid	0.103 kWh	_
Transport for wheat grain (lorry 29 t)	85.295 kgkm	_
Polypropylene packaging	0.0025 kg	_
Transport for packaging (van 3.5 t)	0.0845 kgkm	-
Temple flour	_	1
Wheat feed	-	0.2986
Waste (reject mainly metal and stone)	-	0.0265

4.3.3 WBF/PSBF/MSBF Production

The main input—output for the three foams produced in Greenlight Product Ltd are shown in Table 4.3. The materials and volumes of packaging used for each input (feedstocks) were confirmed by either Greenlight or the relevant suppliers such as Heygates Ltd., KTC (Edibles) Ltd., and Select Products Ltd. The vegetable oil container with HDPE tank and metal frame was estimated as 50 kg (KTC Ltd), whereas weights of other packaging were based on measured data.

As output, the loosefill residues produced during foam manufacturing were reported by Greenlight as 0.05 kg/kg WBF extruded, and 0.03 kg/kg PSBF or MSBF extruded. The difference in residue production could be explained by the improved techniques—WBF was the main product within 2006 and 2007, whereas WBF was replaced by PSBF and MSBF in 2008 due to the more competitive price of potato/maize starch. Loosefill residues along with the packaging for PVOH ended in landfill site (SITA UK Ltd); oil container was delivered back to supplier for reuse; the other three packagings, i.e. PP bag for wheat flour/potato maize starch, paper packaging for talc and soy flour were recycled by different companies (T.D. Williams and RecyleItdot.com Ltd).

All the transportation distances were derived from Google Map according to location of companies/waste treatment sites; capacity of lorry used varied between 7.5 and 20 t.

4.3.4 PVOH Production

As indicated above, there is no publically available data on PVOH production. In current study, a dataset for PVOH was developed in collaboration with Shah [23]. As shown in Fig. 4.3, feedstock VAC was assumed to be produced via the reaction route of C_2H_4 , $C_2H_4O_2$ with O_2 , where the Eco-invent database (V2.0) was applied.

The PVOH in current study has a density of 1.3 g/cm³. In the LCA model, it was assumed that the whole process (polymerization plus alkaline alcoholysis) took 30 min, and before drying process, 50 % of volume of mixture products was PVOH. Electricity and natural gas were assumed as the only energy sources for equipment operation and heat etc., the assumptions are given in Table 4.4 [23].

According to the results reported by previous research on methanol solution polymerization of VAC (AIBN initiator), both the rate of polymerization and polymerization degree of PVAc increase with increasing monomer concentration [11]. Therefore, in LCA polymerization model a mixture of approximately 95 % VAC and 5 % methanol was assumed [11]. Commercial polymerization from VAC to PVAc is not carried out up to 65 % [17], therefore, a conversion efficiency of 65 % with an uncertainty range was assumed [11]. Residue VAC was recovered, then the methanol medium with PVAc enters the alkaline alcoholysis, where the main reaction is presented as Eq. 4.1.

Table 4.3 Inventory for foam production (unit: per kg foam extruded)

	WBF	PSBF	MSBF
Input			
Wheat flour (kg) ^a	8.626E-01	_	_
Potato starch (kg) ^a	_	8.723E-01	_
Maize starch (kg) ^a	_	_	8.964E - 01
PVOH (kg) ^b	1.332E-01	1.235E-01	9.730E-02
Soya flour (kg) ^c	1.905E-03	2.151E-03	2.469E −03
Vegetable oil (kg) ^d	2.900E - 03	4.000E - 03	5.400E - 03
Talc ^c	0	2.000E - 04	9.000E - 04
LDPE pack	3.429E - 02	4.444E-02	3.871E-02
Process water (kg)	9.906E - 02	1.259E+02	1.097E+02
Electricity from national grid (kwh)	1.975E-01	2.561E-01	2.230E-01
Transportation for packed materials ^e			
Road transport for wheat flour (kgkm)	3.159E+02	_	_
Rail transport for potato starch (kgkm)	-	4.811E+01	_
Road transport for potato starch (kgkm)	_	4.006E+02	_
Rail transport for maize starch (kgkm)	-	_	4.944E+01
Road transport for maize starch (kgkm)	_	_	4.117E+02
Waterborne transport of PVOH (kgkm)	2.848E+03	2.640E+03	2.080E+03
Road transport of PVOH (kgkm)	1.102E+00	1.022E+00	8.052E-01
Rail transport for PVOH (kgkm)	1.839E+01	1.705E+01	1.344E+01
Road transport for soya flour (kgkm)	1.627E-01	1.837E-01	2.109E-01
Road transport of oil (kgkm)	5.757E-01	7.941E-01	1.072E+00
Road transport for talc	0	5.592E - 02	2.516E-01
Road transport for packaging (kgkm)	2.428E+00	3.147E+00	2.741E+00
Output ^f			
Greenfill waste (kg) to landfill	5.000E-02	3.000E-02	3.000E-02
PP packaging (kg) to recycle	2.157E-03	2.346E - 03	2.420E-03
Paper bag (kg) to recycle	9.905E - 06	1.318E-05	2.184E-05
PE packaging (kg) to landfill	1.066E - 03	9.880E - 04	7.784E - 04
Drum for soya oil(kg)	1.576E-04	2.174E - 04	2.935E-04
Transportation for output ^f			
Greenfill waste to landfill (kgkm)	8.449E+00	5.069E+00	5.069E+00
PP packaging to recycle (kgkm)	2.155E-01	2.345E-01	2.419E-01
Paper bag to recycle (kgkm)	1.706E-04	2.270E-04	3.761E-04
PE packaging to landfill (kgkm)	1.801E-01	1.670E-01	1.315E-01
Drum reuse (kgkm)	2.968E-02	4.093E-02	5.526E-02

Notes

^a Wheat flour, potato starch and maize starch were packed with polypropylene bag

b PVOH was packed with PE/paper bag

^c Soya flour and talc were packed with paper bags

^d Vegetable oil was packed with big container (1,000 L volume) made of HDPE and metal frame. The density of oil is 0.92 kg/l (KTC (Edibles) Ltd.)

e Both input materials and the related packages was taken into account in transport f Data provided by Greenlight Product Ltd on disposal of loosefill residues and wasted packaging

	Input	Output	Range		Assumption
Polymerization	(t)				
Methanol ^a VAC input ^a AIBN ^a	8.097E-02 1.538E+00 4.049E-04		5.540E-02 1.053E+00 2.770E-04	1.050E-01 2.000E+00 5.260E-04	Conversion 65 % (Uncertainty range50–95 %) ^b
PVAc Hydrolysis (kg)		1	2.770E=04 -	5.200E=04 -	90 % recovery rate ^c
Methanol ^e NaOH ^e PVAc	1.140E+00 9.773E-02 1.955E+00		5.017E-01 1.955E-02	1.779E+00 1.759E-01	Conversion efficiency 90 % in first reactor then reach 100 %
PVOH Methyl acetate		1 1.682E+00	- -	- -	in second reactor ^d 90 % recovery rate ^c
Total energy co	•	PVOH produc	ced)		
Electricity ^r Natural gas ^f	1107.692 34991.469		- 6998.294	- 104974.408	

Table 4.4 Inventory for PVOH production

Notes

f [23]

$$(C_4H_6O_2)_n + nCH_3 - OH \rightarrow (C_2H_4O)_n + nC_3H_6O_2$$
 (4.1)

According to previous studies, for this reaction, normally 0.02–0.2 mol NaOH catalyst per mol of PVAc was used [11], via modifying process, less NaOH catalyst could be achieved, such as 0.006–0.15 mol/mol PVAc [26] and 0.02–0.19 mol/mol PVAc [25]. As for methanol input, 0.37 kg per kg PVAc is required for chemical reaction (Eq. 4.1); according to a patent invented by Ter Jung et al. [25] a smaller amount of methanol input for reaction within a range 0.2–0.4 kg methanol/kg PVAc was reported. In this patent, the additional methanol required as medium for catalyst solution, on average was 5.67 kg Methanol/kg NaOH. In commercial hydrolysis process, total conversion efficiency reaches 100 % [20]. Thus PVAc was assumed to fully convert to PVOH and by-product methyl acetate. Waste solvent leaving hydrolysis process (mixture of methyl acetate and methanol), together with the wasted VAC from polymerization were assumed to be 90 % recovered and recycled internally [11, 20].

In summary, the inventories under 'good practice' (average input, efficient conversion and recovery system) are given in Table 4.4. Uncertainty ranges were used for sensitivity/uncertainty analyses.

4.3.5 Specifications of Case Studies

Based on the system boundary and functional unit defined, products systems modelled and materials involved are specified in Tables 4.5 and 4.6. WBF-based

a [11]

^b [11, 17]

^c [11, 20]

^d [12]

e [11], Ter Jung et al. [25]

coolboxes have been tested in both laboratory and commercial trials in Brunel University and Hydropac Ltd. It was verified that not only WBF with double layers (26 mm) but also single-layer WBF (13 mm thickness) delivered better insulation performances than standard 20 mm LDPE liner, maintaining a temperature below 5 °C for 24 h for the transportation of frozen food [3, 15]. However, WBF applied in display board/construction sector were concept products at laboratory stage in Brunel University and Buro Happold.

As shown in Table 4.5, various densities of WBF were modelled in different case studies. The density of WBF applied in coolbox was derived from the laboratory test data in Hydropac Ltd; the densities of WBF in concept construction products were estimated based on the laboratory results from Brunel University [24]. From the equations they discovered, WBFs with density of 50, 60, 70 kg/m³ were estimated theoretically to deliver equivalent compressive characteristics as different EPS grades (corresponding EPS has 70, 100 and 150 kpa compressive strength at 10 % compression respectively) [5].

As PSBFs/MSBFs were new foams developed recently in Greenlight Product Ltd, no laboratory test has been carried out on their performances e.g. insulation performance. Thus in the LCA study, they were modelled as concept products where their properties and characteristics were assumed to be the same as WBF.

4.3.6 C/N/S Content of Modelled Products

As shown in Table 4.8, C/N/S contents in foams and cardboard calculated based on results presented in Sect. 2.5 were applied in LCA model to estimate the CO₂ sequestration and track the fate of C/N/S elements over product life cycles.

The C content in flour was estimated as 45.56 % on dry mass (Sect. 3.3.4.4); C contained in PVOH was calculated from molar mass, accounting for 54.5 % of dry basis; the C content in soybean oil was estimated from the typical compositions of soybean oil triglycerides (accounting for 99 % of mass) [18, 19]. As shown in Table 4.7, based on the fatty acids present in soybean oil reported by List et al. [18] and Belitz et al. [1] and the chemical structure of triglycerides (single molecule of glycerol, combined with three fatty acids), the C content in soybean oil was estimated as 75.5–78 %. Mean value 77.76 %, which is equivalent to 2.85 kg CO₂ sequestered/kg soybean oil was used in the calculation. As soy flour was only used as lubricant for machinery but not as ingredient an for foams, very trace amounts of C introduced to foams by soy flour were assumed as negligible.

The moisture contents given in Table 2.2 were contained in the received fresh feedstock (wheat flour/starches). But a proportion of these moistures were lost during foam processing. Thus the final moisture contents of finished products were determined in the laboratory as 7.19, 7.85, 7.32 and 4.39 % for WBF, PSBF, MSBF and cardboard, respectively (Table 2.3).

Table 4.5 Specifications for display board, trough mould and concrete formwork

Case studies	Specification	WBF/PSBF/ MSBF	EPS/HDPE
Display board	Service life 3 months Artwork on film rolled on to the board Thickness 10 mm Area 2 m ²	Weight 0.5 kg Density 25 kg/m ³	HDPE with 20 % recycled content Weight 1.7 kg Density: 85 kg/m ³
Trough mould 1	Service life 6 months Supplied volume 9 m ³	Weight450 kg Density 50 kg/m ³	EPS (Filcor 20) with 30 % recycled content Weight 135 kg Density: 15 kg/m ³
Trough mould 2	Service life 6 months Supplied volume 98 m ³	Weight 5,880 kg Density 60 kg/m ³	EPS (Filcor 45) with 15 % recycled content Weight 1,960 kg Density 20 kg/m ³
Trough mould 3	Service life 6 months Supplied volume 51 m ³	Weight 2,550 kg Density 50 kg/m ³	EPS (Filcor 20) with 30 % recycled content Weight 765 kg Density 15 kg/m ³
Trough mould 4	Service life 6 months Supplied volume 138 m ³	Weight 6,900 kg Density 50 kg/m ³	EPS (Filcor 20) with 30 % recycled content Weight 2,070 kg Density 15 kg/m ³
Trough mould 5	Service life 6 months Supplied volume 127 m ³	Weight 7,620 kg Density 60 kg/m ³	EPS (Filcor 45) with 15 % recycled content Weight 2,540 kg Density 20 kg/m ³
Refractory Lining	Service life one-use Shape: dome Coating: epoxy resin Supplied volume 2.4 m ³	Weight 168 kg Density 70 kg/m ³	EPS (Filcor 70) with 100 % virgin EPS Weight 60 kg Density 25 kg/m ³
Formwork for Doha Villa	Service life one-use No coating Supplied volume 335 m ³	Weight 23,450 kg Density 70 kg/m ³	EPS with 100 % virgin EPS Weight 8,375 kg Density 25 kg/m ³

Table 4.6 Specifications for a single coolbox

1			
Input-output	Density (kg/m3)	Quantity (g)	Others
Kraftliner basepaper	136	75.3	Virgin paper
Testliner basepaper	136	75.3	100 % recycled paper
Wellenstoff basepaper	90	65.8	100 % recycled paper
LDPE foam	35	241.99	Thickness: 20 mm
WBF/PSBF/MSBF	25	213.43	Thickness: 26 mm

Notes The insulated coolbox modelled is one 8.5 L corrugated board box with external dimension of 405 \times 270 \times 140 mm (L \times W \times H)

0.090

% received sample WBF (%) PSBF (%) Cardboard (%) MSBF (%) Total Ca 42.707 42.564 43.911 43.775 Biogenic Cb 35.377 37.149 43.911 36.305 Total N^c 0.000 1.280 0.000 0.214

Table 4.7 Element analysis in foams and cardboard

0.087

Total S^c

Table 4.8 Composition of Soybean oil

Soybean oil composition		Study-1 [18] (%)	Study-2 [1] (%)
Fatty acid Composition	Alpha linalenic acid C 18:3	5.40	8.00
(% of total fatty acid)	Linoleic acid C 18:2	54.40	53.00
	Oleic acid C 18:1	23.90	21.00
	Stearic acid C18:0	4.40	5.00
	Palmitic acid C 16:0	11.90	10.00
	Eicosenoic acid C 20:1	0.00	3.50
Estimated Glycerol (% trig	glycerides) ^a	10.22	10.12
Estimated total C content	(% triglycerides)	77.53	77.98

Notes a Estimation based on chemical structure of triglycerides and composition of fatty acid

4.3.7 Distribution Stage

As presented in Table 4.9, transportation distances for products distributions were mainly built on case studies developed in collaboration with manufactures, whereas the capacities of transportation mode (e.g. lorry) were mainly based on assumptions except the coolbox case study.

4.3.8 Other Processes

The electricity production was based on reference year 2008 and the fuel types for electricity generation were derived from national statistics [7]: main sources for UK electricity were coal, natural gas or nuclear, accounting for 88.5 % in 2008, whereas renewable resources including hydropower, wind, solar and biomass only shared 5.6 % of total electricity generation. As for infrastructure input, unit processes derived from Ecoinvent V2.0 were applied as surrogate datasets, e.g. organic chemical plant, corn mill, integrated paper mill, packaging box production unit. Other unit processes including raw-material manufacturing, transportation, fuel mining, processing and delivery were built on GB or EU datasets provided in Ecoinvent database (v2.0).

^a Total C includes the fossil C contained in PVOH and biogenic C sequestered from atmosphere

^b C component sequestered from atmosphere and contained in feedstock

^c Laboratory results (Table 2.3)

Distance (%)	Transportation mode	Data source
Distribution 23	Distribution 28 t lorry	Hydropac data
Distribution 903	Distribution 28 t lorry	
Distribution 50	Distribution 16 t lorry	Assumptions
Distribution 229	Distribution 32 t lorry	Cordek data &assumptions
Distribution 114	Distribution 32 t lorry	
Distribution 710	Distribution 32 t lorry	
Distribution 92	Distribution 32 t lorry	
Distribution 128	Distribution 32 t lorry	
Distribution 100	Distribution 32 t lorry	Assumptions
Distribution 5,209	Freight ship	Assumptions
	Distribution 23 Distribution 903 Distribution 50 Distribution 229 Distribution 114 Distribution 710 Distribution 92 Distribution 128 Distribution 100	Distribution 23 Distribution 28 t lorry Distribution 903 Distribution 28 t lorry Distribution 50 Distribution 16 t lorry Distribution 229 Distribution 32 t lorry Distribution 114 Distribution 32 t lorry Distribution 710 Distribution 32 t lorry Distribution 92 Distribution 32 t lorry Distribution 128 Distribution 32 t lorry Distribution 128 Distribution 32 t lorry Distribution 32 t lorry

Table 4.9 Transportation of products distribution

4.4.1 Contribution Analysis of WBF Production

4.4.1.1 Wheat Flour Milling

Analyzing the unpacked wheat flour production (Fig. 4.6 and Table 4.10), wheat farming is presented as the dominant process causing over 70 % of impacts on most impact categories, especially on ODP, acidification, and eutrophication where above 90 % of impacts was attributable to the farming system.

Apart from wheat farming, electricity was the second resource consumer, contributing 20 % of impacts on abiotic depletion, which was due to the dependency of UK electricity generation on natural gas and hard coal resources, whereas, the diesel consumed in transport or the resources utilized for infrastructure only shared minor burdens.

On GWP100, wheat farming also dominated, but differently, it was shown as a beneficial process by calculating C sequestration. To illustrate this effect, CO_2 up-take during wheat growth was presented as a separate unit process in Fig. 4.6; as indicated as negative scores 'below' the line, the CO_2 sequestered in wheat flour balanced the burdens caused by other processes and led to a wheat flour with a net negative Global warming profile. Regardless of C sequestration, the main contributor to positive score was wheat grain farming and electricity utilized in the mill accounting for 93 and 6 %, respectively.

Similar profiles were found in eutrophication and acidification impact categories where wheat grain farming caused over 97 % of burdens. As analyzed in Sect. 3.5.1, it was mainly associated with N gas flux and N P leaching from soil.

Impacts on human toxicity or eco-toxicity impact categories were mainly driven by the straight N fertilizer production, which resulted in the dominancy of farming system (72–87 % of impacts). Besides, landfill of rejects and electricity

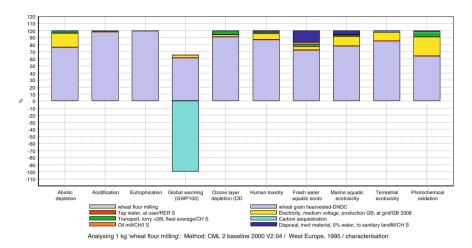


Fig. 4.6 Characterised LCIA profile for milled wheat flour (unit 1 kg flour)

were shown as important elements although they only made minor contributions. The former was mainly associated with fresh water eco-toxicity where the metallic ions released were the main causes. The latter contributed 7–13 % of impacts on all toxicity impacts categories, where the emission from natural-gas and hard-coal based electric generation were the main concerns. Barite water emission from natural gas production was concerned in impacts on marine eco-toxicity; atmospheric mercury emission from hard coal combustion and chromium emission to soil during electricity transmission were found as important contributors to terrestrial eco-toxicity; vanadium ions released from disposal of ash after hard coal burning was associated with fresh water eco-toxicity; barite as well as other toxic compounds brought impacts on human toxicity.

As for POCP and ODP, both impact categories were highly concerned with N fertilizer and field operation during wheat farming, which has been analyzed in Sect. 3.5.1; additional 10–30 % of burdens were caused by transportation as well as electric power generation. Specifically speaking, ODP was mainly attributed to the production and delivery process of fuels utilized for transportation and electricity generation, including CBrF₃ (Halon 1301) emitted during crude oil production, CBrClF₂ (Halon 1211) evolved from transport of natural gas. Different from ODP, the combustion of fuels in vehicle engines or power plants are important contributors to impacts on POCP, e.g. the SO₂ CH₄ and CO released from diesel or hard coal burning.

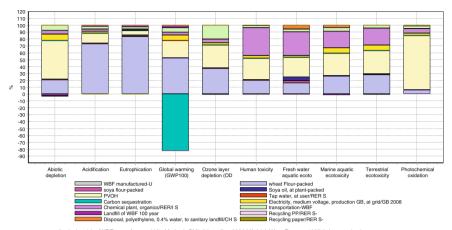
To evaluate the environmental profile of wheat flour from cradle to mill gate, the PP packaging was also taken into account; the contributions of unit processes to the overall impacts caused by packed wheat flour are presented in Table 4.11. The inclusion of packaging led to minor changes in the environmental profile, negative GWP100 scores carried though the packing process indicating wheat flour product with net GWP100 savings. Milled flours were shown as the dominant

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Impact category	Unit	Total	Wheat farming Water	Water	Electricity	Rejects to landfill	Electricity Rejects to landfill Transport of grain Infrastructure	Infrastructure
Abiotic depletion	kg Sb eq	2.28E-03	1.73E-03	1.72E-07	.72E-07 4.55E-04 3.34E-06	3.34E-06	8.10E-05	9.74E-06
Acidification	kg SO2 eq	1.18E - 02	1.15E - 02	1.13E-07	.13E-07 2.03E-04 1.74E-06	1.74E-06	5.73E-05	8.41E - 06
Eutrophication	kg PO4—eq	3.41E - 03	3.38E - 03	8.12E - 09	3.12E-09 1.52E-05	4.74E - 07	1.22E - 05	1.52E - 06
GWP100	kg CO2 eq	-5.01E-01	-5.73E-01	2.53E - 05	5.87E-02	3.03E - 04	1.09E - 02	1.42E - 03
ODP	kg CFC-11 eq	3.51E - 08	3.18E - 08	1.21E-12	.21E-12 1.33E-09	7.63E-11	1.80E - 09	8.44E-11
Human toxicity	kg 1,4-DB eq	1.20E-01	1.05E-01	7.71E-06	9.59E - 03	1.99E - 03	2.22E - 03	1.68E - 03
Fresh water eco-toxicity	kg 1,4-DB eq	1.95E-02	1.40E - 02	4.20E - 06	1.20E-06 1.10E-03	3.34E - 03	4.87E - 04	5.48E - 04
Marine eco-toxicity	kg 1,4-DB eq	4.84E+01	3.77E+01	6.20E - 03	6.20E-03 6.41E+00	2.77E+00	9.03E - 01	5.30E - 01
Terrestrial eco-toxicity	kg 1,4-DB eq	1.49E - 03	1.27E - 03	1.65E-07	1.80E - 04	1.09E - 06	2.41E - 05	1.55E - 05
POCP	kg C2H4	2.97E - 05	1.89E - 05	7.94E-09	8.06E - 06	6.53E - 08	2.07E-06	5.65E - 07

Table 4.11 Contribution analysis of packed wheat flour (per kg packed flour)

Impact category	Total	Packaging production	Wheat farming	Water	Electricity	Rejects to	Transport	Infrastructure
		+ delivery				landfill	of grain	
Abiotic depletion (%)	100.000	3.475	73.271	0.007	19.267	0.141	3.426	0.412
Acidification (%)	100.000	0.136	97.573	0.001	1.718	0.015	0.485	0.071
Eutrophication (%)	100.000	0.051	880.66	0.000	0.444	0.014	0.359	0.044
GWP100 (%)	-100.000	1.020	-115.397	0.005	11.831	0.061	2.192	0.287
ODP (%)	100.000	0.066	90.570	0.003	3.775	0.217	5.129	0.240
Human toxicity (%)	100.000	0.171	986.98	900.0	7.955	1.648	1.841	1.392
Fresh water eco-toxicity (%)	100.000	0.327	71.643	0.021	5.616	17.099	2.492	2.801
Marine eco-toxicity (%)	100.000	0.121	77.961	0.013	13.231	5.715	1.864	1.094
Terrestrial eco-toxicity (%)	100.000	0.053	85.093	0.011	12.106	0.073	1.620	1.044
POCP (%)	100.000	3.616	61.392	0.026	26.190	0.212	6.730	1.834



Analysing 1 kg 'WBF manufactured-U'; Method: CML 2 baseline 2000 V2.04 / West Europe, 1995 / characterisation

Fig. 4.7 Characterised LCIA profile for unpacked WBF (unit 1 kg WBF)

contributor, accounting for 96.4–99.9 % of scores over all impact categories whereas PP packaging production and delivery processes only caused negligible burdens.

4.4.1.2 WBF Production

The characterised LCIA profiles of 'cradle-to-gate' WBF are given in Fig. 4.7, Tables 4.12 and 4.13. Irrespective of LDPE packaging, wheat flour and PVOH are the predominant contributors to environmental profiles of unpacked WBF product system.

In abiotic depletion, landfill of WBF and recycling of PP packaging were presented as negative values below the line (Table 4.12, Fig. 4.7), where the recycled PP and electricity generated from landfill gas combustion were given as 'credits' by following 'avoided product' allocation approach. However, this beneficial effect was overridden by the burdens induced by other processes, amongst which PVOH is presented as a dominant contributor, causing nearly 60 % of impacts. It was mainly attributable to resources (e.g. natural gas and crude oil) consumed during production of feedstocks (C₂H₄, CH₃OH, CO) for PVOH manufacturing. Besides, three other resource consumers were wheat flour production, electricity generation and transportation occupying 39 % of resource depletion in total.

Another impact category dominated by PVOH was POCP, where nearly 80 % of the burdens were attributed to the PVOH component. C_2H_4 and $C_2H_4O_2$, CH_3OH released during production of VAC and its feedstocks (C_2H_4 and $C_2H_4O_2$) were shown as main contributors to POCP burdens. Additional 20 % of POCP was shared by other inputs (infrastructure, electricity, transportation, wheat flour), their

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Impact	Abiotic	Acidification	Acidification Eutrophication GWP100	GWP100	ODP	Human	Fresh water	Marine aquatic Terrestrial	Terrestrial	POCP
category	depletion					toxicity	aquatic ecotox. ecotoxicity	ecotoxicity	ecotoxicity	
Unit	kg Sb	kg SO2	kg PO4—	kg CO2	kg CFC-11 eq	kg CFC-11 eq kg 1,4-DB eq kg 1,4-DB eq	kg 1,4-DB eq	kg 1,4-DB	kg 1,4-DB eq kg C2H4 eq	kg C2H4 eq
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Total	9.50E - 03	1.40E - 02	3.52E-03	2.77E - 01	8.10E - 08	5.16E - 01	1.05E - 01	1.56E+02	4.62E - 03	4.60E - 04
C sequestered	0.00E+00	0.00E+00	0.00E+00	-1.33E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Wheat Flour	2.04E - 03	1.02E - 02	2.94E - 03	8.40E - 01	3.03E - 08	1.04E - 01	1.69E - 02	4.18E+01	1.28E - 03	2.66E - 05
Soya flour ^b	5.30E-06	1.35E - 05	2.78E-05	3.64E - 04	9.73E-11	6.35E - 04	3.42E - 03	1.10E - 01	3.23E-05	3.46E - 07
Soya oil ^b	2.15E-05	3.41E - 05	4.26E-05	6.43E - 03	3.24E-10	1.86E - 03	5.21E-03	4.13E - 01	5.30E-05	1.83E - 06
$PVOH^b$	5.52E-03	2.05E - 03	2.23E-04	4.07E - 01	2.74E-08	1.63E - 01	3.06E - 02	5.18E+01	1.55E-03	3.62E - 04
Water	2.09E - 07	1.38E - 07	9.88E - 09	3.08E - 05	1.48E - 12	9.38E - 06	5.11E-06	7.55E-03	2.01E - 07	9.66E - 09
Electricity	9.33E-04	4.16E - 04	3.11E-05	1.20E - 01	2.72E-09	1.97E - 02	2.25E-03	1.31E+01	3.69E - 04	1.65E - 05
Infrastructure	5.44E-04	4.09E - 04	4.58E-05	7.13E - 02	4.01E - 09	2.11E-01	3.67E - 02	3.78E+01	1.16E - 03	2.99E - 05
Transportation ^a	7.50E-04	5.80E - 04	1.25E-04	1.07E - 01	1.67E - 08	1.83E - 02	3.69E - 03	8.00E+00	2.08E - 04	1.94E - 05
Landfill of WBF	-2.48E-04	2.71E - 04	7.93E-05	5.90E - 02	-6.75E-10	-3.88E-03	-5.53E-04	-3.45E+00	-3.48E-05	4.27E - 06
Recycling PPc	-6.37E-05	-1.06E-05	-1.20E-06	-3.44E-03	1.75E-11	-3.48E-06	-3.15E-05	5.05E - 02	2.22E-06	-8.00E-07
Landfill of PE^c	1.44E - 07	7.59E-08	5.57E-06	1.13E - 04	3.29E - 12	2.48E - 03	6.40E - 03	6.43E+00	8.13E - 08	2.31E - 08
Recycling paper ^c 5.73E-08	5.73E-08	-1.87E-09	-4.83E-09	2.59E-05	4.64E-13	1.78E-06	1.25E - 06	1.38E - 03	1.35E-07	8.07E-10

 $^{^{\}rm a}$ Include transportation of wheat flour and the deliver of wasted packaging or resides to disposal site $^{\rm b}$ Include production and transportation from supplier to Greenlight product 1td $^{\rm c}$ The packagings for feedstocks

individual contribution varied between 4 and 6.5 %. It involved the CO, SO₂, CH₄ emitted either from electricity generation, transportation or from production of metal materials required by chemical plant construction.

As shown in Fig. 4.7, both acidification and eutrophication impacts were dominated by wheat flour production process where N gas flux and N P leaching during wheat farming was the main cause; whereas PVOH component only shared 6.3–14.7 % of burdens, which was mainly caused by the feedstocks production especially those for VAC. Two feedstocks CO and methanol were highly fuel dependent: the former was modelled as the product from combustion of heavy fuel oil, the latter was derived from natural gas; furthermore, CO production was an electricity demanding process. Thus SO₂ and NO_x emissions from combustion of fuels for electricity generation and the feedstock manufacturing played an important role in acidification profiles. In addition, the impact on acidification were partially attributable to the SO₂ and NO_x released from production of C₂H₄, which is another feedstock for VAC. Different from acidification, impacts produced by PVOH on eutrophication was primarily caused by NO_x and COD released, such as the NO_x from diesel burning during transportation, COD released from VAC production, the COD NO_x released from fuel processing and delivery. In both acidification and eutrophication, although the recycling of paper and PP packagings contributed to negative value (Table 4.12), their effects were not sufficient to offset the burdens.

The impact category with significant negative scores was GWP100 where the total CO₂ sequestered in WBF was presented as separate process. As illustrated in Fig. 4.7, this C beneficial effect was mainly overridden by the burdens caused by GHGs emission from the wheat agricultural system and PVOH production, both of which in total accouted for 80 % of positive scores. As analyzed in Sects. 4.4.1.1 and 3.5.1, CO2 flux released from soil, GHGs emitted during field operation and fertilizer production were the dominant factors for GWP100 burdens (positive value) of wheat flour product system. In the case of PVOH, GHGs generated during the life cycle of VAC were the primary cause, which mainly included the GHGs release from fuel combustion either for energy generation or feedstock manufacturing. Besides these two main contributors, the remaining 20 % of the burdens were mainly caused by transportation, electricity infrastructure inputs and disposal of WBF residue. Except landfill, the GHGs during other three processes were mainly derived from fuel combustion; for disposal of WBF residue, although 'green' electricity generated gave credits, the GHGs released either as fugitive gas or via landfill combustion process balanced the benefits brought by renewable energy.

Interestingly, a similar trend appeared across all toxicity impact categories: besides PVOH which shared one third of positive burdens, wheat flour and chemical plant were shown as two main contributors, occupying 16–28 % and 25–40 % of burdens, respectively. Analyzing profiles of PVOH, electricity and infrastructure material involved in VCA manufacturing process were found as the main causes. Impacts on human toxicity were attributed to chromium, arsenic, PAH released from producing construction materials; whereas fresh water/marine

aquatic ecotoxicity was highly related to the water emissions from disposal of slag or ash during metal production or electricity generation, i.e. nickel, vanadium, cobalt, barium, beryllium; burdens on terrestrial eco-toxicity were shared by electricity power transmission, production of infrastructure materials (copper and steel), lignite and heavy fuel oil burning process, which included chromium emission to soil and some atmospheric emissions, e.g. mercury vanadium and arsenic. Therefore, the infrastructure including those concerned in PVOH and WBF production were drivers for environmental profiles on all toxicity impact categories. However, there were uncertainties in the infrastructure inventory, which were tested in sensitivity analysis. Besides the positive burdens, green electric energy generation in WBF landfill and PP recycling brought some benefits (negative values in Table 4.12) by avoidance of burdens for production of petrochemical PP and national grid electricity. These savings are presented as below line but insignificant in comparison with burdens above the line shown in Fig. 4.7. Similar to human and ecotoxicity, one third of impacts on ODP were also contributed by PVOH component; the remaining two third were dominated by wheat flour (37 %) and transportation (21 %). Analysing PVOH only, ODP burdens were primarily derived from production and delivery of fuels (natural gas and heavy fuel oil) utilised for feedstock production, e.g. CBrF₃ emitted from crude oil production and CBrClF2 released from transport of natural gas. This was also the case of wheat flour and transportation processes where ODP profiles were highly related to natural gas and crude oil inputs. Landfill of WBF residue brought beneficial effects on ODP profile (Table 4.12), but it was not sufficient to offset ODP burdens.

Considering the LDPE packaging for WBF the contribution analysis of whole packed WBF product system is shown in Table 4.13, where the biogenic C sequestered in WBF is presented as a separate component. The inclusion of packaging incurred insignificant change in environmental profile over most of the impact categories except abiotic depletion and GWP100, where it led to an increase by approximately 10 and 20 % respectively.

4.4.2 Normalisation of WBF Production

Normalised LCIA results for unpacked wheat flour and unpacked WBF are illustrated in Figs. 4.8 and 4.9, respectively, where the reference system West Europe 95 was applied.

Normalization leads to an interpretation of the relative significance of each individual indicator result where acidification and marine aquatic eco-toxicity are presented as relatively significant for unpacked wheat flour product, followed by eutrophication, abiotic depletion; the normalised indicator results on GWP100 appeared as negative. For unpacked WBF product, the normalisation profiles shifted: marine aquatic eco-toxicity remained as the most significant with abiotic depletion moved to the second place. In addition, indicator results on the other four

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Table 4.15	uonnaunuo	analysis of pac	cked wbr (per	lable 4.13 Contribution analysis of packed with their kg packed with						
Unit %	Abiotic	Acidification	Acidification Eutrophication GWP100	GWP100	ODP	Human	Fresh water aquatic Marine aquatic	Marine aquatic	Terrestrial	POCP
	depletion					toxicity	ecotoxicity	ecotoxicity	ecotoxicity	
Total	100.000	100.000	100.000	100.000	100.000 100.000	100.000	100.000	100.000	100.000	100.000
C sequestration	0.000	0.000	0.000	-380.025	0.000	0.000	0.000	0.000	0.000	0.000
Wheat flour	19.170	71.584	83.101	239.774		20.104	16.113	26.712	27.705	5.592
Soya flour ^b	0.050	0.095	0.786	0.104	0.120	0.123	3.265	0.070	0.698	0.073
Soya oil ^b	0.202	0.240	1.203	1.834		0.359	4.976	0.264	1.145	0.385
$PVOH^b$	51.924	14.401	6.305	116.271		31.435	29.207	33.160	33.466	76.221
Water	0.002	0.001	0.000	0.009		0.002	0.005	0.005	0.004	0.002
Electricity	8.778	2.922	0.877	34.363		3.801	2.150	8.400	7.971	3.481
Infrastructure	5.116	2.875	1.292	20.351	4.933	40.757	35.062	24.174	24.954	6.301
Transportation ^a	7.055	4.079	3.542	30.618		3.533	3.525	5.116	4.499	4.089
Landfill of -2.329 WBF	-2.329	1.903	2.239	16.830	-0.830	-0.749	-0.528	-2.207	-0.752	0.898
Recycling PP ^c -0.600	-0.600	-0.075	-0.034	-0.981	0.021	-0.001	-0.030	0.032	0.048	-0.168
Landfill of PE ^c	0.001	0.001	0.157	0.032	0.004	0.479	6.117	4.112	0.002	0.005
Recycling paper ^c	0.001	0.000	0.000	0.007	0.001	0.000	0.001	0.001	0.003	0.000
LDPE	10.631	1.974	0.531	20.812	0.363	0.157	0.136	0.160	0.257	3.121
packaging ^b										

 $^{^{\}rm a}$ Include transportation of wheat flour and the deliver of wasted packaging or resides to disposal site $^{\rm b}$ Include production and transportation from supplier to Greenlight product 1td $^{\rm c}$ The packagings for feedstocks

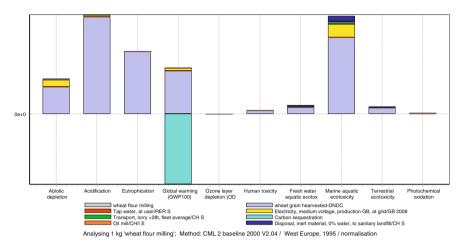


Fig. 4.8 Normalised LCIA profile for wheat flour milling (unit 1 kg unpacked flour)

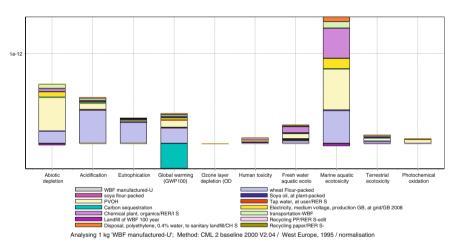


Fig. 4.9 Normalized LCIA profile for WBF production (unit 1 kg unpacked WBF)

impact categories are also of relative significance, i.e. acidification, fresh water eco-toxicity GWP100, and eutrophication.

As seen from Figs. 4.8 and 4.9, the key components driving normalisation profiles are wheat grain farming, PVOH and infrastructure input for WBF production. PVOH and farming system appear to be significant sources of overall environmental burdens; whereas infrastructure is only shown as an important source of normalized marine eco-toxic profile. These three components concern the major options for improvement of WBF product system. For both wheat flour and WBF, C sequestration appears as relatively important component bringing beneficial effects on their normalized LCIA profiles.

Impact category	WBF packed	Unpacked WBF	Unpacked wheat Flour	Packed wheat flour	
Abiotic depletion	7.166E-13	6.405E-13	1.537E-13	1.593E-13	
Acidification	5.208E-13	5.105E-13	4.316E-13	4.322E-13	
Eutrophication	2.840E-13	2.825E-13	2.735E-13	2.736E-13	
GWP100	7.286E-14	5.770E-14	-1.043E-13	-1.032E-13	
ODP	9.750E-16	9.715E-16	4.215E-16	4.217E-16	
Human toxicity	6.827E-14	6.816E-14	1.588E-14	1.591E-14	
Fresh water ecotox.	2.073E-13	2.070E - 13	3.859E-14	3.871E-14	
Marine ecotoxicity	1.377E-12	1.375E-12	4.260E-13	4.265E-13	
Terrestrial ecotoxicity	9.815E-14	9.790E - 14	3.151E-14	3.152E-14	
POCP	5.746E-14	5.567E-14	3.591E-15	3.725E-15	

Table 4.14 Normalized LCIA profiles (kg packed WBF or wheat flour)

The normalisation profiles of packed wheat flour and WBF were evaluated as well. As shown in Table 4.14, relatively speaking, packaging was shown as an insignificant input in terms of normalised LCIA results. Although the results discussed above indicated relative contribution of WBF to environmental problems for the reference region (West Europe) at specific temporal scales, the normalised indicator results are dependent on reference system chosen. The influence of this factor was tested via sensitivity analysis.

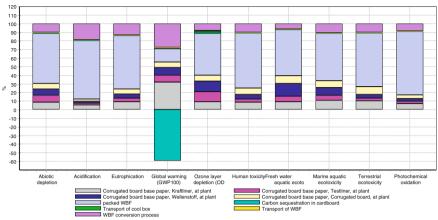
4.4.3 Coolbox Case Study

The LCIA results of coolbox insulated with WBF and its comparison with a LDPE foam equivalent are presented below. The contribution analysis of the cradle-to-gate LCIA for the WBF coolbox followed by comparison between two coolbox systems and finally the LCIA profiles with additional distribution aspects are given.

4.4.3.1 Contribution Analysis of Cradle-to-gate WBF Insulated Coolbox

The LCIA profile for the coolbox insulated with WBF is given in Fig. 4.10 and Table 4.15. The WBF production process is found to be the main cause of the impact on almost all the impact categories except GWP100.

WBF production and conversion processes are the main contributors to abiotic depletion, accounting for nearly 70 % of impacts due to the production of PVOH and wheat flour components. Paper and corrugated board box production contributes approximately 30 % to abiotic depletion, mainly due to the electricity and other energy (natural gas, heavy fuel oil) required by cardboard production system, where Kraftliner and corrugated board making are electricity and heavy fuel oil



Analysing 1 p '-WBF Cool box -double layer'; Method: CML 2 baseline 2000 V2.04 / West Europe, 1995 / characterisation

Fig. 4.10 Contribution analysis of WBF coolbox (unit: per coolbox)

 Table 4.15 Characterised LCIA profiles of WBF coolbox (Unit: per coolbox)

Impact	Unit	Total	Corrugated	Converted	Transportation	
category			board box production	WBF production	Corrugated board box	WBF
Abiotic depletion	kg Sb eq	4.88E-03	1.49E-03	3.33E-03	5.44E-05	1.35E-06
Acidification	kg SO2 eq	5.57E-03	6.82E - 04	4.85E-03	4.21E-05	1.05E-06
Eutrophication	kg PO4– eq	1.52E-03	3.64E - 04	1.15E-03	9.09E-06	2.26E-07
GWP100	kg CO2 eq	2.43E-01	-2.51E-02	2.60E-01	7.78E - 03	1.94E - 04
ODP	kg CFC-11 eq	4.44E - 08	1.77E-08	2.54E - 08	1.21E-09	3.02E-11
Human toxicity	kg 1,4-DB eq	2.14E-01	5.31E-02	1.59E-01	1.33E-03	3.30E-05
Fresh water ecotoxicity	kg 1,4-DB eq	5.21E-02	2.05E-02	3.13E-02	2.68E-04	6.66E-06
Marine ecotoxicity	kg 1,4-DB eq	7.58E+01	2.54E+01	4.98E+01	5.80E - 01	1.44E-02
Terrestrial ecotoxicity	kg 1,4-DB eq	1.97E-03	5.23E-04	1.43E-03	1.51E-05	3.76E-07
POCP	kg C2H4 eq	1.71E-04	2.88E-05	1.41E-04	1.40E-06	3.49E-08

demanding processes, while Testliner and Wellenstoff are natural gas consumers. As seen in Fig. 4.10, resource depletion associated with transport is shown as negligible.

To track the biogenic C present in cardboard, all the CO₂ sequestered during plant growth and contained in corrugated board is illustrated as below line in Fig. 4.10. This C beneficial effect was sufficient to offset the burdens caused by GHG emissions from the cardboard product system, leading to a corrugated board with negative C 'savings'. Regardless of cardboard-C sequestration, Kraftliner was the main contributor to GWP profile of the corrugated board due to large quantity of CO₂ emitted from Kraftliner plant. The same as Kraftliner, CO₂ emitted from other two basepaper making plants (Testliner and Wellenstoff) was the major

GHG; differently, for corrugated board making process besides CO_2 emission, electricity generation from hard coal and natural gas were other GHGs sources. Converted WBF foam with inclusion of biogenic C accounted for over 40 % of positive GWP100 scores, where the conversion process was the main contributor due to the electricity input and WBF residue disposal (CO_2 from home composting).

For the ODP, nearly 60 % of impacts are attributed to WBF production and conversion. Specifically speaking, the main cause was the CBrF₃, CBrClF₂ released from production, delivery of natural gas, crude oil which was utilized for production of PVOH, or the diesel used for field operation and transportation. The corrugated board component of the coolbox contributes less than 40 %, primarily due to fuel (natural gas, fuel oil) and electrical power consumed and transportation involved.

On the toxicity impact categories, the contribution of WBF varied between 60 and 75 % of impacts; as analysed in Sect. 4.4.1.2, electricity transmission and production of infrastructure material, as well as N fertilizer input involved in the WBF production were the main cause. Corrugated board in total incurred 25–40 % of burdens across all toxicity impact categories, where infrastructure, electricity, additives (especially starch input), recycled paper (raw material for Testliner and Wellenstoff) as well as disposal of waste shared most of the environmental scores. Via contribution analysis on corrugated board, it was found that human toxicity mainly resulted from chromium from ferrochromium production (raw material for infrastructure); barite, PAH released from natural gas production and combustion (for electricity generation), arsenic and PAH released from hard coal combustion (for electricity generation). Burdens on fresh water aquatic ecotoxicity were dominated by the water emissions from waste disposal or slag/ash treatment during base paper/cardboard making, metal production, and recycled paper sorting, such as vanadium, nickel and copper ions. As for marine aquatic eco-toxicity, it was highly related to the barite emissions from natural gas production and other metallic ions (e.g. nickel, beryllium, vanadium, barium) released from waste/slag treatment during metal production or basepaper/cardboard manufacturing. Corrugated board totally shared less than 30 % of burdens on terrestrial eco-toxicity, which was primarily attributable to mercury released to soil from starch production, soil emission chromium from electricity transmission as well as mercury atmospheric emission from hard-coal burning (electricity generation) and infrastructure material production (steel ferrochromium).

As shown in Fig. 4.10, WBF production was the main cause of POCP burdens, where the main contributor was identified as PVOH (Sect. 4.4.1.2). Only approximately 15 and 10 % of POCP scores were shared by corrugated board production and WBF conversion processes, which were driven by the SO₂, CH₄ and CO emissions from fuel combustion during either transportation or energy production and delivery processes (electricity generation, natural gas and heavy fuel oil processing and delivery). Besides, CH₄ emission assumed from WBF residue disposal during conversion process also contributed 2.5 % of total POCP score.

Impacts on acidification and eutrophication are dominated by WBF (around 70 %); whereas WBF conversion process incurred 20 % of the acidification potential and 10 % of eutrophication burdens, which was mainly caused by NH₃ emitted from composting of WBF residue. Approximately 10 % of the acidification score and 25 % of the eutrophication profiles was caused by corrugated board component. NO_x and SO_x from basepaper/corrugated board making, energy generation (e.g. electricity), and transportation were the main contributors to acidification. While eutrophication burdens were primarily induced by N, P leaching $(PO_4^{\ 3-}, NO_3^{\ -}, NH_4^{\ +})$ either from potato agricultural system (potato as feedstock for starch) or basepaper/cardboard production process (paper making process plus waste disposal involved), another cause is NO_x gas evolved from basepaper making.

It is worth mentioning that the renewable electric and thermal energy generated from the CHP system [10] during basepaper making offered 'negative' values to all impact categories via avoided grid electricity and fossil fuel based heat production. However, it was not sufficient to offset the burdens caused by corrugated board product system. In summary, the production (including transport and energy required) of raw materials is the main contributor to the environmental burden of the WBF foam insulation in most impact categories except GWP, where the WBF conversion process dominates. The primary causes for the environmental burdens of WBF in most impact categories were wheat grain farming and PVOH production. Another component of coolbox i.e. corrugated board delivered significant environmental burdens, which was driven by energy required, waste treatment, involved additives e.g. starch input as well as emissions from either fuel combustion or cardboard/base paper making processes. Infrastructure appeared as an important contributor particularly to toxicity impacts.

4.4.3.2 Comparison of WBF and LDPE Insulated Coolbox Production Stage

The characterised LCIA profiles of cradle-to-manufacturer-gate LDPE and WBF insulated coolboxes are compared in Fig. 4.11, where transportation represent the delivery of converted foam and cardboard box to coolbox manufacturer for further assembly process. It was shown that the LDPE coolbox incurred a higher environmental burden than the WBF coolbox in most impact categories except eutrophication and fresh water aquatic eco-toxicity. For these two systems the modelled corrugated board input was the same, indicating that the WBF delivers a much lower contribution to environmental impacts of the coolbox on most of the impact categories than in the case of the 'conventional' coolbox using LDPE foam insulation.

Contribution analysis indicated that the LDPE foam production (including LDPE production and transformation of LDPE into foam) was the dominant factor, accounting for around 50 % of impacts on eutrophication and fresh water ecotoxicity, 70–99 % of burdens on the rest of impact categories. Actually, the transformation process rather than LDPE production drove the LDPE foam profiles

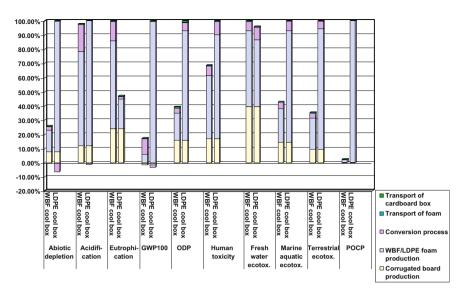


Fig. 4.11 Characterised LCIA profiles for production phase of WBF and LDPE (unit: per coolbox)

on most impact categories where energy consumed during transformation including electricity, natural gas and heavy fuel oil were the main causes. But on POCP, pentane emitted from the transformation process dominated the POCP profiles. LDPE production only shared 25-55 % of impacts on GWP100, acidification, eutrophication and abiotic depletion whereas on the remaining impact categories, its contribution was insignificant. Generally, the LDPE conversion process only incurred less than 10 % of environmental burdens of coolbox and moreover produced beneficial effects on abiotic depletion, GWP100, acidification and POCP. These environmental savings were brought about by the recycling LDPE residue during conversion where recycled LDPE was assumed as a substitution for virgin petrochemical LDPE. The positive burdens of the conversion process were mainly induced by the electricity and transportation inputs, whereas the infrastructure modelled was another important contributor to impacts on toxicity impact categories. As discussed in the study scope (Sect. 2.1.2.2), some transportation processes involved in LDPE production were omitted from the system boundary and their inclusion would increase the environmental burden of the LDPE coolbox system.

4.4.3.3 Distribution of Coolbox

The effect of adding coolbox distribution scenarios (local 23 km and long distance 903 km) to the LCIA profile of the whole coolbox production stage is presented in Fig. 4.12. Local distribution had a negligible effect on the overall impact and

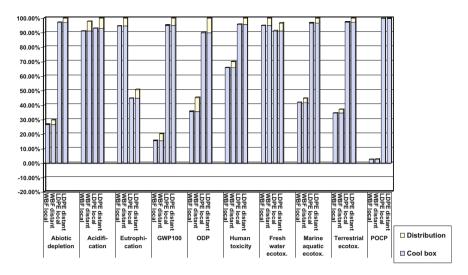


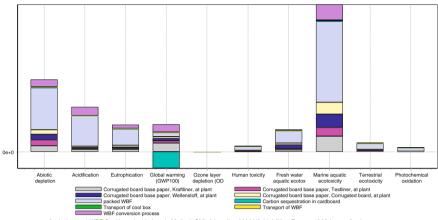
Fig. 4.12 Characterised LCIA profiles for distribution phase of WBF and LDPE coolbox (unit: per coolbox)

long-distance distribution increases the environmental burden by between 5 and 25 % dependent upon the specific impact category. The inclusion of the distribution step does not change the relative comparison between WBF and LDPE coolboxes. In both local and long-distance delivery cases, the environmental profiles of WBF coolbox are still better than LDPE coolbox in almost all impact categories except eutrophication and fresh water eco-toxicity.

4.4.3.4 Normalization of WBF/LDPE Coolbox

Normalized LCIA results are given in Figs. 4.13 and 4.14, which indicates a shift in significance of the impact category results. Indicator results for marine aquatic eco-toxicity are relatively most significant for both LDPE and WBF coolboxes. Irrespective of marine toxic profile, the impacts on abiotic depletion appear as relatively significant for the LDPE coolbox, followed by POCP, GWP, and acidification; in the case of WBF coolbox, the relative significance of impact category results ranked as abiotic depletion, acidification, eutrophication, followed by fresh water eco-toxicity and GWP100. ODP impacts appear to be of little significance for both coolbox systems. As indicated in Fig. 4.14, the environmental advantage of the WBF-insulated coolbox to the conventional LDPE coolbox is shown as relatively significant; whereas the superior eutrophication profile of LDPE foam to WBF insulation appeared as insignificant.

Analysing normalised LCIA profiles for WBF coolbox, WBF production appeared to be relatively important as a source of abiotic depletion, toxicity, acidification and eutrophication due to emission/leaching from the agricultural system, energy demanded for PVOH production, electricity as well as infrastructure



Analysing 1 p '-WBF Cool box -double layer'; Method: CML 2 baseline 2000 V2.04 / West Europe, 1995 / normalisation

Fig. 4.13 Normalised LCIA results for production phase of WBF coolbox (unit: per coolbox)

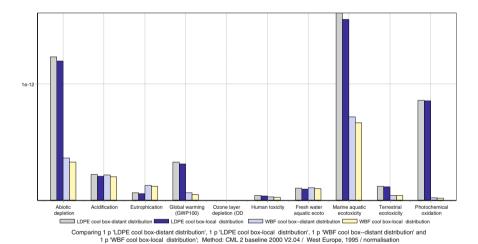


Fig. 4.14 Normalised LCIA results for distribution phase of WBF/LDPE coolbox (unit: per coolbox)

material involved in WBF manufacturing. The cardboard component was also significant as a source of abiotic depletion, GWP100, and marine eco-toxicity, which was caused by the energy and infrastructures concerned in basepaper/corrugated board production as well as the $\rm CO_2$ emitted during paper making process. These relatively significant contributors indicated the major options for improvement of the WBF coolbox. However, these normalised LCIA profiles only gave indicative information on the relative contribution of the coolbox to environmental problems at a specific temporal and spatial scale; other reference systems could bring different outcomes.

4.4.4 Display Board Case Study

4.4.4.1 Characterised LCIA Results for WBF/HDPE Display Board

The characterisation profiles for the production (cradle-to-gate) of 1 kg WBF/ HDPE material and WBF/HDPE display board are given in Figs. 4.15 and 4.16. Petroleum-based HDPE with 20 % recycled content showed better performance than WBF in five impact categories i.e. acidification, eutrophication, ODP, marine and terrestrial eco-toxicity, whereas on the remaining impact categories, WBF appeared environmentally superior to HDPE polymer. Compared with the environmental profiles of per kg polymers, inclusion of display board production stage reversed the results in acidification, ODP, terrestrial eco-toxicity, where the WBF display board delivered less impact than conventional display board due to the lighter weight assumed for WBF display board. It is also indicated in Fig. 4.16 that the residue recycling during HDPE display board production brought beneficial effects on most impact categories due to the avoidance of virgin HDPE making assumed. However, electricity required and residue disposal involved in the recycling process (fate of residue: 80 % landfill, 20 % incineration) brought extra eco-toxic impacts, which included the environmental burdens on marine aquatic and terrestrial systems, mainly caused by vanadium ion emission during HDPE landfill and chromium soil emission during electricity transmission, respectively.

The inclusion of distribution phase (Fig. 4.17) brings insignificant changes to the comparison results between WBF and HDPE display board. But the transportation distance assumed here represents a local delivery; a case study on long-distance delivery might reverse the outcomes on eutrophication and terrestrial eco-toxicity impact categories due to the advantages of WBF over HDPE in terms of weight.

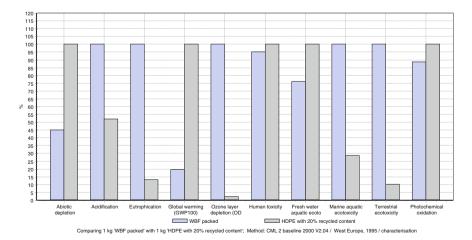


Fig. 4.15 Characterised LCIA profiles for WBF/HDPE (unit: per kg polymer)

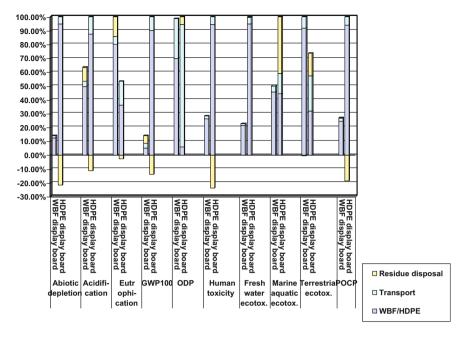


Fig. 4.16 Characterised LCIA profiles for production of WBF/HDPE display board (unit: per display board)

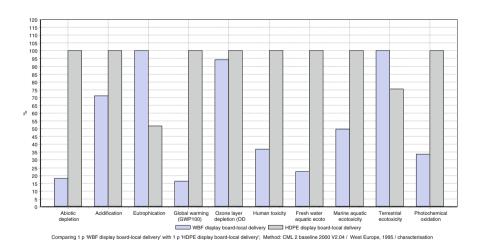


Fig. 4.17 Characterised LCIA profiles for distribution phase of WBF/HDPE display board (unit: per display board)

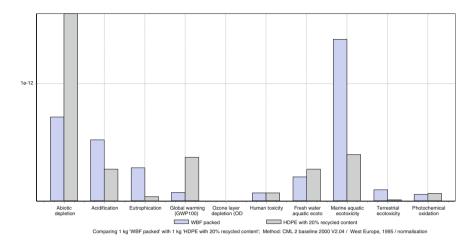


Fig. 4.18 Normalised LCIA profiles for WBF/HDPE (unit: per kg polymer)

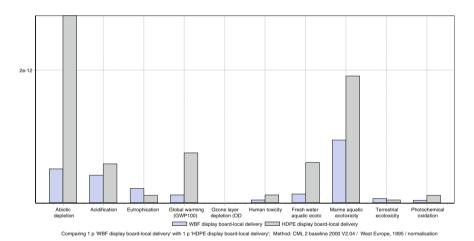


Fig. 4.19 Normalised LCIA profiles for distribution phase of WBF/HDPE display board (unit: per display board)

4.4.4.2 Normalised LCIA Results for WBF/HDPE Display Board

Normalised LCIA results for production of 1 kg polymer and WBF/LDPE display board at distribution stage are illustrated in Figs. 4.18 and 4.19, respectively.

For HDPE, the magnitude of the abiotic depletion indicator results was carried through from polymer system to final product (display board), appearing as most significant for the given region (West Europe). However, the inclusion of display board production and distribution phase caused a shift in significance of some impact category results, marine eco-toxicity shifted to second place, whereas GWP moved to third place. This marine toxic impact was mainly led by both HDPE

polymer production and HDPE landfill involved in residue disposal during display board production.

Different from HDPE, the inclusion of further processing WBF polymer and distribution of display board did not lead to change in the rank of indicator results. The magnitude of the category indicator results were similar to WBF insulated coolbox (Sect. 4.4.3.4): impacts on marine eco-toxicity are shown as relatively most significant for both WBF polymer and WBF display board, which was mainly driven by manufacturing N fertilizer, crude oil and diesel production, as well as the infrastructure materials involved in WBF product system.

At distribution phase, the environmental advantages of WBF over HDPE display board appeared relatively significant, but its disadvantages on eutrophication and terrestrial eco-toxicity are shown as negligible. However, the normalised comparison results only gave relative information to a selected reference system (West Europe 1995).

4.4.5 Case Studies on Trough Mould and Concrete Formwork

To compare WBF with different EPS grades, five trough mould case studies and two concrete formworks are given as examples. The characterised LCIA results for converted EPS/WBF as well as their products at production and distribution phase are shown in Figs. 4.20, 4.21, 4.22, 4.23 and 4.24.

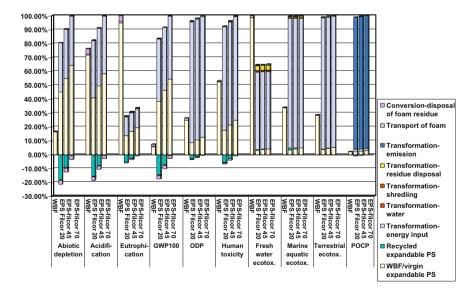


Fig. 4.20 Characterised LCIA profiles for converted WBF/EPS (unit: per kg)

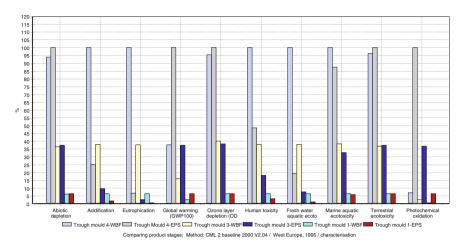


Fig. 4.21 Characterised LCIA profiles for distribution of WBF/EPS (Filcor 20°) trough mould (unit: per trough mould)

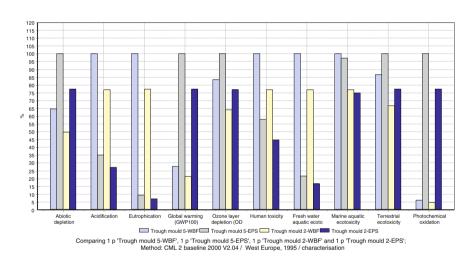


Fig. 4.22 Characterised LCIA profiles for distribution of WBF/EPS (Filcor $45^{\$}$) trough mould (unit: per trough mould)

4.4.5.1 Characterised LCIA Profiles for Converted WBF/EPS

As illustrated in Fig. 4.20, for the converted EPS/WBF products with the same weight (1 kg), WBF delivered the better environmental performance in comparison with different grade EPS (Filcor 20, 45, 70) in almost all impact categories, except acidification, eutrophication and fresh water aquatic eco-toxicity, where the contributors were wheat agricultural system (NH₃ emission and N/P leaching) and the infrastructure involved in WBF production respectively. WBF foam production

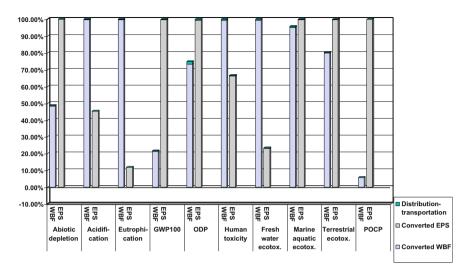


Fig. 4.23 Characterised LCIA profiles for distribution of WBF/EPS refractory lining (unit: per refractory lining)

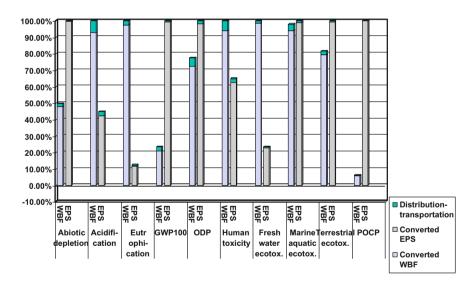


Fig. 4.24 Characterised LCIA profiles for distribution of WBF/EPS formwork for Doha Villa (unit: per formwork)

was shown as the dominant factor driving environmental profiles, whereas the impacts caused by transportation (from foam supplier to conversion company) were negligible; the residue disposal (home composting) only shared a minor contribution to the impacts on acidification, eutrophication, and GWP100, which was attributable to the gas emission (CO₂, CH₄ and NH₃) estimated in the home composting model.

In the case of converted EPS, residue produced during conversion process was recycled, which brought beneficial effects by avoiding virgin expandable PS production. Recycled EPS content in Filcor 20, 45 was another factor leading to environmental 'savings', which were the major cause for the difference in environmental profiles of various EPS grades. In addition to expandable PS production, transformation process was another main contributor to environmental burdens, especially on ODP, human toxicity and eco-toxicity as well as POCP where 80–95 % of impacts were incurred by transformation. EPS transformation was shown as an energy demanding process; apart from electricity, heavy fuel oil and natural gas inputs led to high ODP and toxic impacts due to emissions from their production, transportation and combustion, e.g. atmospheric emission vanadium, nickel from heavy fuel oil burning, CBrClF₂ from natural gas transportation, PAH released during natural gas burning. Besides, pentane release owing to the use of pentane as blowing agent during transformation was another factor bringing environmental problems, which dominated the POCP impacts.

4.4.5.2 Characterised LCIA Profiles for WBF/EPS Trough Mould

As discussed in Sect. 4.3.5, according to equations discovered by Brunel university [24] the density of WBF was estimated as 50, and 60 kg/m³ to deliver equivalent compressive characteristics as EPS grade (Filcor 20 and 45) containing 30 and 15 % recycled content, respectively. Case studies are given in Figs. 4.21 and 4.22 to compare Filcor 20, 45 with the corresponding WBF concept trough moulds at the distribution stage, respectively. Via contribution analysis, it was found that the transportation process involved in the distribution phase only made a minor contribution to overall environmental profiles of both WBF and EPS trough mould (less than 2 %), the manufacturing stage was the primary cause.

In contrast with Fig. 4.20, comparison results on acidification, human toxicity, and marine eco-toxicity presented in Figs. 4.21 and 4.22 reverse due to the different density of WBF and EPS modelled. On these three impact categories, trough moulds made of either Filcor 20 or 45 delivered better performance than WBF concept products. In addition, another potential factor influencing the comparison results was EPS grades. Owing to the high recycled content in Filcor 20, WBF only showed marginal advantages to Filcor 20 trough moulds (see Fig. 4.21) on terrestrial eco-toxicity, abiotic depletion, and ODP; whilst WBF represented a significant 'savings' on these impact categories than trough mould manufactured with Filcor 45. In general, the advantages of WBF trough mould over conventional products were carried through from manufacturing to distribution phase on five impact categories (GWP, POCP, abiotic depletion, ODP, and terrestrial ecotoxicity); especially on both GWP100 and POCP, the WBF were environmentally superior to EPS products, which were caused by the GHGs from expandable PS production and fuel combustion during EPS transformation, as well as the pentane emitted from transformation process. The similarity between two outcomes (Figs. 4.21 and 4.22) indicated that in the cases of trough moulds, the recycling content in EPS is not a significant factor driving the LCIA comparison between EPS and WBF.

4.4.5.3 Characterised LCIA Profiles for WBF/EPS Concrete Formwork

Different from trough mould, EPS foams modelled as formwork to construct simple or complex geometric structures are derived from virgin material. Here, as shown in Figs. 4.23 and 4.24, a refractory lining and the formwork for Doha Villa were modelled to compare virgin EPS (Filcor 70[®]) and corresponding WBF with an estimated density of 70 kg/m³.

In contrast with Fig. 4.20, only comparison results on acidification and human toxicity shown in Figs. 4.23 and 4.24 reversed due to the greater density estimated for WBF than EPS grade Filcor 70. WBF formwork still showed better environmental performance in most impact categories than conventional EPS products, especially on abiotic depletion, GWP100, and POCP, WBF brought remarkable benefits. It was attributed to two fuel-demanding EPS processes i.e. expandable PS production and transformation: pentane emission and high fuel consumption drove impacts on POCP and abiotic depletion respectively, whereas the GHGs released from expandable PS making and fuel combustion during transformation led to high GWP100 burdens. Although transportations involved in the distribution stage were shown as minor contributors to environmental profiles of both formworks cases, distance could become a critical factor increasing environmental scores substantially. As shown in the case of Doha Villa, the contribution of transportation was of more significance than refractory lining which was caused by the longer distribution distance assumed.

Analysing all the case studies on construction products, it was found that the EPS recycling content and the foam density were factors influencing the comparison profiles between WBF with conventional EPS products. As analyzed in Sect. 4.4.5.1, in comparison with the EPS with recycled content, virgin EPS brought higher resource depletion and ODP GWP100 burdens, which are presented in Figs. 4.23 and 4.24 as a greater advantage of WBF products over Filcor 70 than comparison results given in Figs. 4.23 and 4.24. Interestingly, on marine eco-toxicity, WBF showed a slightly better score than Filcor 70 whereas other EPS grades were environmentally superior to WBF. This trend was different from results revealed in Fig. 4.20 where different EPS grades with identical weight incurred similar marine co-toxic impacts. This could be explained by the difference in density of EPS grades. Generally all case studies indicated that WBF offers promising products, bringing better environmental performance than conventional construction products made of different EPS grades on abiotic depletion, GWP100, ODP, terrestrial eco-toxicity and POCP; regarding the remaining impact categories, they are dependent on the EPS grade and assumptions made for WBF concept

products. However, only comparisons of WBF with three EPS grades were investigated; case studies on other EPS grades, e.g. dense EPS with higher compressive strength or EPS with high recycled content could change the outcomes revealed so far.

4.4.5.4 Normalised LCIA Results for WBF/EPS Construction Products

The normalised results for 1 kg converted WBF and EPS products are given in Fig. 4.25. Increase in recycling content of EPS grade caused a shift in the significance of impact category results: with the beneficial effects brought by resource 'saving', abiotic depletion moving from first place to third place. However, for three EPS grades, the impacts on either abiotic depletion or marine eco-toxicity appeared as the most significant, which were mainly due to fuel consumed for EPS foam production as well as the emissions from fuel production and combustion (vanadium atmospheric emission from heavy fuel burning, barite to water body during well drilling for gas production). Besides, POCP indicator result was also of significance for EPS, followed by GWP100, and acidification; whereas the impacts on the remaining categories were shown as relatively negligible.

As indicated in Fig. 4.25, generally the contribution of 1 kg WBF to the environmental problems for the given region (West Europe) appeared as less significant in comparison with 1 kg EPS. In addition, the same magnitudes of categories indicator results were carried through from the WBF production stage: marine eco-toxic impact is shown as relatively most significant for both WBF foam and WBF concept construction products at production phase.

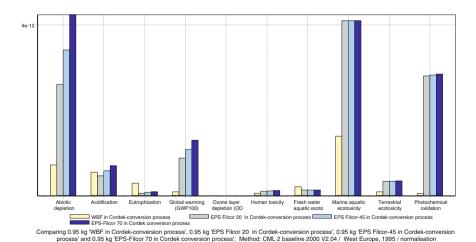


Fig. 4.25 Normalized LCIA profiles for converted WBF and EPS (unit: per kg)

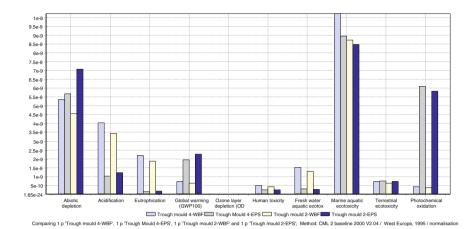


Fig. 4.26 Normalised LCIA profiles for distribution of WBF/EPS trough mould (unit: per trough mould). *Notes* case study 4 Filcor 20, case study 2 Filcor 45

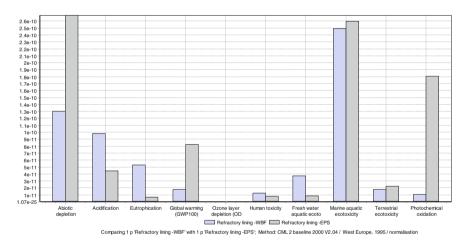


Fig. 4.27 Normalised LCIA profiles for distribution of WBF/EPS refractory lining (unit: per refractory lining)

The comparison of concept WBF and conventional EPS construction products was not based on the weight but on the functional unit defined in the study scope. Their normalized results are presented in Figs. 4.26 and 4.27, where trough mould case study 2 and 4 and refractory lining are given as examples to illustrate the comparison of WBF with lower EPS grade (containing recycled material) and with virgin EPS respectively. Compared with Figs. 4.25, 4.26 and 4.27 indicated that the consideration of product function and inclusion of distribution stage did not shift the rank of category indicator results for individual foam but induced the change in significance of comparison results between WBF and EPS; especially on

abiotic resource, with the increase in EPS recycling content, advantages of WBF over EPS appeared relatively more significant. Besides, another sensitive factor was EPS density modelled which caused a relatively significant shift in marine eco-toxic results: WBF was environmentally inferior to low-density EPS grade (Filcor 20, 45) but superior to dense virgin EPS.

Generally marine eco-toxic impacts and abiotic depletion indicator results were of relative significance for all the WBF and EPS construction products modelled. These normalised comparison results offered good insights in the relative contributions of EPS and WBF construction products to environmental problems in the reference region (West Europe) for the given year (1995).

4.4.6 Comparison of WBF and PSBF/MSBF

Besides WBF, other two biopolymer produced by Greenlight Product Ltd were also investigated including MSBF and PSBF, both of which are starch based but derived from different renewable resources. This section presents the comparison of WBF and two PSBF/MSBF products at both production and distribution phases.

4.4.6.1 Comparison of WBF and PSBF/MSBF at Production Stage

The productions of WBF and PSBF/MSBF are compared in Fig. 4.28. WBF delivers best environmental performance in most of impact categories except acidification, GWP100 and POCP, where NH₃ emission from wheat farming (contributed to acidification) and high PVOH input (contributes to GWP and POCP) induced WBF with higher burdens than alternative starch-based foam. In POCP, both MSBF and WBF scored slightly better than PSBF, whereas in abiotic depletion, ODP, GWP100, eutrophication and all eco-toxicity impact categories, MSBF incurred higher impacts than the other two products, mainly due to emissions from maize farming (e.g. soil emission metolachlor resulted from pesticide application, higher NO₃⁻ emissions) and the intensive energy inputs to maize starch production (higher natural gas/electricity consumption than potato starch).

Contribution analysis in Fig. 4.29 illustrated the beneficial effects brought by CO₂ sequestration in GWP100 were not sufficient to offset the GWP burdens caused by feedstock making (PVOH, starch or flour) and foam manufacturing processes. Generally, the main contributors for foams were PVOH and starch/flour; the contribution of other trace components i.e. soy oil, talc and soy flour were marginal. Wheat flour appeared to be environmentally superior to pure starch, which could be partially explained by the relatively less energy and resource demanding processing of wheat to flour for WBF rather than the extra processing to derive more purified starch from potato and maize. However, this was considered as a tentative indication at present time due to the use of database information for the alternative starches rather than the primary data used for the

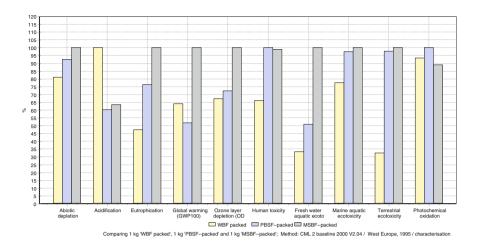


Fig. 4.28 Characterised LCIA profiles for WBF/PSBF/MSBF (unit: per kg packed foams)

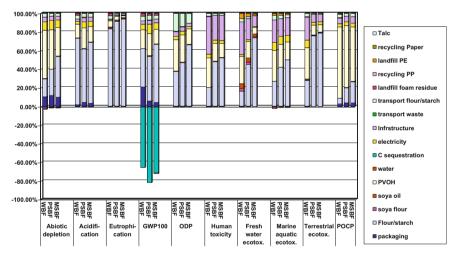


Fig. 4.29 Contribution analysis of WBF/PSBF/MSBF (unit: per kg packed foams)

wheat flour inventory. Besides, PVOH component incurred 20–50 % of impacts on most impact categories, except eutrophication and POCP. The former was driven by NO_3^- leaching and NH_3 flux in agricultural system, whereas, PVOH only shared 2–6 % of burdens; the latter were dominated by PVOH (60–76 %), which was attributed to the C_2H_4 , $C_2H_4O_2$, CH_3OH emissions during VAC and its feedstock productions.

Some similarities between WBF and PSBF/MSBF were found: the share of the foam making process (except infrastructure) which including energy consumption

transport or disposal involved, in total accounted for less than 20 % of overall environmental burdens; but the impacts caused by infrastructure on toxicity impact categories were not negligible, ranging between 10 and 40 %. However, the influence of infrastructure needs to be evaluated in sensitivity analysis. Actually the waste disposal during foam production brought some minor 'savings' by energy substitution or avoidance of paper/plastic making, these effects are shown in Fig. 4.29 as unnoticeable in comparison with the positive scores above line.

4.4.6.2 WBF and PSBF/MSBF Concept Products at Distribution Stage

As described in Sect. 4.3.5, PSBF/MSBF concept products were modelled, where they were assumed to deliver identical properties as WBF (e.g. thermal performance). As shown in Figs. 4.30, 4.31, 4.32, 4.33 and 4.34, five case studies are given as examples to illustrate the comparison of different biopolymer against equivalent petrochemical polymer (LDPE/HDPE/EPS) at the distribution stage.

The advantages of WBF over MSBF/PSBF were carried through from production to distribution phase where WBF only appeared as significantly environmental inferior to both MSBF and PSBF in acidification. On GWP100 and POCP, WBF incurred slightly higher impacts than one alternative starch foam; however, the differences in their environmental performance are negligible in comparison with the great advantage of biopolymer over petrochemical polymers.

Generally all the biopolymers delivered much better performance in comparison with LDPE and HDPE on most impact categories except ODP, eutrophication, fresh water and terrestrial eco-toxicity. But in the case of construction products, only on GWP100 and POCP three biopolymers were environmentally superior to

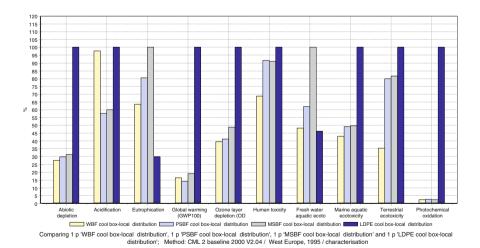


Fig. 4.30 Characterised LCIA profiles for local distribution of WBF/MSBF/PSBF coolbox (unit: per coolbox)

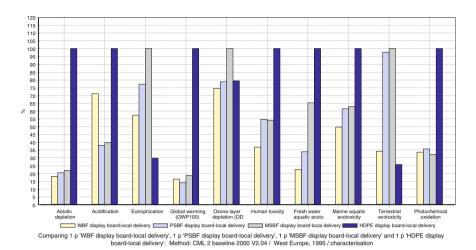


Fig. 4.31 Characterised LCIA profiles for distribution of WBF/MSBF/PSBF display board (unit: per display board)

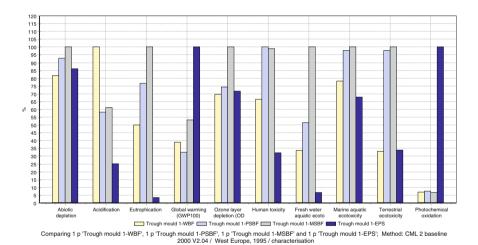


Fig. 4.32 Characterised LCIA profiles for distribution of WBF/MSBF/PSBF trough mould-1 (unit: per trough mould)

all EPS grades; whereas the comparisons of biopolymer and EPS on other impact categories were dependant on the biopolymer feedstock and EPS recycling content. For instance, EPS products led to higher ODP and terrestrial ecotoxic impacts than WBF but not other biopolymers derived from maize or potato starch; on abiotic depletion, advantages of biopolymers over EPS declined with increase in EPS recycling content due to the beneficial effects by avoiding virgin expandable PS production.

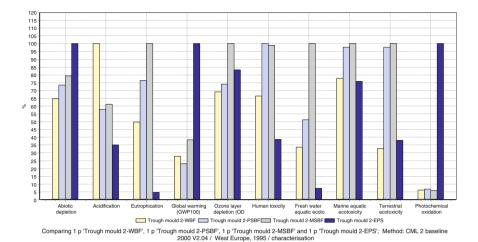


Fig. 4.33 Characterised LCIA profiles for distribution of WBF/MSBF/PSBF trough mould-2 (unit: per trough mould)

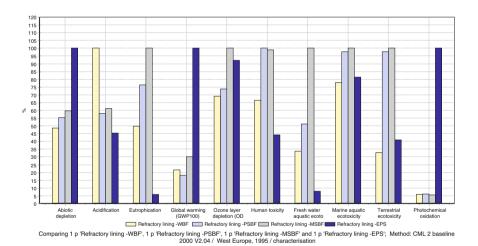


Fig. 4.34 Characterised LCIA profiles for distribution of WBF/MSBF/PSBF refractory lining (unit: per refractory lining)

4.5 Sensitivity Analysis

The sensitivity analyses were conducted to analyse the influences of scenarios and key parameters on indicator results, which include the C/N dynamic modelling approach, PVOH model, and infrastructures etc. The thresholds defined in Sect. 2.3.1, i.e. 10 % change in LCIA results for one product system or change in comparison ranking were used as sensitivity criteria. Mainly five case studies are

given as examples to represent the applications of WBF as thermal insulation packaging, display board, and construction products in comparison with PE (LDPE/HDPE) and various EPS grades. The outcomes from other void-formers and concrete formworks are not shown here as they gave similar results to the trough moulds and refractory lining illustrated below.

4.5.1 Sensitivity Test on N₂O Modelling Approach

As indicated in Sect. 3.6.1, the GWP100 profiles of wheat grain were sensitive to the choice of model and boundary defined. The sensitivity analysis was also carried out on polymer production and final application levels; here the sensitivity of comparison results between WBF and petrochemical polymers to modelling approaches are presented.

As discussed in Chap. 3, IPCC gave higher estimation of N_2O field emission than DNDC modelling approach; by using IPCC method approximately 77 % of total N_2O flux was estimated as direct emission, the rest N_2O released via the indirect pathway was either caused by leaching or atmospheric deposition. The GWP100 profiles of WBF derived from six fields by using different modelling approach are compared in Figs. 4.35, 4.36, 4.37, 4.38 and 4.39, where coolbox, construction products and display board are given as examples.

Generally across six fields, 1.5-3.5 % of GWP100 indicator results for WBF products were attributable to DNDC simulated N_2O whereas IPCC-estimated N_2O emission shared higher GWP burdens (5–14 %). In addition, GWP100 profiles for WBF construction products were more sensitive to N_2O modelling approach than WBF coolbox or display board case studies, which could be explained by the

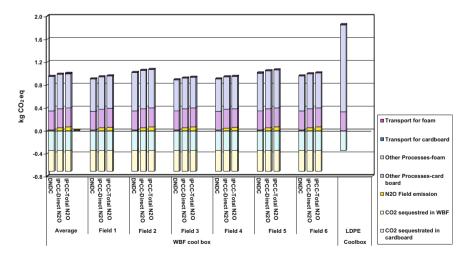


Fig. 4.35 Comparison of DNDC and IPCC modelling approach -characterised GWP100 profiles for production of coolbox (unit: per coolbox)

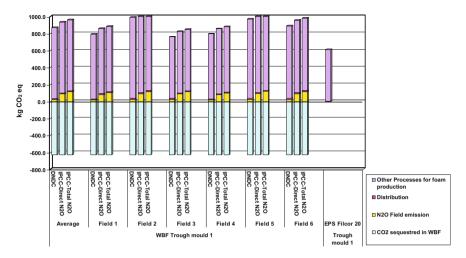


Fig. 4.36 Comparison of DNDC and IPCC modelling approach-characterised GWP100 profiles for distribution of trough mould-1 (unit: per trough mould)

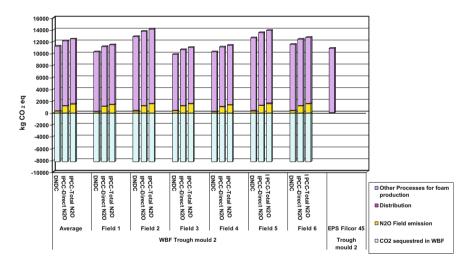


Fig. 4.37 Comparison of DNDC and IPCC modelling approach-characterised GWP100 profiles for distribution of trough mould case 2 (unit: per trough mould)

different density of WBF assumed. In the case of trough mould and refractory lining where WBF with greater density was modelled, IPCC simulated N_2O brought approximately 25–70 % increase in GWP100 score compared with DNDC approach, but IPCC estimated N_2O only increased GWP100 burdens of coolbox or display board by 15–25 %.

In addition, across all case studies, GWP100 scores varied between fields. Regardless of modelling approach, generally WBF products derived from Fields 1,

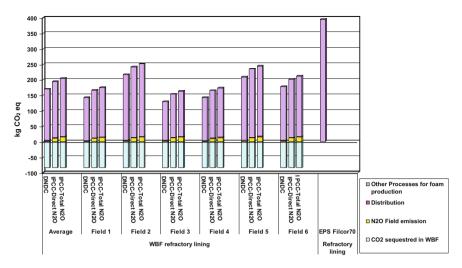


Fig. 4.38 Comparison of DNDC and IPCC modelling approach—characterised GWP100 profiles for distribution of refractory lining (unit: per refractory lining)

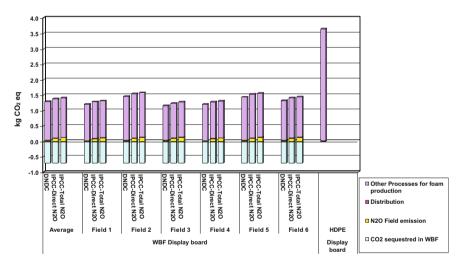


Fig. 4.39 Comparison of DNDC and IPCC modelling approach—characterised GWP100 profiles for distribution of display board (unit: per display board)

3 and 4 represented the best cases, showing GWP100 burdens below average; whereas the other three fields was environmentally inferior to average WBF products. It indicated that the comparison between six fields were not sensitive to N_2O estimation but driven by other factors such as C field emissions. Although the GWP100 burdens of WBF products varied with fields and modelling approaches, these factors did not produce significant effects on the comparison between

polymers: as illustrated in Figs. 4.35, 4.36, 4.37, 4.38 and 4.39, overall GWP100 scores of all WBF scenarios are superior to their equivalent petrochemical products (EPS/LDPE/HDPE) due to the benefit from C sequestration in WBF.

Therefore, different modelling approaches (system boundary) is a sensitive parameter for GWP100 scores of WBF products, especially those applied in the construction sector; but it is not a critical factor for comparison profiles of WBF with equivalent petrochemical polymer in the cases studied, nor the sensitive parameter for comparison between the 6 fields.

4.5.2 Sensitivity Analysis on PVOH Model

A theoretical model for PVOH production was developed to fill in the data gap. However, a great uncertainty was introduced to the PVOH dataset by using literature data and expert estimations. Based on the data range given in Table 4.4, two scenarios (best and worst cases) for PVOH production were established; sensitivity analyses were carried out on five case studies (Figs. 4.40, 4.41, 4.42, 4.43 and 4.44) to test the influence of PVOH scenarios on the LCIA results of WBF and its comparison with petrochemical polymers at the distribution stage.

Generally, the LCIA profiles of WBF on acidification and eutrophication appeared as less sensitive to PVOH scenario than other indicator results, with the change in environmental score below the threshold 10 %; it was due to the fact that driving factor of acidification/eutrophication impacts was wheat flour whereas PVOH was shown as an insignificant contributor.

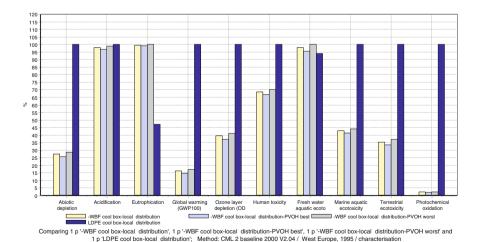


Fig. 4.40 Sensitivity analysis on PVOH model-characterised LCIA profiles for local distribution of coolbox (unit: per Coolbox)

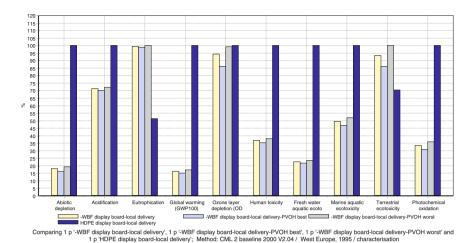


Fig. 4.41 Sensitivity analysis on PVOH model-characterised LCIA profiles for distribution of display board (unit: per display board)

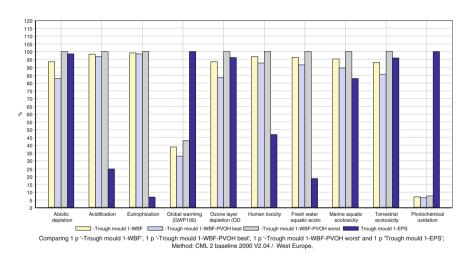


Fig. 4.42 Sensitivity analysis on PVOH model-characterised LCIA profiles for distribution of trough mould-1 (unit: per trough mould)

As given in Figs. 4.40 and 4.41, PVOH scenarios did not play an important role in the comparison between PE (LDPE and HDPE) and WBF applied in the specific coolbox insulation or display board case studies: with either best or worst scenarios for PVOH, WBF always delivered better environmental performance than LDPE/HDPE on most impact categories.

In addition, three EPS grades with various recycling contents were also concerned in sensitivity tests. Figures 4.42, 4.43 and 4.44 present the comparison

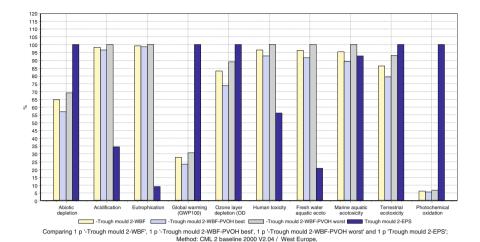


Fig. 4.43 Sensitivity analysis on PVOH model-characterised LCIA profiles for distribution of trough mould-2 (unit: per trough mould)

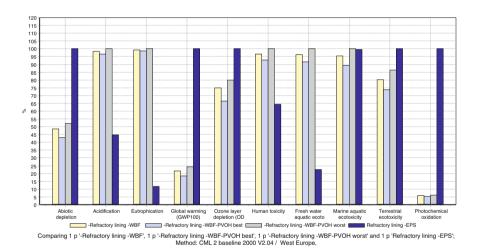


Fig. 4.44 Sensitivity analysis on PVOH model-characterised LCIA profiles for distribution of refractory lining (unit: per refractory lining)

between WBF and Filcor 20, 45 and 70, respectively; it is indicated that on most impact categories PVOH is not a sensitive factor in terms of LCIA comparison results, however, on abiotic depletion, marine and terrestrial eco-toxicity PVOH scenario could lead to slightly different findings. WBF with PVOH worst scenario represented a marginally higher resource consumer than Filcor 20 whereas the other two WBF scenarios appeared as environmentally superior to corresponding EPS products on abiotic depletion; besides, PVOH worst scenario reversed the

comparison results between WBF and Filcor 20 on terrestrial eco-toxicity; as for another eco-toxicity impact category (marine), WBF with best PVOH scenario showed a better score in contrast with filcor 45 and 70, whilst the PVOH worst scenario brought WBF with higher or equivalent marine eco-toxic impacts to corresponding EPS.

Construction applications were more sensitive to PVOH scenarios than other case studies investigated; but overall PVOH model was concluded as a parameter producing insignificant effects on LCIA comparison profiles between WBF and petrochemical polymers. However, this conclusion might change if other potential applications of WBF are considered.

4.5.3 Sensitivity Analysis on Infrastructures

Via the analysis presented in this chapter, infrastructure was indicated as an important contributor to environmental profiles of biopolymer, especially on toxicity impact categories (such as results shown in Figs. 4.7 and 4.29). However, the unit processes for infrastructures were based on a surrogate database derived from Ecoinvent V2.0 rather than the primary inventory due to the deficiencies in datasets. To test the effects of these infrastructure datasets on indicator results, sensitivity analyses were performed. As shown in Figs. 4.45, 4.46, 4.47, 4.48 and 4.49, environmental profiles of WBF products including and excluding infrastructure processes are compared; furthermore, the comparison results between WBF and petrochemical polymers are presented.

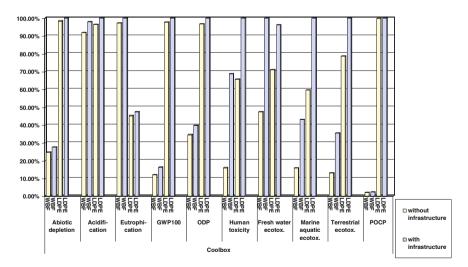


Fig. 4.45 Sensitivity analysis on infrastructure-characterised LCIA profiles for local distribution of coolbox (unit: per coolbox)

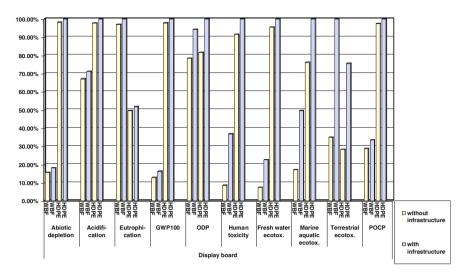


Fig. 4.46 Sensitivity analysis on infrastructure-characterised LCIA profiles for distribution of display board (unit: per display board)

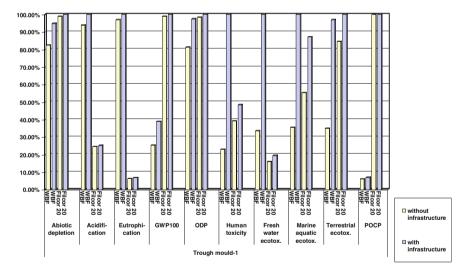


Fig. 4.47 Sensitivity analysis on infrastructure-characterised LCIA profiles for distribution of trough mould-1(unit: per trough mould)

Amongst all the category indicator results, human and eco-toxicity impacts appeared as most sensitivity to infrastructure processes. Excluding the infrastructures, toxic impacts of both bio- and petrochemical polymers decreased considerably, especially for WBF products where approximately 60–80 % decline

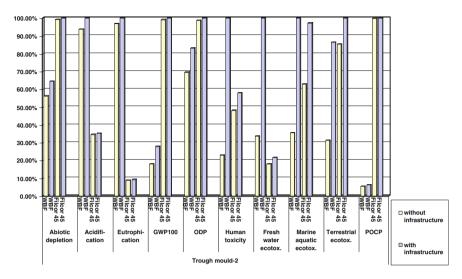


Fig. 4.48 Sensitivity analysis on infrastructure-characterised LCIA profiles for distribution of trough mould-2(unit: per trough mould)

was observed. Infrastructure was also a sensitive parameter for the WBF on abiotic depletion, GWP100, ODP and POCP, its exclusion causing decrease of impacts by 10–35 %; whereas infrastructure processes produced minor or insignificant influences on other impact categories. This was confirmed by the outcomes of contribution analysis that infrastructures were the dominant factor driving environmental profiles of WBF on toxicity impact categories and acted as an important contributor to toxic scores across all case studies.

Generally, the LCIA comparison between WBF products and equivalent petrochemical polymers at the distribution stage on most impact categories was not sensitive to infrastructure element, except toxicity scores. Exclusion of infrastructures brought WBF greater advantages over PE/EPS on toxicity, especially human toxicity and marine eco-toxicity, on which the comparison of WBF with low-grade EPS (Filcor 20, 45) was reversed by excluding infrastructures (Figs. 4.47, 4.48 and 4.49). This was due to greater influence of infrastructure on toxic profiles of WBF than PE/EPS.

Only three construction products are presented here as examples, similar results were also found in other trough moulds and concrete formworks. Via discussion above, it was indicated that the assumptions made or parameters applied regarding infrastructure could significantly influence the toxic impacts of WBF based products, but not the comparison between WBF and petrochemical polymers.

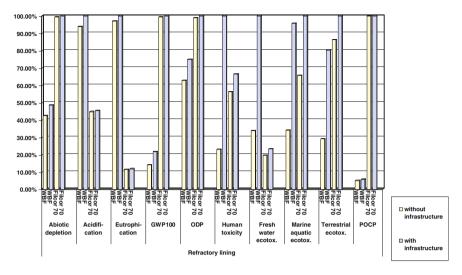


Fig. 4.49 Sensitivity analysis on infrastructure-characterised LCIA profiles for distribution of refractory lining (unit: per refractory lining)

4.5.4 Sensitivity Analysis on Conversion Process

As defined in product system (Sect. 2.1.2.2), due to the deficiency in datasets for display board and construction products, energy and infrastructure inputs to conversion processes were omitted. But in another case study coolbox conversion inventory was developed and included, which gave good indications: conversion process brought insignificant effects on comparison profiles of WBF and LDPE (Fig. 4.11). To test the sensitivity of LCIA profiles to these parameters in display board and construction product cases, identical energy and infrastructure inputs as coolbox were assumed for the process where WBF/HDPE/EPS block are converted to final products.

As illustrated in Figs. 4.50, 4.51, 4.52 and 4.53, generally the inclusion of conversion processes increased LCIA profiles by approx 3–20 %, except terrestrial toxic scores of HDPE and GWP100 scores of WBF construction products as well as the POCP impacts caused by EPS. The former two showed substantial increases (over 40 %), which meant the conversion process was a sensitivity parameter for HDPE and WBF in terms of terrestrial eco-toxicity and GWP respectively where the chromium emissions from electricity transmission and GHGs released from fuel combustion during conversion processes were main causes. On the contrary, no noticeable change was observed in the latter one, which indicated that conversion process was negligible in comparison with the driving factor (pentane emission) for POCP indicator results of EPS.

In terms of LCIA comparisons of WBF with petrochemical polymers, conversion scenario was presented as an insignificant parameter for display board, but an important factor for construction case studies, especially those comparisons

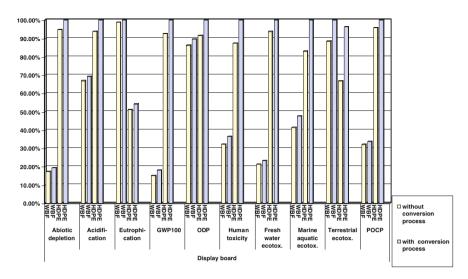


Fig. 4.50 Sensitivity analysis on conversion process-characterised LCIA profiles for distribution of display board (unit: per display board)

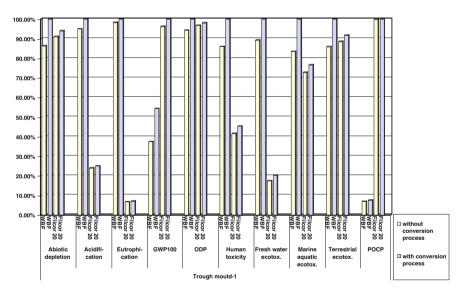


Fig. 4.51 Sensitivity analysis on conversion process-characterised LCIA profiles for distribution of trough mould-1 (unit: per trough mould)

showing marginal differences. Compared with low EPS grade (Fig. 4.51), WBF only had marginal advantages on abiotic depletion and terrestrial eco-toxicity, which was insufficient to offset the extra resource consumption and eco-toxic burdens brought by the conversion process (it brought higher burdens to WBF than

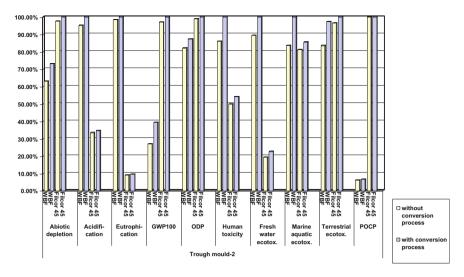


Fig. 4.52 Sensitivity analysis on conversion process-characterised LCIA profiles for distribution of trough mould-2 (unit: per trough mould)

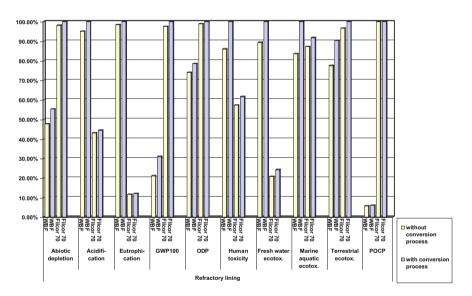


Fig. 4.53 Sensitivity analysis on conversion process-characterised LCIA profiles for distribution of refractory lining (unit: per refractory lining)

EPS due to the greater density of WBF). Similarly, although Filcor 70 was marginally inferior to WBF on marine eco-toxicity, the inclusion of conversion scenario reversed the comparison results due to the greater density modelled for WBF than EPS.

In summary, the conversion process not only influenced the indicator results of both WBF and petrochemical polymers, but also was shown as a sensitive parameter for comparison of WBF with EPS especially with low EPS grade. However, it should be borne in mind that the conversion scenario presented here was a surrogate dataset derived from manufacturers who convert polymer for insulation packaging; in the real case of either display board or construction products, the energy or infrastructure inputs might be considerably different from coolbox case study, which could lead to different findings.

4.5.5 Sensitivity Analysis on WBF Coolbox Scenario

As discussed in Sect. 4.3.5, not only WBF with double layers (26 mm) but also single-layer WBF (13 mm thickness) was verified by both laboratory test and commercial trial that they delivered better insulation performances than standard 20 mm LDPE liner [3, 15]. Thus the WBF insulation thickness was considered as a parameter, to which the sensitivities of LCIA profiles of WBF coolbox were examined. As indicated in Fig. 4.54, environmental scores were sensitive to the tested parameter, showing approx 25–45 % decline by reducing WBF insulation to a single layer. Generally, the decrease in insulation thickness drove WBF as significantly superior choice to LDPE insulation. Not only the advantages of WBF over LDPE were enhanced (e.g. acidification score) but also the disadvantages of WBF to LDPE were reversed (e.g. fresh water eco-toxic impacts). Therefore, WBF insulation thickness was considered as a sensitive parameter for coolbox case study.

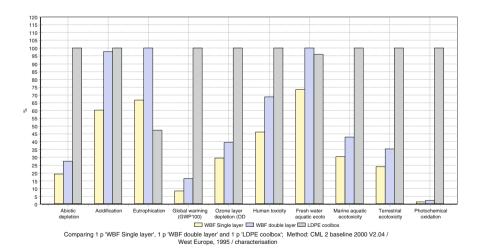


Fig. 4.54 Sensitivity analysis on WBF insulation scenario-characterised LCIA profiles for distribution of coolbox (unit: per coolbox)

4.6 Discussion 215

4.6 Discussion

In summary, the 'cradle-to-gate' LCA profiles of WBFs have been evaluated in multi case studies to address the basic question 'is there a general environmental advantage for WBFs over petroleum-based foam?' The case studies were conducted to compare the LCA performance of WBFs with conventional polymers (HDPE/LDPE/EPS) in various applications. In addition, comparison was also undertaken between WBF and two additional developments of biopolymers derived from potato and maize starches.

The key findings from this chapter were:

- Throughout 'cradle-to-gate' life cycle stages of WBF, the wheat agricultural system was the major contributor to the acidification and eutrophication burdens due to the NH₃ gas flux and N leaching. Farming system together with PVOH dominated GWP100 and ODP impacts whereas PVOH appeared as the main cause of abiotic depletion and POCP, which was attributable to the resource consumed during production of feedstocks for PVOH and gases evolved from VAC and its feedstock (C₂H₄, C₂H₄O₂) manufacturing. Apart from these two contributors, infrastructure was the driving factor for impacts of WBF on human and eco-toxicities. Other factors such as the packaging produced minor influences on environmental profile of WBF.
- The beneficial effects brought by CO₂ sequestration during wheat growth were carried through from wheat grain production to flour milling stage, inducing wheat flour with a negative GWP100 score. However, the C sequestration benefit was not sufficient to offset the burdens caused by PVOH component and CO₂ release from the wheat agro-ecosystem, which led to the WBF having a positive GWP100 burdens. Besides, the disposal of residue/waste packaging generated during WBF production (landfill of WBF residue and recycling of PE/PP packaging,) also brought benefits by avoidance of plastic making or energy substitution.
- As summarised in Table 4.16, at the production stage, generally WBF-based products scored better than or equal to conventional petrochemical polymers on four environmental impact categories—abiotic depletion, GWP100, POCP and ODP; but WBF appeared environmentally inferior to all conventional polymers on eutrophication due to the emission/leachate from the wheat agricultural system. The WBF alternative delivered higher terrestrial eco-toxic impacts than HDPE in the display board application but not in the other polymers. In the remaining impact categories, generally WBF showed better/equal environmental performance compared with PE (LDPE or HDPE) but incurred higher burdens than EPS. Actually WBF has the potential to offer even greater environmental advantages over LDPE as insulation for the coolbox due to the fact that WBF insulation with single layer was verified via commercial trial to deliver better performance than standard LDPE insulation. The reduction of WBF thickness from 26 to 13 mm led to a WBF coolbox with lower impacts than LDPE in all impact categories except eutrophication. Further LCA

	Production stage					
Impact category	Cool	Display	Trough	Trough	Concrete	
	Box	board	mould-	mould-	formwork	
	LDPE	HDPE	Filcor 20	Filcor 45	Filcor 70	
Abiotic depletion						
Acidification						
Eutrophication						
GWP100						
ODP						
Human toxicity						
Ecotoxicity Fresh water						
Ecotoxicity Marine						
Ecotoxicity Terrestrial						
POCP						

Table 4.16 Comparison of WBF with petrochemical polymers

Notes

- WBF lower impact than petrochemical polymer
- WBF higher impact than petrochemical polymer
- WBF similar impact to petrochemical polymer

outcomes showed that the inclusion of distribution stage only brought insignificant change in the LCIA profiles.

- Generally, similar magnitudes of category indicator results were carried through
 from WBF production into its distribution phases. Normalised LCIA profiles
 indicated that for WBF, the marine eco-toxic impacts were of most significance;
 in addition, the indicator results on the other five impact categories also
 appeared relatively significant, i.e. abiotic depletion, acidification, eutrophication, fresh water eco-toxicity and GWP100.
- WBF appeared to offer the lowest impact on most impact categories in comparison with alternative biopolymer derived from potato or maize starch (Table 4.17), but both PSBF and MSBF gave better acidification scores than WBF. The principal reasons for this were the relatively lesser energy demanding processing for wheat conversion to flour for the WBF than the extra processing to derive purified starch from potato and maize. The high NH₃ fluxes from wheat agricultural system simulated by the DNDC model were the main driving factor for the acidification score of WBF. However, only indicative information for the alternative starches was available at the present time due to the use of database information for rather than the primary data and process-oriented modelling approach used for the WBF inventory. Based on MSBF/PSBF product scenarios established (Table 4.17), both starch-derived bio-polymers

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	Production	Distribution (vs petrochemical)				
Impact category	PSBF/MSBF vs WBF	Cool- Box LDPE	Display board HDPE	Trough mould-1 Filcor 20	Trough mould-2 Filcor 45	Concrete formwork Filcor 70
Abiotic depletion						
Acidification						
Eutrophication						
GWP100						
ODP						
Human toxicity						
Ecotoxicity						

Table 4.17 Comparison of MSBF/PSBF with petrochemical polymers

POCP Notes

Fresh water
Ecotoxicity
Marine
Ecotoxicity
Terrestrial

 MSBF& PSBF lower impact than WBF; MSBF& PSBF lower impact than petrochemical polymer

 MSBF & PSBF higher impact than WBF; MSBF & PSBF higher impact than petrochemical polymer

MSBF or PSBF lower impact than WBF; MSBF or PSBF lower impact than petrochemical polymer

appeared as environmentally superior to petrochemicals in GWP100 and POCP but as inferior in many other impact categories. Especially in comparison with EPS, PSBF/MSBF did not present as promising biopolymers. However, this is only an approximation as these comparisons were based on the assumption that MSBF/PSBF would deliver the same properties as WBF. So far no laboratory research has been conducted to compare the performance of MSBF/PSBF with conventional polymers in various applications, thus more in-depth research could lead to different LCIA results.

• For the PVOH product system, VAC production appeared as the dominant contributor to the impacts on all impact categories. This study suggests that the contribution of PVOH was significant in energy consumption and ODP and POCP impacts; and this is in agreement with a previous study on maize starch-based loosefills [8] where a PVOH inventory derived from patent and German generic data was applied. However, their PVOH data was undisclosed and apart from this, no publically accessible PVOH datasets were found despite PVOH being a commonly used polymer [12]. In the present LCA model, uncertainty was introduced in PVOH inventory by the use of literature data and expert estimations due to the absence of validated datasets. Based on the theoretical PVOH model developed, the sensitivity of indicator results to the choice of PVOH production scenarios was analyzed. Across all the case studies examined,

the PVOH model was shown to be an insignificant parameter for the comparison of the LCIA results between WBF and LDPE/HDPE but was a sensitive factor for comparison of WBF with EPS. This conclusion was valid for the case studies examined and for a fossil based PVOH as modelled here. Actually, as reported by Flieger et al. [13], PVOH can be derived from renewable resources (e.g. bio-ethanol) which could benefit the environmental profile of WBF. Thus the inclusion of outcomes obtained so far could change by including other WBF applications or modelling bio-PVOH. In addition, further work towards a reliable LCA inventory for PVOH is recommended.

- In the LCA inventory, surrogate datasets were used to model the inclusion of
 infrastructure inputs and so were subject to sensitivity analysis. It was found that
 infrastructure was a critical parameter for LCIA profiles of WBF, especially
 toxicity impacts, but it was not a factor producing significant influence on the
 comparison between WBF and petrochemical polymers. However, these
 conclusions were generalized from limited case studies; it may not represent other
 applications.
- In system boundary definition, processes for conversion of polymers into display board or construction products were omitted due to missing data. Thus the identical inputs (energy infrastructure etc.) as the coolbox were applied as surrogate data in sensitivity analysis. It was found that the conversion process could be a sensitive factor for environmental profiles of WBF products as well as their comparison with low EPS grade. However, this only offered indicative information about the potential impacts of conversion processes. As in the display board and construction sector, the property of converted polymers is different from LDPE, thus the energy consumed as well as the infrastructure involved in LDPE insulation conversion might not be a good representative of HDPE or EPS.
- As discussed in Chap. 3, compared with IPCC approach, DNDC accounts for regional agro-eco-system difference and agriculture managements. Therefore, sensitivity analysis on N₂O modelling approaches is also to investigate the sensitivity of indicator results to the system boundary definition. The results indicated that modelling approach (system boundary) was a sensitive parameter for the GWP100 scores of WBF products but not for the comparison profiles between WBF and equivalent petrochemical polymers. Besides, the comparisons between WBF derived from six fields were not sensitive to system boundary definition and six fields gave consistent outcome: WBF is environmentally superior to HDPE/EPS/LDPE on GWP100 at production stage.
- Most of the results presented above were based on laboratory research except the coolbox case study, which was verified at both lab and commercial trial levels. Although WBF was indicated as a potential polymer delivering better environmental performance than petrochemical products, substitution of HDPE/ EPS by WBF in display board and construction sectors is still uncertain. To achieve the equivalent performance as petrochemical polymers, more in-depth research needs to be carried out on WBF, such as application of laminations on WBF. These uncertain factors may affect the environmental advantages of WBF relative to conventional polymers.

4.6 Discussion 219

4.6.1 Key Findings

The dominating contributors to cradle-to-gate environmental impacts of WBF were identified as: the wheat farming system (C and N gas fluxes and diesel consumption) and the production of feedstock for PVOH (resources consumption and gases evolved from VAC, C₂H₄ and C₂H₄O₂ manufacturing).

A case-by-case approach is necessary for comparison between WBF and petrochemical polymers. But a general 'cradle-to-gate' environmental advantage of WBF-based products over conventional petrochemical polymers was recognised for abiotic depletion, GWP100, POCP and ODP.

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Chapter 5 End-of-Life Scenarios

5.1 Introduction

To reduce the negative effects of landfilling of waste on both natural environment and human health, EU legislation has entered into force since 1999 to divert waste from landfill [24]. However, in UK waste treatment systems especially MSW disposal, landfill still dominates followed by recycling composting and energy recovery [13, 15].

Biological treatment options together with recycling and incineration provide diverse options for separate waste streams i.e. bio-degradable and non-biodegradable wastes [44]. AD, especially offers a unique technology which generates bio-energy and beneficial soil conditioner. Another newly developed technology is MBT which incorporates mechanical and biological treatments and supplements to other disposal routes [14]. However, compared with the progress in EU, AD and MBT technologies have undergone slow development in UK; there are only 2 AD plants and 7 MBT systems operating to treat MSW in UK, the MBT system and AD plant modelled in this study is represented as a good case study [14, 44].

Publicly available LCAs on waste treatment were reviewed. Generally the waste hierarchy was supported by previous LCAs i.e. recycling is environmentally preferable to incineration and further this was preferable to landfill [26, 9, 45, 58]. However, number of LCAs conducted to compare different waste treatment routes is rather small especially serious data gap was found for biological treatment. There is also a lack of transparency in most LCAs in terms of methodology and assumptions, which makes it difficult to compare their results [68, 11] and as pointed out by Cleary [11], only selective impact categories were concerned in most of published LCA studies.

In the current study product-specific waste streams and their components were assessed in some detail and particularly included biological waste treatments. In this way the present work goes beyond many of the previous studies and models which have focused largely on the MSW/BFMSW. Diverse end-of-life scenarios

were modelled in this study, especially an AD scenario which was built on the data developed from a UK commercial AD plant and on novel laboratory results obtained from lab-scale AD research.

5.2 Product System and System Boundaries

As shown earlier (Fig. 2.3), post-consumer WBF-based products were assumed to be disposed in various waste treatment routes, including AD, composting, landfill, recycling, and incineration. The systems studied and system boundaries for each end-of-life scenario are defined as below.

5.2.1 Anaerobic Digestion

In the current study, AD was modelled as an option for disposal of WBF-based products mainly due to the fact that AD is suggested as a potentially preferred diposal routes. The UK government encourages AD development to assist with achieving waste management and renewable energy targets. It is predicted that AD will become a more widely established technology in the UK by 2020 [16].

The AD system modelled was based on the case study developed in collaboration with the a UK commercial AD plant. This AD plant, as a part of a 25 year waste treatment project, mainly digests the biodegradable solid waste separated from mixed wastes in Ball Mill (MBT) located at a UK industrial estate [64]. The Ball Mill treats waste collected via local waste management system in total approx 110,830 t/year, the source-segregated waste includes 5 % metals, 35 % organic waste for AD treatment, 40 % RDF (for the cement industry), and 20 % residues which are sent to landfill [64, 57].

The MBT system involves a sorting step followed by ball milling and trommel sieves to reduce particle size and separate waste based on particle size into further separation streams in which a series of separation processes are employed such as magnetic and eddy current separation (to remove metal), hydro-pulpers/mix separators (to remove light and heavy fractions) and air classifier (to remove light material). The separated organic fraction with particle size less than 50 mm is transferred to enclosed containers and transported to the AD plant [64].

The UK commercial AD plant modelled is a wet (dry solid less than 15 %), continuous feeding multiple-stage digestion system operated at mesophilic temperature. As shown in Fig. 5.1, the AD process includes pre-treatment and two-stage digestion. In the first stage, mainly hydrolysis and acidification occur which can be coincident with some degree of acetogenesis. In the second stage, the methanogenesis process dominates with certain degree of acetogenesis. The whole AD plant is comprises of two hydrolysis tanks with a capacity of 400 m³ each and three digesters (capacity of each digester is 2,500 m³), and a gas tank with a total

capacity of 600 m³. The AD plant is operated for 24 h a day and 7 days per week and fed almost everyday (except for maintenance period). On average, approx 90 ton solid organic waste (with 51.7 % total solid) is processed per day.

As illustrated in Fig. 5.1, the waste entering AD plant is tipped into the reception hall then fed by conveyor into a mixing tank, where slurry is produced by addition of process water. Feedstock undergoes further pre-treatment: the sand and inert fines are separated from the feedstock and the solid content is controlled by dewatering process. The removed sand accounting for approx 20 % of raw waste delivered to AD plant ends up in landfill; another 35 % fraction of waste is separated as RDF, which potentially could be used as fuel, but is currently sent to landfill. However, these three by-products from AD process are only produced

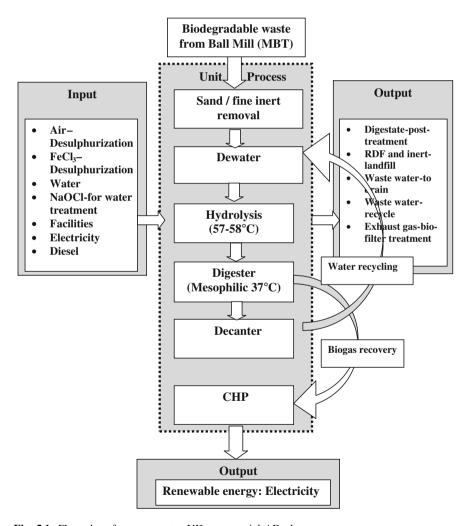


Fig. 5.1 Flow chart for process at a UK commercial AD plant

when the BFMSW is the feedstock, in the case of WBF/PSBF/MSBF, sand RDF and inert are excluded from system boundary.

Then the pre-treated wastes together with process water to make up 300 m³ feedstock are fed into the hydrolysis tank which is operated at 57 °C for over 5 h and then cooled down to 32 °C. This thermophilic temperature is not only a first hydrolysis step but also a hygienisation treatment to ensure the pathogen-free digestate as the final product when used as a soil conditioner [44]. Then the 300 m³ hydrolyzed feedstock is divided to three streams and fed into three AD digesters respectively (approx 100 m³ each). The OLR to digesters varies with BFMSW composition; based on the laboratory results from the commercial AD plant modelled, the average OLR over a three-month period (January–March 2009) is approx 2.393 g COD/L/day with a CV of 0.184.

The AD digester is operated at approx 37 °C; pH is monitored, ranging between 6.2 and 7.2. To ensure the dispersion of feedstock throughout the AD digester, a mechanical mixing system is applied which is composed of rotating blades; mixing is also aided by the generated biogas, which constantly bubble through the digester contents. The biogas production and energy generation are monitored, samples are collected daily and lab results (total solid, COD, sulphite, ammonia, sulphide) are used for process control purpose to maintain desired digestion conditions.

Biogas is the main product from AD digester, with a composition of 65 % CH₄, 32 % CO₂, and 1 % O₂. On average the yield of biogas is about 10,000 m³/day. The biogas is collected in the gas tank prior to combustion in the CHP system to generate electricity which is approx 1.2 kWh/m³ biogas (range 0.7–2.0 kWh/m³) and heat. Currently, 100 % of the renewable electricity is exported, while the electricity required for operations at the AD plant are 100 % imported from the national grid; the thermal energy produced from the CHP is not used and a separate diesel boiler is used to provide heat supply. It is clear from this that a proportion of the energy available form this AD system is wasted. However, according to the experts working on-site [57], in the future the efficiency of energy utilization will be optimized as, in the original design of this AD system,—heat from the CHP plant was to be the main heating source for the AD plant and only 'surplus' electricity after satisfying the energy requirement for the AD plant operation ('parasitic' load) will be exported.

In addition to biogas, around 300 m³ of digestates per day is produced from the three digesters, entering post-treatment stage, i.e. dewatering, and aerobic treatment. Dewatered and post-treated digestate is applied to the landfill site for the land reclamation purposes. The separated digest water (about 300 m³/day) is partly recycled internally (150 m³/day) via the water-cleaning system and the remains are sent to the drain. Apart from treated water, fresh water supplied by a local water supplier is incorporated into each new cycle (150 m³/day). All the water is stored in a water tank; prior to storage, NaOCl provided by Ineos is used for the water treatment.

Besides CHP, aerobic composting, waste water treatment, other two essential post-treatment processes are biogas upgrading and exhaust gas control. As some of the S contained in feedstock is released as H₂S, which is toxic and highly corrosive

to gas engines [44], it need to be removed prior to biogas utilization. In the AD plant studied, two technologies were applied for biogas desulphurization: one is addition of FeCl₃ supplied by Oasis Environmental Ltd; the second is oxidation of H₂S by introducing air. As for the exhaust treatment, the odorous areas including reception, pre-treatment and post-treatment areas are enclosed to eliminate off-gas escape and a biofilter technology is used which consist of woody biomass populated with microbes capable of degrading odorous contaminants present in exhaust gas [44].

Therefore, two AD systems were modelled, one was the scenario based on current operation at the UK commercial AD plant modelled, and the other was the optimized AD system. As discussed above, main inputs concerned in AD of WBF/MSBF/PSBF based products included infrastructure, chemicals, electricity and diesel fuel, water input as well as the electricity consumed for pre-treatment of biodegradable waste in MBT; the renewable energy and digestate produced, waste water and the potential gas emissions were taken into account as main outputs. As a multiple-product system, an 'avoided burdens' allocation approach was applied to the digestate and electricity produced.

5.2.2 Composting

Industrial and home composting systems were modelled, which are defined in Fig. 5.2.

In comparison with industrial composting, home composting was a simpler system with less energy input where a standard PE compost bin was the only infrastructure input and no energy was required for operation or collection. Two operational modes were simulated: active and passive compost. The former referred to an aerobically operated composting achieved by regularly turning the compost pile; the latter was defined as an anaerobically operated composting which was assumed to be poorly-maintained and so anaerobic zone were prevalent. Both scenarios were considered since there are risks that domestic compost bins may not be properly mixed nor well aerated under the oxygenating assistance of earthworms [39]. Active composting was applied as a default mode while the passive mode was modelled to test the sensitivity of LCIA results to potentially different home composting practices.

Besides home composting, in the UK open-air mechanical turned windrows are dominating commercial composting technology, accounting for 79 % of composted waste in 2007 [59]. Thus a composting system derived from WRATE software was simulated [23], which reflected UK open-air windrow composting of green waste. The biodegradable wastes i.e. foams/cardboard collected were assumed to be separated from the general waste streams and shredded to particles size of less than 50 mm; treated material was then placed into windrow piles. At the beginning of composting process the piles were turned approx every 5 days; at the end of process, the frequency of turning was reduced; after 12 weeks the

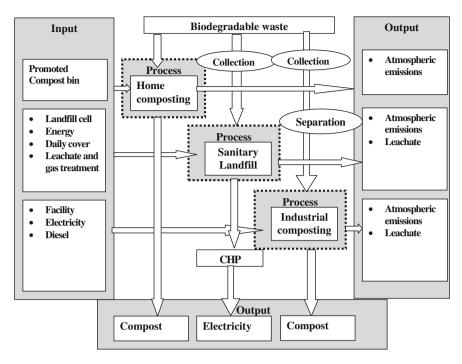


Fig. 5.2 Comparison of composting and landfill scenarios

compost process was effectively complete. Diesel and electricity were used for turning and weighing purpose respectively; apart from energy input, infrastructure was the main input; it was assumed no additional water was needed due to the self-contained water and rain water.

In addition, a 'silo cage' composting system was used as a representative invessel industrial composting technology for comparison with open-air windrow composting. The silo cage composting system modelled was based on the technology applied in TEG Group PLC [23], which is a vertical flow thermophilic composting system. The scenario assumed was: delivered organic waste was loaded into the silo, then rapid degradation was achieved by the accelerated microbial activity under thermophilic temperatures; the vertical temperature gradient in the organic waste created a chimney effect, which draws air up from the open base of the silo. Therefore, energy was saved by excluding forced aeration, turning or agitation operations. The residence time of the bio-waste varies between 10 and 21 days, after which, the composted waste was unloaded and further stabilized in a static pile before being packed. The main inputs include additional water, infrastructure, electricity consumed for system operation and diesel consumed for on-site delivery tasks.

For all three composting scenarios, the main final product was stabilized mature compost used as a soil improver or fertilizer. Trace gas emissions released from the degradation of biodegradable waste depended upon the process and conditions, e.g. temperature and aeration. Generally, NH₃ and CO₂ emissions are considered to occur in the aerobic composting process [49] and CH₄ and N₂O may be released under the anaerobic conditions [8, 37].

5.2.3 Landfill

As described in Fig. 5.2, sanitary landfill was another waste management option for WBF/PSBF/MSBF and cardboard. A representative small-scale four-cell landfill site with a total area of 15 ha and a capacity of 2,250,000 t was simulated, where a typical engineered clay liner and clay cover were assumed [23] as the leachate barrier to prevent odours and surface water ingress. Apart from installation of the cap and liner, other processes and operations modelled included: the delivery of waste to the site reception area, confirmation of acceptance of waste, compaction of the wastes by a steel-wheeled landfill compactor during the operational period and the placement of daily soil cover to oxidize the fugitive CH₄ passing through cell surface [23].

Regarding the temporal boundary, an approach recommended by Obersteiner et al. [47] was applied; a medium time-period of 100 years was selected for current model because the fate of compounds thereafter (up to an infinite time horizon) is uncertain and unpredictable. The 100 year time boundary includes three periods, i.e. operation, post-closure monitoring and medium time periods; the operation period was assumed as 5 years, which was followed by a 25 year monitoring period [47]. During the first 30 years, leachate collection, treatment system and an effective impermeable bottom liner as a leachate barrier was modelled. After the monitoring period, it was assumed that leachate treatment system ceased and liners deteriorated to permit the leakage of leachate.

Generally, in other studies modelling whole MSW, landfill gas was only captured in the post-closure monitoring period which suggests that landfill gas generated during operation period or after the monitoring period is considered to be directly released to atmosphere [47, 40]. However, it is also the case that many landfill sites utilise landfill gas from other adjacent landfills and hence would collect all the gas that was available [23]. Thus the same modelling approach as the WRATE model [23] was applied for the landfill scenario: the landfill gas collection system was assumed to run over whole simulation period and utilize the maximum landfill gas produced from landfilled materials being studied (foams/cardboard).

In summary, the main infrastructure inputs to the landfill scenario include cell liner/cover/cap, equipment for cell compaction, cover placement etc., biogas and leachate collection systems, biogas plant and leachate treatment system. Other inputs e.g. chemicals for leachate treatment were considered to be negligible. Electrical energy recovered from landfill gas was the main product from landfill process, another co-product—thermal energy—was assumed to be wasted and gases and leachates released from the landfill site e.g. CO₂, CH₄, and NH₄⁺ were included within the system boundary.

5.2.4 Recycling and Incineration

Recycling and incineration were modelled as alternative disposal routes for cardboard, where infrastructure and auxiliary material input, energy consumption, short-term or long-term emissions, residue waste treatment were taken into account. Both scenarios were derived from the Ecoinvent database v2.0 [27]. In the incineration scenario, it was assumed that 100 % of net electrical energy generated (1.55 MJ/kg cardboard) was exported and 100 % thermal energy (3.23 MJ/kg cardboard) was recovered [27]; in the recycling scenario, recycled board was modelled as the main product. For both scenarios, a system expansion allocation approach was applied where the 'avoided burdens' of the equivalent quantity of electrical power generated by the UK average electricity supply and average thermal mixes and of emissions associated with the EU average production of core board were credited to the incineration and recycling systems respectively.

5.3 Anaerobic Digestibility of WBF/MSBF/PSBF Based Products

The Biochemical Methane Potential (BMP) assays were conducted in triplicate in 165 ml serum bottles with 100 ml mixture of media, inoculum and substrates incubated at 37 °C (see Sect. 2.4.1) to investigate the biodegradability of WBF/PSBF/MSBF based products. These laboratory results were used to develop the LCA inventory simulating the fate of products modelled under the AD scenario.

The inocula used in BMP assay were collected fresh from a mesophilic continuous-feed, two-step digester (as defined in Sect. 5.2.1), where the OFMSW main feedstock was fed at an average OLR of 2.393 g COD/L/day. The TSS and VSS concentration of biomass was 50.56 ± 3.74 g/L and 25.01 ± 3.02 g/L. The activity assay were performed in triplicate in 39 ml serum bottles with 20 ml mixture of media, inoculum and model substrates to determine the activity of different trophic groups involved in each metabolism step of the AD process.

5.3.1 Activity of Inocula

Although there have been numerous papers published on the anaerobic biodegradability of different materials, it is difficult to directly compare these literature data due to different test conditions (e.g. inoculum used) and protocols applied [2]. Thus, relevant activity assay data is essential to provide indicative information on the performance of various trophic groups involved in the AD metabolism steps. However, only few publications on AD concern activity assessment, especially

assay of the individual populations. A comprehensive review was conducted by Rozzi and Remigi [54], covering most of the studies on this topic. They pointed out that majority of literature reviewed focused on acetoclastic activity, whereas little information is available on the hydrolytic and acetogenic activity assessment. To harmonize the batch assay, a protocol was proposed by Angelidaki et al. [2], was used in the current study.

In the complex metabolism pathway of the AD process, five trophic groups are involved i.e. hydrolysing bacteria, acidogenic bacteria, acetogenic bacteria, aceticlastic and hydrogenotrophic methanogens [54]. Therefore, those intermediate molecules involved in each metabolic step can be used as model substrates in tests and the rates of substrate consumption are good indicators of bacterial activities. In this study, four substrates including glucose, \(\alpha \)-cellulose, and different fatty acids (VFA) were used in BMP assay with 2 g VSS/L pre-incubated inocula. The theoretical CODs of model substrates calculated based on Eq. 2.18 and the characterized inoculum activities expressed as cumulative methane yield or conversion efficiency are presented in Table 5.1 and Figs. 5.3 and 5.4.

The SMPR presented in Fig. 5.3, was obtained by dividing the daily methane yield by the VSS of inoculum; only the period of maximum biogas production was analyzed because after 25 days there was no significant further CH₄ production observed. Although non-acclimatised inocula was used in assay, no lag phase was found for glucose and only a short lag phase occurred in the case of VFA and cellulose (1 day and 2 days respectively). This was not only due to these being easily digestible substrates but also attributable to the initial high activities of the microorganisms present in the inocula which were presumed to have been already adapted to the sugar/cellulose/VFA contained in BFMSW in the AD system. The short lag phase for cellulose can be explained by the essential hydrolysis step to convert cellulose into sugars.

As indicated in Fig. 5.3, a non-linear SMPR was found for the model substrates. The SMPR results for all the substrates over the first 7 days showed a rapid decomposition phase followed by a sharp decrease towards the baseline. In the case of glucose and acetic acid, negative SMPR appeared, which can be explained

Table 5.1 Activities of tropnic groups (SD is indicated in brackets)						
Population ^a	Substrate	Theoretical COD (g/g VS)	Cumulative CH ₄ (ml/g VSS)	Conversion efficiency (%) ^c		
Hydrolytic	α-cellulose ^b	1.18	145.064 (3.428)	60.067 (1.428)		
Acidogenic	Glucose ^b	1.07	136.098 (2.694)	62.527 (0.299)		
Acetogenic	Propionic acid ^b	1.51	319.861 (24.057)	100.204 (7.536)		
	Butyric acid ^b	1.81				
Acetoclastic	Acetic acid ^b	1.07	197.638 (5.703)	89.926 (2.595)		

Notes

^a Inoculum VSS = 2 g/L

^b Theoretical CH₄ potential: 1 g COD equivalent to 0.395 L CH₄ at 35 °C and one atmosphere

^c Conversion efficiency = measured BMP/theoretical BMP*100 %

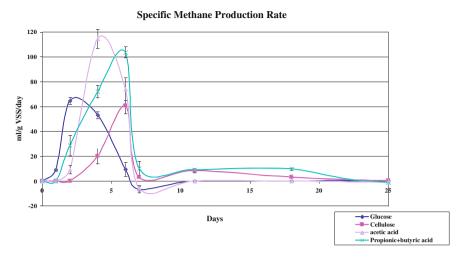


Fig. 5.3 Specific CH₄ production rate (ml CH₄/g VSS/day)

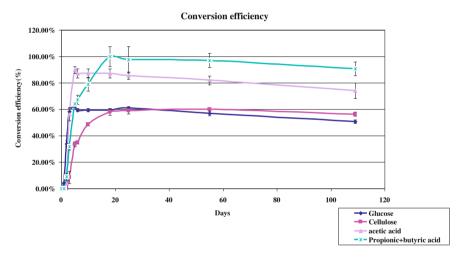


Fig. 5.4 Conversion efficiency (measured CH₄/theoretical CH₄)

by the fact that the feedstock nearly stopped CH₄ production whereas the blank bottles were still producing CH₄ due to cell lysis caused by nutrient deficiency [4]. After the first 7 days, the BMP assays fed with acetic acid and glucose showed a constant trend without significant CH₄ produced, whereas the propionic acid/butyric acid and cellulose assays showed further digestion, which brought a slightly increased SMPR followed by a decline to zero CH₄ production. Compared with the specific activity on acetate proposed by Angelidaki et al. [2]. in their protocol (39.5 ml CH₄/gVSS/day), the SMPR obtained in the present experiments was higher, which indicated that the inoculum performance in this study reached

the standard level, although activity was slightly lower than the accelatic activities found by Rozzi et al. [55].

As presented in Fig. 5.4, the cumulative CH₄ yield was expressed in terms of conversion efficiency where the theoretical CH₄ was calculated by the method indicated in Sect. 2.4.3.3 (1 g COD equivalent to 0.395L CH₄ at 35 °C and at one atmosphere) [60]. It was shown that the occurrence of maximum cumulative CH₄ yield varied with substrates: for the readily methanogen-metabolized compound acetic acid gave the first CH₄ yield peak, which occurred in day 6, followed by glucose and propionic/butyric acid (day 7 and day 18 respectively); cellulose showed a gradually increasing curve with maximum CH₄ production appearing in day 55. The declining trend after 55 days can be explained by a higher 'background' CH₄ production occurring in the blanks than in the sample bottles due to starvation-induced cell lysis in the blanks over this time period. The ultimate CH₄ potential for each substrate is given in Table 5.1; approx 247 ml CH₄/gCOD and 237 ml CH₄/g COD were yielded from digesting glucose and cellulose respectively, which corresponded to 60.1 and 60.9 % conversion efficiency. As for VFAs, high utilization was achieved; nearly 100 % of theoretical CH₄ potential of propionic/butyric acid was released, whereas in the case of acetic acid conversion efficiency reached 89.9 %.

The results from different model substrates are indicators of activities of trophic groups. The insignificant lag phase, combining with the over 60 % conversion efficiency for cellulose and glucose, suggested relatively high hydrolytic and acidogenic activities respectively. The high SMPR and satisfactory conversion efficiency for VFAs, indicated a good performance of acetogens and aceticlastic methanogens. Besides aceticlastic methanogens, hydrogenotrophic methangens also play a key role in methanogenesis over the whole AD process as this bacterial group is responsible for maintaining the low partial pressure of H₂ required for the satisfactory functioning of intermediate trophic groups [54]. By monitoring the consumption of substrates i.e. H₂/CO₂ or the production of CH₄, the hydrogenotrophic activity can be assessed. This was not included in current study but could be assessed in future work. Overall, the activity assay results obtained suggested highly active trophic groups present in inocula supporting the likely presence in well-managed AD systems of microbial populations with good inherent abilities to undertake degradation of WBF materials.

5.3.2 Biodegradability of WBF/PSBF/MSBF Products

The BMP assays were carried out at I/S ratio of 1:1 and 3:1 to determine the biodegradability of the materials studied; the final concentration of added substrates (WBF/PSBF/MSBF and cardboard) were about 2 g COD/L. Gas and liquid samples were collected to determine the biogas composition and VFAs concentrations; the results not only represent the digestibility of the materials under anaerobic conditions in presence of the specified inocula but also give good

indication of the potential energy recovery from the studied materials in the UK commercial AD plant modelled or similar AD systems.

5.3.2.1 Biogas Production

The cumulative CH₄ and biogas production at I/S ratio of 1 are given in Figs. 5.5 and 5.6. No lag phase was observed for almost all the substrates except cardboard, which showed a very short lag phase (1 day), which indicates a good level of activity for all the trophic groups present in the inocula. Digestion of different substrates gave similar biogas compositions: cumulative biogas produced over the 115 day period was mainly composed of 53–55 % CO₂ and over 45 % CH₄; some trace amount of gases such as H₂, H₂S may be contained in the biogas but it was not investigated as (1) the limitation of the equipment (2) it was modelled in LCA based on the literature data which were considered as reliable.

As shown in Fig. 5.5, within the first 10 days a rapid digestion was observed for all substrates; especially the biodegradable foams, and cumulative CH₄ production from foam digestion increased substantially over the first 5–6 days followed by a plateau period. The CH₄ yielded from digestion of cardboard rose gradually after 10 days. According to statistic analysis ($\alpha = 0.05$, see Sect. 5.3.2.5), the digestibility of WBF was statistically greater than PSBF/MSBF within the first 5 day incubation period during which the cumulative CH₄ yield reached 249.9 \pm 6.2 ml/g VS equivalent to 208.2 \pm 5.2 mlCH₄/gCOD. This is probably due to the starch and protein contained in the wheat flour component of WBF providing both C and N nutrients for microorganisms, whereas only a C-source was supplied in the

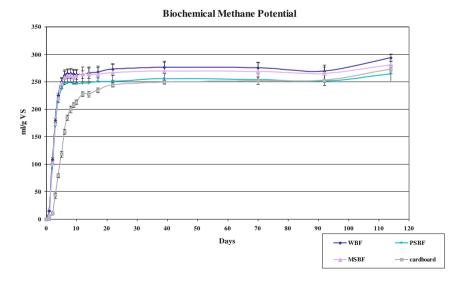


Fig. 5.5 BMP at I/S ratio = 1 (Error bar shows SD)

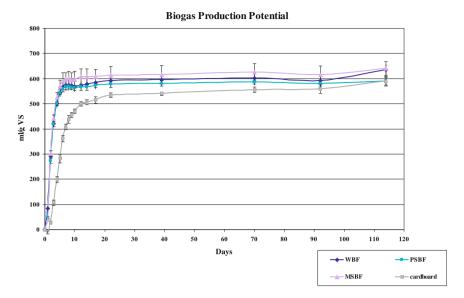


Fig. 5.6 Biogas production potential at I/S ratio = 1 (Error bar shows SD)

purified starch of the other substrates. Generally, the foams in these BMP assays had greater CH_4 yields than results reported by previous studies on biopolymer materials: Russo et al. [56] reported less than 40 ml/g COD CH_4 produced within 4 days from BMP bottles fed with maize starch/PVOH blends having similar starch/PVOH ratios to the MSBF foam used in the present study (w/w % 90:10) which produced 219.3 ml \pm 6.2 CH_4 /gVS equivalent to 178.2 \pm 5.03 ml/g COD within the first 4 days. This may be due to possibly differences in experimental conditions but this is difficult to ascertain due to a lack of transparency in their study. However, it also seems very likely that the structure of the starch and wheat flour foams in the present study was a substantial aid to their rapid breakdown in the AD conditions. As expected, the cardboard underwent the slowest degradation rates in comparison with the foams. This may be explained by the impeded access to cellulose by the complex three-dimensional structures formed between cellulose hemicellulose and the lignin component being highly recalcitrant to biodegradation in the AD system [62].

As reported by Monson et al. [44], an optimum CH₄ could be expect at a C:N ratio ranging between 20 and 30; the WBF substrate gave a C:N ratio of approx 34.2 (Table 4.8), which is close to this optimum range. Therefore, as expected, WBF gave the highest ultimate CH₄ yield on the basis of per g VS, followed by the MSBF, cardboard and PSBF (Table 5.2). As shown in Table 5.2, the conversion efficiency was calculated, where the equivalent theoretical CH₄ was estimated based on the lab-derived COD results (1 g COD equivalent to 0.395 L CH₄ at 35 °C and at one atmosphere) [60]. The final conversion efficiency of WBF was

•	COD	Ultimate CH ₄	Ultimate CH ₄	Conversion
	(g COD/g VS)	(ml/g TS fed)	(ml/g VS fed)	efficiency (%)
I/S ratio = 1				
WBF-1	1.199 (0.174)	296.404 (6.732)	293.736 (6.671)	61.947 (1.407)
MSBF-1	1.254 (0.449)	281.277 (6.822)	280.922 (6.813)	57.795 (1.402)
PSBF-1	1.173 (0.252)	265.342 (12.988)	264.141 (12.929)	58.315 (2.854)
Cardboard-1	1.267 (0.153)	304.916 (8.829)	272.777 (7.899)	54.697 (1.584)
I/S ratio = 3				
WBF-3	1.199 (0.174)	290.790 (4.961)	288.173 (4.916)	60.774 (1.037)
MSBF-3	1.254 (0.449)	280.799 (4.068)	280.445 (4.063)	57.698 (0.836)
PSBF-3	1.173 (0.252)	262.321 (5.341)	261.134 (5.317)	57.651 (1.174)
Cardboard-3	1.267 (0.153)	255.951 (3.017)	228.973 (2.699)	45.913 (0.541)

Table 5.2 Biodegradability of WBF/MSBF/PSBF products (SD is indicated in bracket)

slightly higher than PSBF and MSBF, achieving 62 %, and the results indicated that over 55 % biodegradability is reachable for all the tested substrates.

5.3.2.2 I/S Ratio Effects on CH₄ Production

The different I/S ratio was explored, the conversion efficiency and ultimate CH₄ potential at I/S ratio of 3 and 1 are compared in Table 5.2 and Fig. 5.7. The SMPR are presented in Figs. 5.8 and 5.9, which are expressed as daily CH₄ yield on the basis of VS loaded and inoculum VSS respectively.

There was no lag phase observed at I/S ratio of 3, in the first day, CH₄ was yielded from all the tested materials; the biogas compositions found at I/S ratio of 3 was very similar to the results obtained at I/S ratio 1: CH₄ accounted for 45–47 % (v/v) of biogas yielded. Analyzing the SMPR, a similar trend was shown at both I/S ratios. During the first 4 day incubation period, daily CH₄ yield from digestion of WBF/MSBF/PSBF increased substantially, which was followed by a sharp drop, approaching 'zero baselines' at day 8. The negative SMPR of foam samples at day 9 and 10 was attributable to the gas produced in the blank control bottle from cell lysis due to starvation in the absence of a C-source, whilst no significant CH₄ yield from sample bottles. After day 10, only trace amounts of CH₄ were produced from the foams at both I/S ratios, thus SMPR curve remained constant. As expected, slower degradation rates were found in the BMP assay of cardboard than the foams, which led to gradually increased SMPR over the first 7 days followed by a decline to 14 days after which there was no significant CH₄ production from cardboard as indicated by the plateau in the SMPR curve.

Despite similar SMPR trends, the CH₄ production rates varied between the I/S ratios. Generally, high I/S ratios resulted in a statistically greater daily CH₄ yield per substrate loaded at the initial phase of AD process (approx 6–8 days for foams and 10 days for cardboard); high I/S ratio also brought higher maximum SMPRs, but induced lower gas emissions per unit inoculum VSS over the initial digestion period (Figs. 5.8, 5.9). This suggests that high initial concentrations of biomass can bring

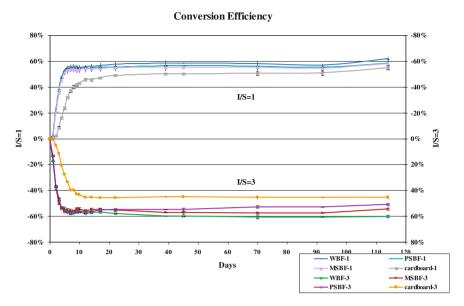


Fig. 5.7 Conversion efficiency (I/S ratio = 1 & 3) (Error bar shows SD)

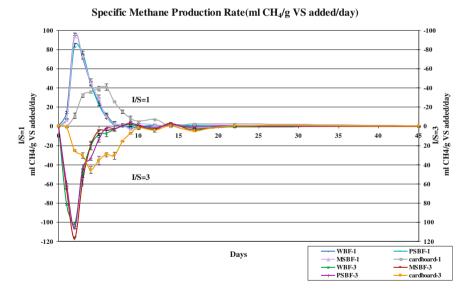


Fig. 5.8 SMPR (mlCH₄/gVS added/day at I/S ratio of 1, 3) (Error bar shows SD)

about a rapid initial degradation, but a decline in the specific inoculum activity due to a deficiency of nutrients. This results are consistent with previous studies on the effects of I/S ratios [52, 63]. Trzcinski and Stuckey [63] found that at high I/S ratios

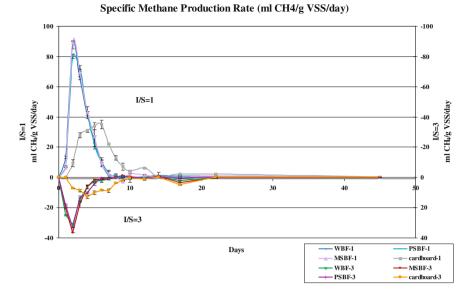


Fig. 5.9 SMPR (ml CH₄/gVSS/day at I/S ratio of 1, 3) (Error bar shows SD)

CH₄ yield occurred in the first days during which a lag phase appeared when using low I/S ratios; Raposo et al. [52] observed that an I/S ratio of 1 brought a longer CH₄-production period and a greater SMPR (ml CH4/g VSS) but lower maximum CH₄ production per load compared with I/S ratios of 1.5, 2 and 3.

Statistical analysis indicated that SMPR of WBF is significantly higher than PSBF/MSBF in the first 2 days at both I/S ratios (1 and 3) which may be due to the more balanced C/N nutrients supplied by WBF stimulating the micro-organism populations at the beginning of decomposition. After day 2, insignificant difference in SMPR curve was found for three biodegradable foams; maximum daily CH₄ yield from foam digestion occurred at day 2: at ratio 1 and 3, SMPR for three foams ranged between 84.6 and 94.6 ml/g VS added/day and 102.2-117.2 ml/g VS/day respectively, which corresponded to 80–89.2 mlCH₄/gVSS and 31.2– 36.7 mlCH₄/gVSS per day. The maximum SMPR occurrence (day 2) and the range for three foams at I/S ratio 1 coincided with the results observed in BMP assay of glucose (day 2 maximum SMPR occurred 64.6 \pm 2.9 ml/g VSS/day). On the contrary, although the SMPR trend of cardboard agreed with that of cellulose, its maximum SMPR differed from the model substrate. Maximum SMPR of cardboard approx 35.1 ml CH₄/g VSS/day occurred on day 6 at I/S ratio of 1, whereas a maximum SMPR of double that (60.8 \pm 6.4 ml/g VSS/day) was found on day 6 in bottle fed with cellulose). This could be lower level for cardboard can be explained by the strong association between cellulose, hemicellulose and lignin, which impeded access to cellulose.

Although different I/S ratios gave some differences in the SMPR profiles, the ultimate CH₄ production and conversion efficiency did not vary significantly

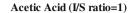
between the I/S ratios. As indicated in Fig. 5.7, in the case of foams (WBF/MSBF/ PSBF) and cardboard most of the CH₄ was produced within the first 5 days and 12 days respectively, after this rapid-increase phase, conversion efficiency reached a plateau. At I/S ratio of 3, WBF was still shown as the substrates with greatest ultimate biodegradability, which producing 288.2 \pm 4.9 ml cumulative CH₄ per g VS over the 115 day period, equivalent to a conversion efficiency of $60.8 \pm 1 \%$. The two other starch-based foams delivered very similar final conversion efficiency, approx 57.7 % at I/S ratio of 3, which was similar to the finding at I/S ratio 1. In contrast, the BMP assay fed with cardboard at I/S ratio 3 resulted in much less ultimate CH₄ production per mass of substrate loaded than the assay at I/S ratio 1, only 45.9 \pm 0.5 % conversion efficiency achieved. This may be attributable to the increase in cell lysis caused by the C nutrient deficiency after an initial rapid digestion phase at the high I/S ratio, during which the most readily hydrolyzed C source was consumed while the access to remaining C was impeded by the bonding between lignin and cellulose/hemicellulose. However, the ultimate CH₄ production from the batch assays on cardboard in this study at both I./S ratios was higher than the results reported in a previous study i.e. 217 ml CH₄/gVS yielded from cardboard digestion within 237 days at I/S ratio of 1.5 [33]. This could be due to the difference in inoculum used in batch assay carried out by Jokela et al. [33]. Actually, in a largescale AD system, a higher conversion efficiency of cardboard can be expected due to the balanced nutrients provided by the mixed organic feedstock.

5.3.2.3 Process Indicator-VFA

As one of the most important parameters in AD, the concentration of VFAs in BMP bottles over the digestion period was analyzed including acetic acid, propionic acid, butyric acid, valeric acid, caproic acid. No significant quantities of VFAs were detected after day 12, the VFA concentrations within first 12 day incubation period are presented in Figs. 5.10, 5.11, 5.12, 5.13, 5.14.

As shown in Figs. 5.10–5.13, at I/S ratio 1, in general the fermentation products from digestion of WBF/PSBF/MSBF were dominated by acetic acid, and n-butyric acid, propionic acid. Different from foams, acetic acid and propionic acid were the most prevalent VFAs in BMP bottle fed with cardboard, besides, n-butyric acid only accounted for small proportion. These findings were confirmed by previous studies where the predominant VFAs produced from digestion of maize starch/PVOH blends (90:10 % w/w) were acetic acid, n-butyric acid followed by propionic acid [56]; the similar VFA compositions were reported in the batch assays on potato solid waste [67].

The VFA distributions varied over the digestion period, which provided information on the metabolic pathways. For three foam substrates (WBF/MSBF/PSBF), n-butyric acid made up less than 50 % of VFAs in the first 2 days, with 5–12 % of the total VFA was contributed by propionic acid at day 2, rising to 16–28 % at in day 3–4. This pattern was not only caused by substrate characteristics but also due to pH regulation. In previous research, the high proportion of n-butyric acid was



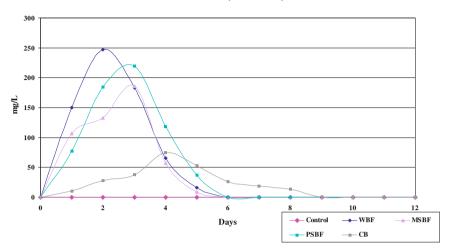


Fig. 5.10 Acetic acid concentration at I/S ratio of 1

Propionic Acid (I/S ratio=1)

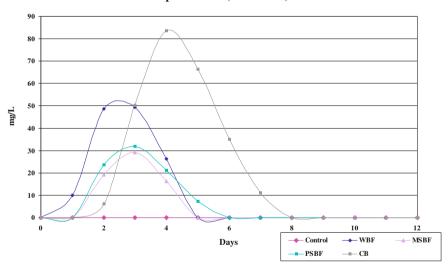


Fig. 5.11 Propionic Acid concentration at I/S ratio of 1 *Notes* CB = cardboard

considered as being due the starch present in the substrate [5, 67]. Additionally, it has also been reported that the lower the pH (within the range 4.5–8.0), the higher the propionic acid was observed and that pHs of 5.9–6.2 encouraged more butyric acid production [50, 31]. Therefore, the high starch content of the foams and the neutral

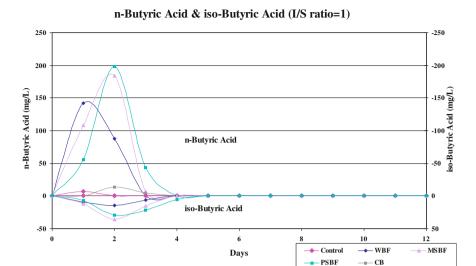


Fig. 5.12 Butyric acid concentration at I/S ratio of 1 *Notes CB* cardboard

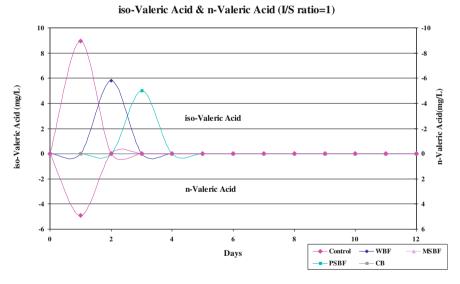


Fig. 5.13 Valeric acid concentration at I/S ratio of 1 Notes CB cardboard

pH value in BMP bottles are likely to have favoured butyric acid production. However, these two acids were only intermediate products further utilized by acetogens, which caused a decrease in their concentration: n-butyric acid and propionic acid reached full degradation in day 4 and day 6 respectively. Unlike these

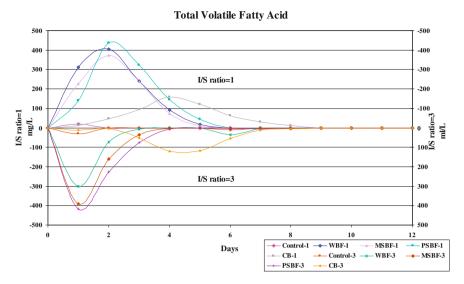


Fig. 5.14 Total VFAs at I/S ratio of 1 and 3 *Notes CB* cardboard

two acids, acetic acid was always prevalent in the VFAs, increasing from 47–55 to 100 % within the first 5 days; due to a number of metabolic pathways to form acetic acid, including conversion of VFAs to acetate [62] and direct formation from fermentation of carbohydrates and protein [50]. In the case of cardboard digestion, only small proportions of n-butyric acid were found (27 % at day 2); whereas propionic acid and acetic acid dominated, remaining constant as 55 and 40–45 % respectively during days 3–6. Afterwards, acetogic degradation of propionic acid/n-butyric acid resulted in a predominance of acetic acid, making up 100 % of the cardboard VFAs at day 8. Because the acetic acid formed can be directly utilized by methanogens, it is considered as the major precursor of CH₄ [67]. Comparing patterns of acetic acid and methane, it was found that the timing of the acetic acid peak (day 2/3 for WBF/PSBF/MSBF and day 4 for cardboard) coincided with the occurrence of maximum SMPR (Fig. 5.7); the plateau period i.e. zero acetic acid production which occurred in day 6 and day 9 for foams and cardboard respectively, matched well with the CH₄ production curves.

As shown in Figs. 5.10–5.13, all VFA production pattern showed similarities i.e. a sharp increase followed by a decline to zero, but the quantities of VFAs produced varied with the substrates and I/S ratios. At day 1 for I/S 1 higher VFAs production was observed from WBF digestion than PSBF/MSBF, which is attributed to stimulation effects on the bacteria produced by the favourable C/N nutrient present in WBF. During the second day, the higher n-butyric acid concentrations were found in bottles fed with MSBF/PSBF than WSBF at I/S ratio 1 can be explained by the higher starch content in MSBF/PSBF; however, at day 2 WBF was still the substrate with the highest acetic acid yield due to the actogenic

degradation of butyric acid produced on day 1. From day 3, bottles fed with PSBF and MSBF showed higher acetic acid and n-butyric acid concentrations than WBF. Amongst all the substrates at I/S ratio 1 digestion of the cardboard brought the highest propionic acid profiles, primarily formed from the carbohydrates contained in the cardboard [50]. Comparing I/S ratios, VFAs compositions did not differ (not presented here), but it was found that the high I/S ratio brought a rapid total VFA formation in the initial digestion phase (day 1), but led to a lower maximum total VFAs concentration and the shorter period over which VFA formation occurred.

In addition, in this study, it was found that straight-chain forms were the dominant VFAs in all the batch assays, e.g. more n-butyric acid and n-valeric acid produced than their isomers (Figs. 5.12 and 5.13). Similar results have been reported in previous batch assays carried out on similar substrates [67, 56]. Wang et al. [65] indicate that the decomposition rates of VFAs (C₂-C₆) with a straight chain (normal form) were greater than their respective branched isomers suggesting that foams and cardboard provide easily digestible intermediate VFAs for bacteria. In the current study, the longer the chain in the VFA, the smaller chance that it was found in the batch assay bottle, e.g. no caproic acid was found in any BMP bottle. This finding is consistent with those of Wilson et al. [67] and Russo et al. [56] in studies of VFA production from starch-based materials. The higher molecular weight VFAs, i.e. iso-butyric acid and the three isomers of valeric acid are considered to be associated with the fermentation of proteins [50]. This was also observed in the present study as trace amount of iso-valeric acid were observed only from WBF digestion (the higher concentration of both iso-valeric acid and n-valeric acid fond in the control bottles were considered to be due to cell lysis due to nutrient deficiency).

5.3.2.4 PVOH and Protein Assay

After 115 days incubation period, liquid samples were collected from each serum bottle running at the I/S ratio of 1; the protein and PVOH remaining were estimated by using a modified Lowry assay [51] and a colorimetric method [34, 25] respectively (Sects. 2.4.3.5 and 2.4.3.6). As shown in Table 5.3, the PVOH and wheat protein concentrations were calculated from the composition of foams (Table 2.3); all the data are expressed in terms of 100 ml solution per one serum bottle (100 ml media, inoculum and substrates).

The concentrations of PVOH remaining in the serum bottles after 115 days incubation were based on the formation of PVOH-iodine-boric acid blue complex. In comparison with MSBF/PSBF, more PVOH residues were detected in WBF sample bottles approx 4.8 ± 0.3 mg PVOH remained which is equivalent to 17.4 ± 2.5 % of the initial PVOH input; only a small fraction of PVOH remained in bottles fed with MSBF and PSBF $(8.1 \pm 1.6$ % and 3.6 ± 0.8 % of the input amount respectively). This finding gives an approximation of PVOH degradation in the presence of inocula collected from AD plant, the degraded PVOH may be presented as compounds with shorter molecule chains as well as being fully

orackets)					
	Substrates input	/BMP bottle ^a	Remains after 115 day digestion/bottle		
	PVOH (mg/100 ml)	Wheat protein (mg/100 ml)	PVOH remained ^b (mg/100 ml)	Extracellular protein/ wheat protein ^c (mg/100 ml)	
Control WBF	0.000 (0.000) 27.445 (0.000)	- 17.523 (0.000)	0.000 (0.000) 4.776 (0.300)	3.338 (0.248) 4.104 (0.160)	
MSBF PSBF	19.921 (0.049) 27.012 (0.019)	- -	1.609 (0.336) 0.959 (0.219)	3.546 (0.152) 3.499 (0.158)	

Table 5.3 Estimation on biodegradability of PVOH and wheat protein (SD is indicated in brackets)

Notes

metabolised. The high biodegradation of PVOH indicated can be partly explained by the highly active inocula but may also be attributable to the relatively low molecular weight of the PVOH component in the foams. Generally, PVOH with low molecular weight is considered to be more rapidly degradable than higher molecular weight variants [41, 10]. In a comparison study of PVOH-2000 and PVOH-14000, the high molecular weight fraction was found as a residue left in the media, while PVOH-2000 reached over 75 % biodegradability in river sediments after 125 day incubation [41]; similar degradation rates have also been reported by Liu et al. [38] (66 % degradation of PVOH-1799 in 22 days). However, in future work, other methodologies could be applied to further investigate the biodegradation of PVOH under anaerobic digestion.

The results determined by modified Lowry assay primarily represented the secreted extracellular protein after separating intracellular protein by 0.22 μm filter (Table 5.3). Actually the similar method was applied in previous studies to determine total soluble protein and extra-cellular protein [4, 42]. The results in the current study were considered as reasonable indications of soluble extra-cellular protein. The wheat protein degradation could also be estimated by the difference in protein content between bottles fed with WBF and those fed with MSBF/PSBF which contained similar amounts of C source derived starch/PVOH components but no protein.

Generally, it is believed that soluble microbial products (including extracellular protein) can be produced in response to stressed condition e.g. limitation of nutrients [6]. However, in the current study, it was found that there was no significant difference in the soluble protein present in control bottles without feeding and the sample bottles fed with MSBF/PSBF which may be attributable to long digestion period which led to the nutrient deficiency occurring in sample bottles. Total proteins present in control bottles and MSBF/PSBF sample bottles ranged between 3.34 and 3.50 mg, which is equivalent to a range of 0.0167–0.0177 mg protein/mgVSS. This result is similar to the findings in previous study by Aquino and Stuckey [4]: they reported approx 0.01 mg protein/mgVSS present in a reactor

^a The total substrates input in 165 ml serum bottle with 100 ml liquid

^b PVOH left in the liquid phase after 115 day incubation

^c Total protein determined after cellular proteins were removed by 0.22 μm filters

continuously fed with glucose and above 0.03 mg protein/mgVSS in bulk solution under stressed nutrient conditions.

In comparison with the blank bottles and sample bottles fed with the other two foams, only slightly higher protein contents were found in WBF sample bottles, which may be caused by small fraction of wheat protein being left as residues (approx 3.2–3.5 % of the initial wheat protein) or higher extracellular protein produced during metabolism of WBF. It is not possible to simply separate the influence of these two factors on protein content results however, it is suggested that most of the initial wheat protein was degraded. As for the fate of protein-N, it should be explored in future study.

5.3.2.5 Statistical Analysis

Statistical analyses in the form of one-tailed Mann-Whitney test were performed at significance level $\alpha = 0.05$, to determine the magnitudes of CH₄ yields from four substrates (WBF, PSBF, MSBF and cardboard) at I/S ratio of 1 over the digestion period and test the hypothesis that higher I/S ratios led to greater biodegradability.

Cumulative CH_4 yield per VS loaded was analyzed, the results confirmed that at significance level $\alpha=0.05$, CH_4 produced from WBF digestion was statistically greater than PSBF and cardboard throughout the whole digestion period; whereas WBF statistically showed higher CH_4 production than MSBF in the first 5 days, but not over the rest of digestion period; there was no significant difference between cumulative CH_4 yields from PSBF and MSBF, however, the CH_4 productions from both foams were statistically higher than cardboard substrates in the first 40 days after which the differences were not statistically significant. Statistical test on the conversion efficiency of different substrates indicated that within the first 4 day incubation, WBF showed higher biodegradability than other substrates (PSBF/MSBF/cardboard), but in the rest of incubation period, the difference between the biodegradability of WBF and PSBF/MSBF was not statistically significant.

Statistical analysis at significance level $\alpha=0.05$ suggested that the I/S ratio of 3 resulted in a statistically greater CH_4 production per unit of substrate loaded at initial phase of process (first 6 days for WBF/MSBF, first 8 days for PSBF and first 10 days for cardboard) than with the I/S ration of 1, after which, the ultimate cumulative methane yielded from foam substrates did not differ significantly with I/S ratio. However, the high I/S ratio produced significantly more ultimate CH_4 yield from cardboard digestion.

5.3.3 Discussion: Biodegradability and Element Flow

The calculated C balances from the laboratory work are presented in Table 5.4. 68–75 % of the total C contained in foams was released as biogas; if assuming that all gasified C was biogenic not fossil origin, approx 82.8–86.9 % of the C

sequestered from atmosphere and contained in the foams was converted to CO₂ or CH₄. C present in PVOH residue in the liquid phase only made up a small fraction of total C. The rest of the C was partially utilized by microorganisms for cell synthesis, but a fraction of the C could also be present in liquid phase as molecules produced from PVOH degradation. In the case of cardboard, it was estimated that approx 62 % of total C was gasified; representing about 75 % of the C contained in cellulose and hemi-cellulose released as biogas (lignin is assumed to be nonbiodegradable in AD). As a relatively non-degradable component under anaerobic digestion, lignin was assumed to remain in the digestate. Therefore, a high gasification efficiency of degradable C was achieved for all the substrates under this study: over 70 % of degradable C was released as biogas (CO₂, CH₄). However, the composition of biogas observed in the laboratory-scale test was 53–55 % CO₂ and just over 45 % CH₄ which it would be desirable to further optimized to higher CH₄ levels at industrial scale in the anaerobic digester. In a well controlled commercial scale AD system (high inoculum concentration, stabilized process parameters and co-digestion with other organic waste), a biogas with over 60 % CH₄ proportion could be expected. Moreover, in the presence of an acclimatized inoculum a higher conversion efficiency of the less biodegradable components e.g. PVOH may be achievable. Therefore, in future research, effects of acclimatization of biomass and influence of I/S ratio on the biochemical methane potential could be explored.

In addition to C, other elements contained in the substrates such as N, S, Mg are also released during digestion. Many trace elements such as Mg can be utilized by microorganisms as nutrients [44], whereas N and S releases are mainly concerns with upgrading of biogas or in tail gases treatment in AD model. As these two elements were present in WBF and in cardboard (see Table 4.8), their element flows and distributions are discussed below.

Actually during digestion of wheat protein, inorganic nitrogenous products can be produced. As summarized by Kayhanian [35], metabolic pathways to degrade protein include hydrolysis of protein to alpha-amino acids, which are sequentially

Toble 5.4	Carbon	halanaa in	anaarahia	digastion	(CD ic	indicated	in brackets)
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Table 5.4 Carbon (WBF	PSBF	MSBF	Cardboard
	M DI.	LODI	MSDI	Carubbaru
C mass flow (g/g Ta	S)			
Total C	0.469	0.461	0.457	0.458
Biogenic C	0.389	0.382	0.399	0.458^{a}
CH ₄ yield as C ^b	0.157 (0.004)	0.141 (0.007)	0.151 (0.004)	0.131 (0.004)
CO ₂ yield as C ^b	0.182 (0.01)	0.174 (0.003)	0.194 (0.011)	0.153 (0.004)
C balance (% total	C)			
CH ₄	33.363 (0.758)	30.699 (1.503)	33.028 (0.801)	28.627 (0.829)
CO_2	38.733 (2.088)	37.873 (0.733)	42.389 (2.371)	33.390 (0.829)
PVOH residue	2.969 (0.427)	0.610 (0.137)	1.027 (0.204)	_

Notes

^a Biogenic C in cardboard includes 0.378gC/g TS is derived from cellulose and hemi-cellulose ^b Density $CH_4 = 0.717$ g/L; Density $CO_2 = 1.977$ g/L

utilized by hydrolyzers and acetogens and eventually degraded by methanogens. During the digestion of a few amino-acids, N-containing purines and pyrimidines are produced, which are further degraded by bacteria to release NH₃. Dissolved NH₃ can exist in equilibrium with NH₄⁺ [44] or may be converted via nitrification and denitrification pathways [62], through which intermediate products NO₃⁻, NO₂⁻ or gases (NO, N₂O, N₂) can be produced. In the case of cardboard, initial N present could be either biologically solubilized into NH₄⁺-N or that bound to the woody biomass may remain intact during digestion [33];—the N-distribution may also depend on pre-treatment of the woody substrate. In summary, initial N compounds may be converted into several forms during wheat protein degradation or cardboard digestion and these can either be utilized for microbial cell synthesis [44] or recovered as mineralized components present in digestate or lost as volatilized NH₃ and denitrification-induced gases.

As for the S flow, its distribution has been studied in AD of waste water. It was found that during the microbial decomposition (oxidation) of organic matter, S is present in sludge either as soluble ionic form e.g. SO_4^{2-} or bound to metals (Fe, Cd, Zn, Cu, Hg); the sulphide is primarily formed under anaerobic condition when depletion of dissolved oxygen (major electron acceptor) occurs which induce SO_4^{2-} acting as an alternative electron acceptor and transformed into H_2S , S^2 via biochemical reaction [17]. After FeCl₃ desulphurization treatment majority of sulphide is bound to free ions Fe^2 brought by the addition of FeCl₃; as reported by Dewil et al. [17], typically after digestion, approx 99.8 % of S mainly is remained as insoluble $Fe(HS)_2$ and $Fe(HS)_3^-$ whereas minor fraction of S was found in soluble form; only 0.02 % of S was released as H_2S component of biogas. Similar S flow was also found in another study conducted on various full-scale AD plants [18]. These results gave good indications of the S flow throughout the digestion of cardboard/foams.

An in-depth study could be carried on the distribution of the multiple elements during digestion of solid waste, which were excluded from the scope of the current study. Thus, in the current LCA model, element flows of N/S were estimated based on the emission factors derived from previous studies but the specific new results on the biodegradability and C element flows obtained from the current laboratory experiments were applied. These, together with other inventory analyses, are presented in the Sect. 5.4.

5.4 Anaerobic Digestion Scenarios

The AD scenarios for disposal of WBF/MSBF/PSBF products were built on the empirical results from measurements in the UK commerical AD plant for disposal of BFMSW and the laboratory results of the biodegradability test.

5.4.1 Inventory for BFMSW Treatment in AD Plant

The inventory data was developed in collaboration with the UK commercial AD plant presented in Table 5.5. Considering the daily variability of input-output data for the AD plant (data range given in Table 5.5), the mean values calculated for the three-month period January–March 2009) was used as the 'default' LCA inventory.

5.4.1.1 Pre-Treatment by Ball Mill

In addition to the electricity consumed in the AD plant operation, the energy required for the mechanical separation process by Ball Mill was also taken into

Table 5.5 Anaerobic digestion of BFMSW (January–March 2009)

Input-output			Total Solid	d content
	Quantity	Range	TS (%)	Range (%)
Material and gas flow				
Input				
Raw feedstock (t/day)	89.72	47.30-111.10	51.73	43.58-57.62
FeCl ₃ ^a (kg/day)	8.58	-	_	_
NaOCl ^b (kg/day)	4.50	_	_	_
Air flow (m ³ /day)	1177.38	482-1851	_	_
Hydrolysis tank-1 ^c	_	_	7.89	2.33-11.83
Hydrolysis tank-2 ^c	_	_	8.15	3.75-15.97
Digester-1 ^c	_	_	4.00	1.16-13.08
Digester-2 ^c	_	_	2.94	0.53 - 5.23
Digester-3 ^c	_	_	3.73	0.47 - 15.85
Output				
Digestate cake (t/day)	16.43	8.0-20.0	43.96	17.40-59.63
RDF(t/day)	34.48	11.36-63.54	41.66	33.08-50.34
Sand(t/day)	18.63	9.0-49.12	50.81	19.02-77.02
Biogas (m³/day)	9719.13	5501-13570	_	_
Energy and water flow				
Input				
Electricity (kwh/day)	1704.70	1116-2801	_	_
Diesel (L/day)	1000	-	_	_
Fresh water (m ³ /day)	150	_	_	_
Recycled water (m ³ /day)	150	_	_	_
Output				
Electricity (kwh/day)	12000.10	5106.7-19635	_	_
Wasted water ^d (m ³ /day)	150	_	1.62	0.07-4.08

Notes

^a FeCl₃ 40 % (w/w) solution, density = 1.43 kg/L

^b NaOCl 16 % (w/w) solution, density = 1.26 kg/L

^c Laboratory tested results: total solid content of feedstock in hydrolysis tank or digester

^d Digest water from dewater process is recycled internally

account. With average 12 operational hours per day assumed, approx 12,000 kWh is consumed in the Ball Mill per day to process 600 t MSW, 36 % of which is the organic fraction digested in the AD plant; therefore, the electricity consumption derived per unit of organic waste was 20 kWh/t.

5.4.1.2 By-Products from Pre-Treatment

On average, 89.7 t waste/day (includes non-biodegradable components) were processed in the AD plant (Table 5.5). After pre-treatment, 36.61 t of upgraded waste mainly containing the organic fractions together with approx 300 m³ water were fed into the hydrolysis tank. The removed components including the inert fraction/sand and the RDF were produced as by-products and sent to the landfill site. However, unlike the BFMSW, these sand/inert materials and RDF are not by-products from digesting foam wastes and so their disposal was excluded from the AD scenario for foam-based products.

5.4.1.3 Biogas Production

Generally it takes 25 days to digest BFMSW in the modelled UK commercial AD system. Biogas was generated as the main product from the digester, varying from 78.23 to 169.21 m 3 /t waste, mainly composed of 65 % CH $_4$, 32 % CO $_2$, and 1 % O $_2$. The composition and yield of biogas (average 116.76 m 3 /t waste) is consistent with the biogas production observed in other EU BFMSW-treatment AD plants (range 85–135 m 3 /t bio-waste) [44].

5.4.1.4 Biogas Upgrading and Water Treatment

Biogas produced was assumed to be upgraded by a desulphurization process. On average, 1,177 m³ air plus 8.58 kgFeCl₃ per day were introduced into the AD digester to remove H_2S . After oxidation by the oxygen molecules from air and precipitation by bonding to ionic iron (from FeCl₃) to form insoluble Fe (HS)₂ and Fe(HS)₃, only trace amounts of H_2S are present in the biogas, which is below the detection limit of the AD biogas monitoring system and was thus considered as negligible.

Besides FeCl₃, another chemical added to the AD system is small amounts of NaOCl for water treatment purposes. Both chemicals were produced in UK: NaOCl was produced by Ineos Chlor Limited at Runcorn and FeCl₃ supplied by Oasis Environmental Ltd at Runcorn and was derived from FeCl₂ which is a byproduct from steel production process. The FeCl₂ produced in steel mills (main one is located in Llanwern) was transported to Runcorn, where the FeCl₂ is converted to FeCl₃ 40 % solution. 23–26 t batches of FeCl₃ were delivered to Huddersfield then 4,000 L FeCl₃ packed with a tank was transported to AD plant.

To model these two chemical inputs, typical European production processes for 15 % NaOCl and 40 % FeCl₃ (Eco-invent v2.0) were selected to represent UK case study, additional transportation between suppliers and AD plant were included as unit processes.

5.4.1.5 Biogas Utilization

Upgraded biogas was transferred to the on-site CHP system to generate heat (wasted) and electricity (exported to grid), which is approx 1.2 kWh/m³ biogas (range 0.7–2.0 kWh/m³). Thus 12,000 kWh/day electricity is produced, which is 100 % exported; this figure is lower than the design capacity of the system (36,000 kWh/day) [57]. Assuming the biogas calorific value is 21.48 MJ/m³ [44], the electrical conversion efficiency in the modelled UK AD plant was estimated as approx 20.35 % (range 11.61–33.38 %), which is very close with observed values for in EU AD plants (20–25 %) but lower than the theoretical efficiency (30–35 %) [44]. Actually, in most of AD systems, up to 50 % of the energy contained in biogas is converted to thermal energy [44]; in other words, in the case of the modelled AD plant, most of the energy content in the biogas—the thermal energy—is unutilised.

Currently, the electricity consumed by the modelled AD process (1,704 kWh/day) was 100 % imported from the national grid; while diesel was the only energy source for heat supply. Based on the current energy balance, around 15.7 % (range: 7.6–31.3 %) of electricity generated from CHP system was estimated to be sufficient for AD plant operation. In comparison with other European AD plants, where the percentage of generated electricity used on-site (parasitic load) ranged between 10 and 40 % [44], the UK commercial AD plant modelled is efficient in terms of its electrical energy utilization.

5.4.1.6 Digestate

Besides the renewable energy produced, post-treated digestate cake (16.43 t/day with 43.96 % TS) is produced and used as a product for landfill cover at the Landfill site. Despite that currently this product is distributed internally free of charge, it could be sold as a commercial product. Actually, a UK survey has suggested that over half of UK composted material including AD digestate was sold (57 %) and the rest was either used on-site (29 %) or distributed free of charge (14 %) and the price fluctuates, averaging at £9.85 per tonne [44]. Therefore, digestate were modelled as a co-product which has economic value and brings benefits.

An 'avoided burdens' allocation approach was applied to the AD electricity and AD digestate produced. The equivalent quantity of electrical power generated by the average electricity supply mix for the UK grid and equivalent quantity of

compost produced via composting process (dry matter basis) were allocated as 'credits' to the modelled AD system.

5.4.1.7 Post-Treatment of Off-Gas

The exhaust gases from the AD plant include fugitive gaseous emissions from pipes or reactors and gas emitted from fuel or biogas combustion [43]. As described in Sect. 5.2.1, exhaust gases except those emitted from diesel combustion, were captured in the enclosed AD system and treated prior to being released to atmosphere. It was assumed that the woodchips applied in bio-filter was negligible compared with large amount of organic waste treated, thus it was omitted from the inventory.

5.4.2 Inventory for Digestion of WBF, PSBF/MSBF Products

Despite the difference in the scales of BMP lab test and industrial AD plant, results obtained from BMP assay could give good indications on digestibility of test material and their energy recovery potential. Actually, a previous study was carried out to compare different scale AD reactors, including BMP pilot scale and industrial scales, it was indicated that ultimate biogas and CH₄ yield from BMP assay and large-scale reactor and their evolution of gas production were similar [30]. Based on the laboratory and industrial data as well as the assumption that labderived data on digestibility and ultimate biogas yields could represent the behaviour of the materials digested in the industrial plant, the inventories for the AD scenarios treating WBF, PSBF/MSBF products are given in Table 5.6. However, there are uncertainties in these inventories as the representativeness of lab data has not been explored in this research. The modelled UK commercial AD plant is a two-stage digestion system with continuous feeding of mixed organic wastes, whereas the BMP assay was a batch feeding lab-scale test. These different conditions could lead to different digestion 'performance'. In further research, comparisons should be carried out to explore the digestibility of WBF, PSBF/ MSBF products under BMP and in a pilot-scale (or commercial scale) two-stage continuous feeding AD system. Moreover, the behaviors of these three biopolymers in mixed bio-waste streams under AD condition should also be explored.

The infrastructure inventory was obtained from WRATE model [23].

5.4.2.1 Energy Input

As shown in Figs. 5.5 and 5.7, foams and cardboard achieved 85–90 % of the ultimate methane production within 5 days and 17 days respectively. An additional one day is needed for the hydrolysis step at the industrial scale AD system

Table 5.6 AD inventory for WBF/PSBF/MSBF products

	WBF	PSBF	MSBF	Cardboard
Unit: per kg received waste				
Baseline scenario input				
Electricity ball mill (kwh)	2.000E-02	2.000E-02	2.000E-02	2.000E-02
Electricity for AD (kwh) ^a	2.684E-02	2.491E-02	2.730E-02	6.949E-02
Fresh water (m ³)	1.672E-03	1.672E-03	1.672E-03	1.672E-03
Recycled process water (m ³)	1.672E-03	1.672E-03	1.672E-03	1.672E-03
FeCl ₃ (kg)	5.174E-04	0.000E+00	0.000E+00	4.464E-04
NaOCl (kg)	5.016E-05	5.016E-05	5.016E-05	5.016E-05
Air flow (m ³)	7.099E - 02	0.000E+00	0.000E+00	6.126E-02
Diesel (MJ) ^b	3.696E+00	3.430E+00	3.760E+00	9.569E+00
Baseline scenario output				
Digestate cake (kg) ^C	1.357E-01	1.342E-01	1.046E-01	1.698E-01
Gasified C (kg) ^d	3.156E-01	2.928E-01	3.210E-01	2.723E-01
Total biogas (m ³) ^d	5.861E-01	5.438E-01	5.961E-01	5.057E-01
Bio-electricity-generated (kwh) ^e	7.117E-01	6.604E - 01	7.239E-01	6.141E-01
Bio-heat generated (MJ) ^f	6.294E+00	5.840E+00	6.402E+00	5.431E+00
Waste water (m ³)	1.672E-03	1.672E-03	1.672E-03	1.672E-03
Best scenario energy balance				
Bio-electricity export (kwh)	6.849E - 01	6.355E-01	6.966E - 01	5.447E-01
Renewable-heat input (MJ)	3.696E+00	3.430E+00	3.760E+00	9.569E+00
Diesel consumed (MJ) ^b	0	0	0	9.534E-02
Transportation				
Waste (ball mill—AD plant) (kgkm)	4.989E+00	4.989E+00	4.989E+00	4.989E+00
FeCl ₃ (kgkm)	4.588E-02	0.000E+00	0.000E+00	3.959E-02
NaClO (kgkm)	8.152E-03	8.152E-03	8.152E-03	8.152E-03
Digestate-to landfill (kgkm)	7.466E+00	7.387E+00	5.759E+00	9.345E+00

Notes

was included so 6 and 18 days were assumed as representative operational times for foam and cardboard degradation respectively. According to daily electricity consumption listed in Table 5.5, around 15.7 % of electricity generated was utilized on-site for AD plant operation; about 0.586 L diesel was used per 1 kWh renewable electricity. On average it takes 25 days to digest BFMSW and therefore, the energy consumed for AD of the foams and cardboard accounting for their various digestibilities was estimated based on the assumption that same amount of electrical and thermal energy as used per unit of BFMSW per day.

^a Digestion periods for foams and cardboard were assumed as 6 days and 18 days respectively

^b Diesel density = 0.85 kg/L; net calorific value = 43.4 MJ/kg [21]

^c It was assumed that 100 % of remained C, and N, S was present in digestate cake

^d Laboratory data; gasified C include CH₄-C and CO₂-C

^e Estimated from the average electrical conversion efficiency in AD plant (1.2kWh/m³ biogas) ^f Net calorific value of biogas was assumed as 21.48 MJ/m³ and the 50 % of the energy contained in biogas was converted to thermal energy [44]

5.4.2.2 Biogas Upgrading

Air flow and FeCl₃ used for desulphurization was estimated based on the data reported by AD plant i.e. 0.9 mg FeCl/m³ biogas and 0.12 m³ air/m³ biogas. As no S elements are contained in MSBF/PSBF, zero air/FeCl₃ input was allocated to these two substrates. Water flow and inputs of NaClO were calculated from the daily consumption data listed in Table 5.5 where the same daily requirement as for the usual biowaste processing at modelled UK AD plant was assumed for the foams or cardboard.

5.4.2.3 Biogas Production

As indicated in Table 5.6, the C degradation and biogas production was obtained from BMP assay. Lab-derived biogas composition differed from the gas composition from BFMSW degradation reported in AD plant, which could be attributable to the two-stage continuous feeding systems where mixed organic wastes were codigested, providing more optimum condition than batch feeding BMP assay. Actually this assumption was confirmed by previous studies. It was found that in two-stage AD system longer SRT is achieved which enables better degradation efficiencies and higher biogas yield [44]. This proportional relation between degradation rate/biogas production and SRT was confirmed by previous study [48]. Moreover, co-digestion system enables adjusting C:N ratio ideally for CH₄ production [66]. Therefore, it was assumed that under industrial scale digestion where highly active bacteria were present, higher conversion efficiency of C from CO₂/ C₂H₄O₂ to CH₄ were achieved from foam/cardboard digestion. According to assumed biogas composition with typical 60-65 % CH₄ and electrical conversion efficiency derived from AD plant, the electricity generation was estimated; whereas wasted thermal energy was calculated based on the assumptions that net calorific value of biogas was 21.48 MJ/m³, 50 % of which was converted to heat [44]. In LCA model, a scenario reflecting current AD technology was built, where the thermal energy generated was wasted, while 100 % of renewable electricity was exported, instead, electrical energy imported from national grid was used for AD system. However, an optimized AD process could be expected in near future. Therefore, the best scenario with an improved efficient energy utilization system was modelled and applied in sensitivity analysis. In best scenario, heat from CHP was assumed to be main thermal energy source, diesel was assumed as surplus source to provide extra heat required; only surplus electricity after satisfying the energy requirement for AD plant operation was assumed as exported products. As shown in Table 5.6, in best scenario, the renewable energy recovered from biopolymers can meet the heat required for the AD process (surplus renewable thermal energy was assumed to be wasted); but in the case of cardboard, surplus diesel input is required. This indicated that, according to the data reported by the studied AD plant, their AD system is not optimised in terms of thermal energy utilization.

5.4.2.4 Direct Emissions

Based on the results reported by Dewil et al. [17], it was assumed that only 0.02~% of S was emitted as H_2S present in biogas and the remaining S was retained in sludge as insoluble iron sulphide complex after the FeCl₃ desulphurization treatment. N_2O emission was considered as negligible following IPCC guidelines. Released NH_3 was estimated according to the equation developed by Anthonisen et al. [3] and an on-line model [1], both of which were based on the pH and temperature dependent relationship between NH_4^+ and free NH_3 .

During the biogas utilization stage, oxidized gases were released (Table 5.7). These together with fugitive gases and emissions from fuel combustion comprised three exhaust gas sources during AD process [43]. In AD scenario, complete biogas combustion was assumed, thus SO₂, NO_x and CO₂ were considered as main products. Besides, the second source was the fugitive gas i.e. the unintentional leakage escaped from opened reactor during operation/maintenance where the major component of biogas CH₄ was the main concern. In previous studies, a low fugitive loss was estimated (0–3 % of CH₄ produced) [43]; as stated by IPCC CH₄ emissions could be close to zero 'where the technical standards for biogas plants ensure that unintentional CH₄ emissions are flared' [32]. In the model of AD plant, a good practice was assumed, i.e. uncontrolled CH₄ loss was considered as insignificant; fugitive loss of other trace gases was also negligible. The third exhaust gases source was diesel combustion, where IPCC Tier 1 approach [32] and EMEP-EEA Tier 1 approach [22] were applied to calculate potential emissions (Table 5.7).

5.4.2.5 Digestate

Besides gasified C, the remained C including un-degraded or partially digested fractions together with other elements e.g. mineralized N or insoluble S are contained in the digestate comprising digested biomass, undigested organic material, anaerobic bacteria and digestion intermediates (Monson et al. [44]. It was assumed that 100 % of residual C, N and S were either transformed to mineralized forms or remained as undigestible fractions left in the digestate. As presented in Table 5.6, approx 0.10–0.17 kg digestate was estimated to be produced per kg foam/cardboard feedstock, which is very close to the data reported by the AD plant (on average 0.18 kg digestate/kg feedstock). Here, only 'functional' components contained in digestate and effective for land reclamation were taken into account, (including organic content and nutrients) and so the 'functional equivalent' quantity (dry basis) of compost produced from a generic composting process (Ecoinvent v2.0 database) was allocated as an 'avoided burden' to AD system.

5.4.2.6 Transportation

As indicated in Table 5.6, the transportations involved in delivery of organic waste from the Ball Mill to AD plant, delivery of chemical inputs and disposal of

WBF **PSBF MSBF** Cardboard Unit: Per kg received waste Emissions from biogas combustion^a CO₂ (kg) 1.157E+00 1.074E+00 1.177E+00 9.985E-01 NOx as NO2 (kg) 5.480E-04 0.000E+000.000E+009.160E - 05SO₂ (kg) 3.496E - 070.000E+000.000E+003.590E-07 Emissions from diesel combustion^b CO₂ (kg) 2.739E-01 2.542E-01 2.786E-01 7.091E-01 1.109E-05 1.029E-05 2.871E-05 CH₄ (kg) 1.128E-05 N₂O (kg) 2.218E-06 2.058E-06 2.256E-06 5.741E-06 NOx (kg) 6.654E - 046.174E - 046.767E - 041.722E-03 CO(kg) 5.545E-05 5.145E-05 5.639E-05 1.435E-04 NMVOC (kg) 2.957E-06 2.744E - 063.008E - 067.655E - 06SO_x (kg) 1.700E-03 1.578E-03 1.729E-03 4.402E - 03TSP (kg) 1.109E - 051.029E - 051.128E-05 2.871E-05 PM10 (kg) 7.393E-06 6.860E - 067.519E-06 1.914E-05 PM2.5 (kg) 3.696E-06 3.430E-06 3.760E-06 9.569E-06

Table 5.7 Emissions from AD of WBF/PSBF/MSBF products

Notes

digestate were included in the inventory. The Eco-invent v 2.0 databases were used to represent the UK transportation process.

5.5 Composting Model

Composting was simulated as another potential biological waste treatment option, where the UK site-specific composting parameters and infrastructures derived from WRATE model was used in model development. To estimate the gases released from degradation of waste materials (foams or cardboard) under composting system, a multi-input inventory approach described by Obersteiner et al. [47] was applied, which takes into account the laboratory-determined elements embodied in the waste and release factors for each element developed from literature data. During meta-analysis, only the results derived from experiments which were carried out under conditions similar to those defined in our composting scenarios were considered. This approach directly associates the waste composition with resulting emissions, gives estimations of element flow in a waste-specific manner; using this approach the specific conditions of different composting scenarios were taken into account. The detailed inventory development is given in Appendix C.

The estimated gas releases from decomposition of waste materials (foam/cardboard) in composting are given in Table 5.8. Another exhaust gas source

^a Complete combustion assumed

^b Tier 1 approach [32, 22]

^c The majority of SOx is SO₂ [22]

Per kg received waste		WBF	PSBF	MSBF	Cardboard
Active home composting	CO ₂ (kg)	1.317E+00	1.283E+00	1.342E+00	9.396E-01
	CH ₄ (kg)	1.228E-02	1.196E-02	1.251E-02	8.761E-03
	N_2O (kg)	1.024E-03			1.711E-04
	NH ₃ (kg)	9.190E - 03			4.694E - 04
Passive home composting	CO_2 (kg)	1.013E+00	9.870E-01	1.032E+00	7.228E-01
	CH ₄ (kg)	1.228E-01	1.196E-01	1.251E-01	8.761E-02
	$N_2O(kg)$	2.012E-03			3.362E-04
	NH ₃ (kg)	8.426E-03			3.418E-04
Industrial composting	CO_2 (kg)	1.330E+00	1.296E+00	1.351E+00	1.367E+00
	CH ₄ (kg)	1.240E - 02	1.209E-02	1.260E-02	1.274E-02
	N_2O (kg)	6.458E-04			3.893E-05
	NH ₃ (kg)	9.482E-03			5.716E-04

Table 5.8 Assumption of N/C gaseous emission factors

assumed was diesel combustion, where IPCC Tier 1 approach [32] and EMEP-EEA Tier 1 approach [22] were applied to estimate the emissions. Besides gasified C/N, the remained fractions were assumed to be contained in mature compost and applied as fertilizer and soil improver (see Table 5.9). The undecomposed organic C can enhance SOM to compensate for the SOM loss caused by intensive agriculture; other elements provides essential nutrients for plant growth [19]. In composting models, the active nutrients (N, S) present in compost were considered as beneficial products. By using 'avoided burdens' allocation approach, the equivalent quantities of commonly applied inorganic N and S fertilizers (NH₄NO₃ and Kieserite) were assumed as 'avoided' products.

However, other potential N gaseous losses (N_2 and NO) was not modelled in composting 'base-line' scenarios, because there is no precise measured data available [61, 28]. As Fukumoto and Inubushi [28] indicated, the difference between the total N loss and the sum of NH_3 , N_2O ranged between 13.3 and 27.8 % of initial N, depending on NO_2^- accumulation. The later figure (27.8 %) which was derived from the tests without addition of mature compost was considered as more representative of the composting modelled in current study thus applied in LCA sensitivity analysis. Sensitivity analysis is presented in Chap. 6 where both N_2 and NO gases were taken into account as potential emissions.

5.6 Landfill Model

In landfill scenarios, highly efficient gas and leachate collection systems were modelled, where assumptions of energy recovery and leachate treatment were mainly obtained from results presented by Manfredi and Christensen [40], Renou et al. [53] and WRATE model [23]. Engineered clay bottom liner and clay cap together with soil cover were modelled; 100 % efficiency for bottom liner was

5.6 Landfill Model 255

Per kg received waste		WBF	PSBF	MSBF	Cardboard
Active home composting	C (kg)	6.947E-02	6.817E-02	5.036E-02	1.763E-01
	N (kg)	4.581E-03			1.644E-03
	S (kg)	8.740E - 04			8.974E-04
Passive home composting	C (kg)	6.947E - 02	6.817E-02	5.036E - 02	1.763E-01
	N (kg)	4.581E-03			1.644E-03
	S (kg)	8.740E - 04			8.974E-04
Industrial composting	C (kg)	6.574E - 02	6.451E-02	4.766E - 02	5.682E-02
	N (kg)	4.581E-03			1.644E-03
	S (kg)	8.740E-04			8.974E-04

Table 5.9 Chemical properties of mature compost assumed

assumed for the first 30 year, after which, deterioration of barrier was taken into account. Besides, a top biological CH₄ oxidation layer with efficiency of 0.1 was simulated which took into account both CH₄ diffusion through cap and CH₄ escape via cracks/fissures [32]. The multi-input inventory approach was used to estimate the emissions/leaching from landfill [47]: the composition of foams and cardboard were correlated with emission factor developed by data-mining to estimate the potential fate of each chemical element embodied in the waste material. The detailed landfill inventory developments are given in Appendix D. The calculated energy balances and chemical element fates are summarized in Tables 5.10 and 5.11.

As shown in Table 5.10, 100 % of the heat produced from landfill gas combustion was not recovered; taking into account the in-plant electricity consumption, the net electric energy exported varied between 3.8 and 3.9 MJ for per kg foams, but much less surplus electric energy was produced from landfilled cardboard due to its low biodegradability. Besides electricity input, diesel consumption during on-site operation was also considered.

As presented in Table 5.11, within 100 year time horizon, uncollected landfill gases containing CH_4 , CO_2 , and trace amount of H_2S , NH_3 , N_2O and N_2 diffused through the landfill cover or escaped via cracks/fissures; only 10 % of diffused CH_4 was oxidized by oxidation cover. Collected landfill gas underwent complete combustion in CHP system where oxidized products CO_2 , N_2O , and SO_2 plus trace amount of un-destructed H_2S fraction were main emissions. Besides, another exhaust gas source—diesel combustion was also included in LCA model where IPCC Tier 1 approach [32] and EMEP-EEA Tier 1 approach [22] were adopted to estimate emissions.

The C/N leachate and storage were modelled in current LCA study. Up to 80 % of TOC and 99.5 % of $\mathrm{NH_4}^+$ were removed during leachate treatment; the total leachate over 100 years including the portion discharged to surface water and the untreated fractions released to ground water are presented in Table 5.11. There was no S leachate assumed; however, the precipitated HS $^-$ could be oxidized and emitted slowly to aquatic recipients as $\mathrm{SO_4}^{2-}$ in long-term when complete degradation of organic material achieves and landfill turns to aerobic [46].

Table 5.10 Energy balance of landfill scenarios

MJ/kg received waste	WBF	PSBF	MSBF	Cardboard
Total Electricity generated ^{a, b}	4.436E+00	4.323E+00	4.515E+00	2.169E+00
Thermal energy generated ^{a, b}	6.654E+00	6.485E+00	6.773E+00	3.254E+00
Electricity exported	3.914E+00	3.815E+00	3.984E+00	1.914E+00
Diesel consumption ^{c, d}	8.701E-02	8.701E-02	8.701E-02	8.701E-02

Notes

Table 5.11 C. N and S fate

Kg/kg received waste	WBF	PSBF	MSBF	Cardboard
C fate				
CO ₂ fugitive from landfill	6.788E - 02	6.615E-02	6.909E - 02	3.319E-02
CH ₄ fugitive from landfill	2.216E-02	2.159E-02	2.255E-02	1.083E-02
CO ₂ from CH ₄ oxidation	6.770E - 03	6.598E - 03	6.891E-03	3.310E-03
CO ₂ from biogas plant	1.220E+00	1.189E+00	1.242E+00	5.967E-01
TOC leachate	5.677E-04	5.571E-04	4.116E-04	3.724E-02
Stored C	6.723E - 02	6.597E - 02	4.874E - 02	2.093E-01
N fate				
NH ₃ fugitive	1.554E-04	_	_	1.399E-05
N ₂ fugitive	2.884E - 04	_	_	2.161E-05
N ₂ O fugitive	2.386E-05	_	_	1.608E-06
NO ₂ from biogas plant	1.276E-02	_	_	1.010E-03
NH ₄ ⁺ leachate	5.422E-05	_	_	6.708E-04
NO ₂ ⁻ leachate	1.663E - 04	_	_	4.778E-05
NO ₃ ⁻ leachate	0.000E+00	_	_	1.920E-05
Stored N	0.000E+00	_	_	9.878E-04
S fate				
H ₂ S fugitive gas	4.643E - 05	_	_	4.768E-05
H ₂ S from biogas plant	4.179E-06	_	_	4.291E-06
SO ₂ from biogas plant	7.787E-04	_	_	7.996E-04
HS ⁻ precipitated	4.506E-04	_	_	4.627E-04

Simulated results showed that a significant fraction of C remained in landfill system within 100 years, which accounted for 11.5–15.5 and 47.7 % of total C content for foams and cardboard respectively. This C sequestered in the landfill represented potential CO₂/CH₄ emissions in longer period: for fossil C (e.g. PVOH-C) GWP burdens under infinite timeframe could be expected; in the case of biogenic C (e.g. cardboard-C), uptake of CO₂ during plant growth would be partially balanced by the CO₂ emission. As indicated in Table 5.11, a fraction of N (46 %) contained in cardboard was also stored in landfill site, which may be

^a Density $CH_4 = 0.717 \text{ kg/m}^3$, $CO_2 = 1.977 \text{ kg/m}^3$

b Net calorific value of landfill gas is 19 MJ/m³ [20, 12]

^c Diesel consumption derived from WRATE model [23]

^d Diesel density = 0.85 kg/L; net calorific value = 43.4 MJ/kg [21]

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removed through leachate or gas proportionally in a longer time horizon. Such influences of temporal boundary on environmental profiles were analyzed in sensitivity analysis.

5.7 Discussion

In summary, various end-of-life scenarios as well as their inventory development are presented in this chapter. The main findings are as follows:

- 1. The activity assay conducted on inocula confirmed that highly active microbial populations were present (hydrolic, acidogenetic bacteria, acetogens, aceticlastic methanogens); the BMP assays carried out at I/S ratio 1 and 3 indicated that higher I/S ratios led to greater CH₄ production per unit of substrate loaded in the initial phase but not over the whole digestion process. Generally, the BMP assay indicated that approx 58-62 % biodegradation of WBF/MSBF/ PSBF is achievable under anaerobic conditions; statistic analysis suggested that WBF was the most biodegradable polymer with greater cumulative CH₄ production and conversion efficiency than the alternative starch-based foams, especially within the modelled initial incubation period; whereas the biodegradability of cardboard varied between 46 and 54 %, depending on the I/S ratio. However, the results derived from lab batch assay only gave indicative information on the biodegradability of WBF/PSBF/MSBF/cardboard; in the industrial scale two-stage continuous feeding AD system where microbial populations with higher activity can be expected due to the optimized conditions, greater biodegradation and energy recovery could be achievable.
- 2. Co-existence of multiple microenvironments were modelled in the end-of-life scenarios, which led to complex multiple C/N transformation processes occurring simultaneously. Comparing the C fates, a similar C distribution was found across the biological treatments and the landfill scenarios i.e. gas emission especially CO₂ being the dominant C loss. Amongst all the waste treatment routes, passive composting induced the greatest fugitive CH₄ release, followed by landfill, where most of the CH₄ emission was collected (90 %) with the rest partially oxidized (1 %) to CO₂. Besides the gas phase, C leachate was only involved in the landfill scenario. A fraction of C was assumed to remain in the solid form, but their fates differed between the biological treatments and landfill: the former brought beneficial effects by using digestate/compost for land reclamation and SOM enhancement purposes; the latter acted as a net C sink where non-active C was assumed to be sequestered C. In contrast to C, only cardboard and WBF were modelled to be involved in the N and S element flows. Amongst the N emissions, NH₃ was modelled to be the dominant gas in all the end-of-life scenarios, but its fate varied: in AD and landfill where gas collection systems are applied, the majority of NH₃ produced is converted to NO_x via gas combustion; but in composting, NH₃ was directly released to

atmosphere. Another important N gas was N₂O. Composting, especially passive composting, was modelled as an important N2O producer; landfill incurred much lower N₂O release than composting, which was attributable to the landfill gas collection system and the further transformation of N2O into N2 via complete denitrification processes (due to the long residence times of N₂O in landfills). Apart from the gas phase, N leachate and N in the solid phase were also included. The former was involved in landfill scenarios; the latter was either modelled as active nutrients in biological treatments for fertilizer/compost substitution purposes or simulated as non-active elements stored in the landfill site. Only gas and solid phases were concerned in S element flows. In the AD system, due to the desulphurization treatments by addition of O₂ and FeCl₃, only trace amount of H₂S were assumed to be present in biogas and eventually converted into SO₂ through biogas combustion. But in the landfill scenarios, large fraction of S (50 %) was either released as fugitive H₂S or as combustion product SO₂, whilst the remaining S was assumed to be precipitated.

- 3. Home composting represented an advantageous option over other waste treatment routes in terms of infrastructure and transportation 'savings'. However, the two different operation modes of home composting were differentiated; in the case of passive composting, these saving effects could be overridden by the greater GHGs released (CH₄, N₂O) from anaerobic zone development.
- 4. Compared with industrial composting, which only acts as an energy consumer, AD and landfill systems export renewable-resource-derived electricity, which are generated via biogas/landfill gas combustion. Despite the similar compositions of AD biogas and landfill gas, the greater CH₄ portion and higher net calorific values were assumed for AD due to the initial aerobic digestion phase in the landfill site. However, interestingly (see Table 5.12) greater surplus electricity export was estimated for landfill than AD mainly due to the different degradation rates and electricity conversion efficiencies modelled in the two scenarios. This suggested that inconsistency in data sources between different scenarios and assumptions made in the LCA model can introduce substantial uncertainty in the outcomes of LCIA comparisons. In the current study, sensitivity analysis was carried out on the key parameters assumed for landfill energy generation—these are presented in Chap. 6.
- 5. AD scenarios were based on primary data collected from industry or laboratory experiments. In the baseline AD scenario, which represented the current technology in the studied AD plant, both electric energy and heat consumed onsite were mainly derived from fossil resources; this baseline scenario showed much greater electricity and diesel consumption than any other disposal routes, which suggested AD as an energy intensive technology. But actually there is great energy saving potential achievable via AD system optimization. In contrast with the baseline scenario, the best case scenario gave a good insight into the potential impacts of future optimized of the AD plant; it was modelled by assuming renewable resource based energy was the main energy source for plant operations with only surplus 'green' electricity exported. Unlike the AD

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Table 5.12 Comparison between AD and landfill scenarios

	WBF	PSBF	MSBF	Cardboard
AD				
Biogas composition	65 % CF	I ₄ 35 % CO	O_2^a	
Net calorific value of biogas	21.48 M	J/m ^{3 b}		
Biogas release (% total C) ^a	72.097	68.572	75.417	62.018
Electricity export (% energy content of biogas) ^a	19.586	19.586	19.586	18.051
Landfill				
Landfill composition	50 % CF	I ₄ 50 % CO	O_2	
Net calorific value of biogas	19 MJ/m	3 C		
Landfill release (% total C)	86.712	87.048	90.482	42.352
Electricity export (% energy content of biogas) ^c	30	30	30	30

Notes

scenario, landfill and composting were modelled by applying multi-input inventory approach. Although there are uncertainties in both scenarios, the most likely biodegradability of each component contained in the foams or cardboard have been estimated via data screening. The potential fate of each element embodied in the foams or cardboard were simulated by associating lab-determined chemical element results with the most representative release factors published in previous studies. This modelling approach was deemed to give good indications on the performance of the studied materials in different end-of-life scenarios; several of the key parameters assumed were also examined via sensitivity analysis. However, in future, further in-depth research is recommended to gain better understanding of the biodegradation of WBF/PSBF/MSBF and element flows in biological treatment systems.

6. Unlike the other end-of-life scenarios, the landfill scenario concerned an important temporal boundary which could be a critical parameter and a main source of uncertainty in LCAs, especially for the impact categories relating to emissions and leachate [36]. In the current LCA model, a surveyable timeperiod (100 years) was defined as the system boundary due to the fates of compounds beyond this time being considered as uncertain and unpredictable [47]. However, previous authors [46, 7] have stated an alternative view—that waste will decompose until all organic matter is exhausted and the landfill will turn to aerobic in the long-term. Thus, as discussed in Sect. 5.6, this temporal boundary issue could influence the fate of chemical elements stored in the materials e.g. precipitated HS-, PVOH-C sequestered and cardboard-N stored, which may be removed either through leachate or gas under an infinite time horizon and eventually released to environment. In the current study, efforts were made to study the sensitivity of the LCIA outcomes to this temporal boundary, but certainly, further exploration and in-depth research is needed on this issue.

^a Laboratory results and data collected from AD plant

^b [44]

c [20, 12, 29]

5.7.1 Key Findings

The highly active microbial populations were present in the inocula studied. Laboratory results indicated that under anaerobic conditions and with active inocula, approx 58–62 % biodegradation of WBF/MSBF/PSBF was achieved whereas biodegradability of cardboard varied between 46 and 54 %.

Amongst various end-of-life scenarios modelled, AD was the most energy-intensive process whereas home composting represented an advantageous option in terms of energy inputs.

The complex multiple C and N transformation processes were modelled. Across the end-of-life scenarios, gas emission especially CO_2 was the dominant C loss. The passive home composting scenario induced the greatest fugitive CH_4 release, followed by landfill. NH_3 was emitted from WBF and cardboard degradation in all the end-of-life scenarios, but its fate varied: in AD and landfill the majority of NH_3 produced is collected and converted to NO_x via combustion; but in composting, NH_3 was directly released to atmosphere.

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Chapter 6 LCA of WBF Products Over Whole Life Cycles

6.1 Introduction

Only few LCA studies (in English) on starch-based blends were found public ally accessible [3, 5, 9, 10]; moreover, the literature review suggested that only limited biological treatments were covered in those LCA models except for two studies [3, 10], which modelled both aerobic and anaerobic degradation. However, the models presented by Estermann et al. [3] and Wang et al. [10] were either based on assumptions or not transparent in terms of inventory data.

Actually, as indicated in previous LCAs, the end-of-life scenarios could play significant role in LCA comparisons of starch-based blends and petrochemical polymers. For instance, landfill acts as a net C sink, depositing fossil C embodied in petrochemical polymers whereas starch-based blends undergo biodegradation and release landfill gas, which offers advantages to conventional polymers in terms of GWP profiles; on the contrary, both fossil and biogenic C are released via incineration; even with lower calorific value, starch-based blends still showed lower GWP impacts and fossil energy consumptions than petrochemical polymers [8].

In the current study, cradle-to-grave LCIA comparisons between WBF and petrochemical polymers were modelled. Based on the inventory presented in Chap. 5, various end-of-life scenarios for WBF waste treatments were modelled.

6.2 Product System

The product systems over the whole life cycles of the WBF products as well as the equivalent petrochemical products are given in Fig. 6.1; their end-of-life scenarios are specified in Table 6.1.

Generally, the infrastructure and auxiliary material inputs, energy consumptions, short-term or long-term emissions and residue waste treatment were considered within the system boundary of end-of-life scenarios. As given in Chap. 5,

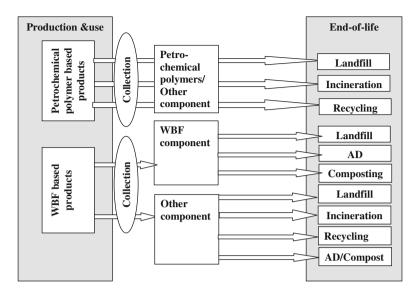


Fig. 6.1 System boundaries of WBF products vs. petrochemical products

'green' electrical/thermal energy and composts were modelled as the major products from biological treatments of WBF whereas in the case of petrochemical polymers, the renewable energy (electricity/thermal) and the recycled polymers were assumed as the products from incineration and recycling processes, respectively. In waste treatment processes, system expansion allocation approach was applied where the equivalent quantity of electrical/thermal power generated by the average UK supply mix and plastics/fertilisers produced via EU average process was assumed as 'avoided products'.

6.3 Inventory Data

6.3.1 End-of-Life Scenarios

The end-of-life inventories for WBF products were given in Chap. 5, where the primary data developed from industry and laboratory experiments were supplemented with other secondary data sources e.g. publications, database and models.

The inventory for waste treatments of petroleum polymers was primarily derived from Ecoinvent database v2.0 but with the inclusion of net energy export from incineration [4]. Key assumptions regarding their end-of-life scenarios are summarised in Table 6.2.

Table 6.1 End-of-life scenarios

Case study		End-of-life	Data source
Cool box	LDPE	LDPE recycled + cardboard recycled	Assumptions
		LDPE incinerated + cardboard incinerated	
		LDPE land filled + cardboard land filled	
		LDPE land filled + cardboard recycled	
		LDPE incinerated + cardboard recycled	
	WBF	WBF anaerobic digested + cardboard recycled	Assumptions
		WBF home composted + cardboard recycled	
		WBF industrial composted + cardboard recycled	
		WBF land filled + cardboard recycled	
		WBF land filled + cardboard land filled	
		WBF home composted + cardboard home composted	
		WBF industrial composted + industrial composted	
		WBF anaerobic digested + cardboard anaerobic digested	
Display board	HDPE	100 % incinerated	Assumptions
		100 % recycled	•
		100 % land filled	
	WBF	100 % anaerobic digested	Assumptions
		100 % home composted	•
		100 %industry composted	
		100 % land filled	
Trough mould	EPS	Case 1 and 2—recycled by Cordek	Cordek Ltd
		Case 3—100 % land filled	
		Case 4 and 5—recycled by EPS foam manufacturer	
	WBF	100 % anaerobic digested	Assumptions
		100 % home composted	
		100 % industry composted	
		100 % land filled	
Concrete	EPS	100 % incinerated	Assumptions
formwork		100 % recycled	
		100 % land filled	
	WBF	100 % anaerobic digested	Assumptions
		100 % home composted	
		100 % industry composted	
		100 % land filled	

6.3.2 Transportation

Table 6.3 present the primary data as well as key assumptions on transportation distance and mode, where the home composting is excluded due to no transportation involved.

End-of-life	Assumptions			References	
Incineration		Electricity export	Thermal energy	Ecoinvent database V 2.0	
	PE	5 MJ/kg	10.02 MJ/kg		
	EPS	4.51 MJ/kg	9.05 MJ/kg		
Recycling	Close-loop recy	veling Substituted products	Electricity consumption	Ecoinvent data base V 2.0 Nextek Ltd	
	LDPE/HDPE EPS	PE granulate Expandable PS	0.75 kWh/kg 0.6 kWh/kg	Caledonian Industries Ltd	
Sanitary landfill	Time horizon: 100 years		_	Ecoinvent data base V 2.0	
		Biodegradability	Electricity export		
	PE	1 %	0		
	EPS	1 %	0		

Table 6.2 Key assumptions for waste treatments of petrochemical polymers

Table 6.3 Transportation data

Case studies	EPS/PE	WBF (except home composting) ^a	Data Source
Coolbox	100 km 16 t lorry	100 km 16 t lorry	Assumptions
Display board	100 km 16 t lorry	100 km 16 t lorry	Assumptions
Trough mould 1	321 km 32 t lorry	100 km 32 t lorry	Cordek Ltd
Trough mould 2	207 km 32 t lorry	100 km 32 t lorry	assumptions
Trough mould 3	100 km 32 t lorry	100 km 32 t lorry	
Trough mould 4	42 km 32 t lorry	100 km 32 t lorry	
Trough mould 5	35 km 32 t lorry	100 km 32 t lorry	
Concrete formwork	100 km 32 t lorry	100 km 32 t lorry	Assumptions

^a Notes No transportation is required for home composting of WBF products

6.4 Cradle-to-Grave LCIA Results

The 'cradle-to-grave' LCIA profiles of WBF and its equivalent petrochemical polymers in various applications are presented in this section; the diverse end-of-life scenarios were compared to identify the optimal option for WBF waste treatment.

6.4.1 Display Board Case Study

The display board is given as an example to interpret the contribution analysis of end-of-life scenarios for WBF products.

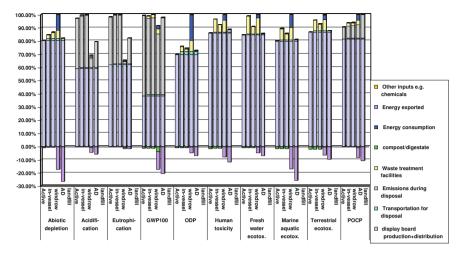


Fig. 6.2 Characterised LCIA profiles for life cycle of WBF display board (unit per display board)

6.4.1.1 End-of-Life Scenarios for WBF Display Board

As given in Fig. 6.2, over the whole life cycle of display board, WBF production process was the dominant factor driving the environmental impacts on most of the impact categories except GWP100, where over 50 % of burdens were caused by the GHGs emitted during WBF disposal.

Irrespective of the WBF production process, the main contributors to impacts of end-of-life scenarios (except AD) on acidification, eutrophication, GWP100 and POCP were the gases and leachate produced from WBF degradation, which were either released directly to environment (e.g. from composting or fugitive gas) or emitted in oxidised form (via combustion). The former i.e. direct emissions dominate the environmental profiles of composting scenarios: NH₃ accounted for over 95 % of both eutrophication and acidification impacts; CO₂ was presented as the most important GHG, sharing 70-90 % of GWP100 impacts. Besides, fugitive gas CH₄ occupied approx 70-90 % of POCP burdens of both landfill and composting systems. The latter (gas emitted from combustion) was involved in landfill scenarios, where N/S oxidized gases (NO_x, SO_x) released from the CHP system accounted for over 90 % burdens on eutrophication and acidification whereas CO₂ emission from biogas/landfill gas combustion was presented as major GHG (over 70 %). Apart from the two exhaust gases sources discussed above, emissions from fuel (diesel) combustion were modelled as a third source: they played significant roles in the environmental profile of AD scenario, which occupied 60-90 % of the positive score on acidification, eutrophication and POCP due to NO_x and SO_x release. Similar to landfill, about 70 % of GWP100 positive score of AD scenario was caused by the CO₂ released from the CHP system.

The inclusion of infrastructure and energy inputs in end-of-life scenarios incurred extra burdens on abiotic depletion, ODP, and toxicity impact categories. Especially for industrial composting where irrespective of negative score, infrastructure input appeared as the dominant factor accounting for above 90 % of the positive toxic score, approximately 90 % of abiotic depletion and 70-95 % of ODP impacts. Their toxic impacts were mainly caused by the emissions from steel production e.g. mercury, chromium, arsenic released to atmosphere and the metallic ions emitted to water (nickel, vanadium); whilst both steel and bitumen production (oil resource depletion as well as CBrF₃ released from oil production) were dominant contributors to ODP burdens and resource depletion. Different from composting system, AD was shown as most energy intensive process. Considering positive environmental scores only, energy consumed in AD scenario especially diesel not only shared approx 15-50 % toxic impacts but also dominated ODP impacts and abiotic depletion (60–70 %) due to crude oil depletion and the emissions from crude oil production (PAH, barite, barium CBrF₃), atmospheric pollutants released from fuel combustion during diesel refinery e.g. vanadium, mercury. Besides, infrastructure also played important roles in the AD process: 50-80 % of toxic impacts were attributable to emissions (chromium/nickel/mercury) from infrastructure material steel production process. However, landfill scenario was exceptional, where infrastructure and energy only made marginal contributions to categories indicator results; as for home composting, the simplicity of the infrastructure system plus the avoidance of energy input brought nearly zero resource depletion ODP and toxic burdens.

Apart from the contributors discussed above, other inputs including chemicals or transportation only incurred marginal impacts (less than 5 %); especially the home composting, no transport is required for WBF disposal. However, it should be borne in mind that the transportation modelled in current LCA was based on assumptions; varying transport input in reality could change the environmental profiles especially on abiotic depletion and ODP where crude oil consumption and CBrF₃ released from oil production dominated.

The products generated from end-of-life scenarios, including energy and compost/digestate, brought environmental credits to 'cradle-to-grave' LCIA profiles of WBF by energy substitution or avoidance of artificial fertilisers. Especially in active home composting and landfill scenarios, a disposal process with negative impacts on ODP and toxicity impact categories were shown because the saving effects were sufficient to offset the burdens caused by the disposal process.

In general, amongst five disposal routes, AD was presented as the best option on acidification, eutrophication, and GWP100 due to less emission evolved and greater 'saving' effects by energy substitution; on the contrary, composting brought high emission profiles (NH₃ and CO₂). AD appeared as the second best choice in terms of POCP and abiotic depletion, however, on other impact categories the advantages gained from electricity and digestate export were overridden by the extra burdens resulting from infrastructure and energy inputs in AD scenarios. Both active home composting and landfill appeared environmentally superior to other biological treatment options on abiotic depletion, ODP, human

and eco-toxicity whereas industrial composting especially in-vessel technology represented the inferior choice on almost all impact categories except ODP where AD incurred highest impacts. This can be explained by the low infrastructure and energy inputs to landfill and home composting systems, high energy/infrastructure consumption but low beneficial products assumed in industrial composting scenarios. However, the landfill modelled here was based on survey able temporal scale (100 years) and the assumption of a highly efficient energy recovery system; an increase in environmental burdens of landfill scenarios could be expected by inclusion of an infinite time horizon and a system with low energy recovery.

6.4.1.2 Comparison of WBF and HDPE Display Board

The 'cradle-to-grave' LCIA comparison between WBF and HDPE is given in Fig. 6.3. Amongst three disposal options for HDPE, recycling appeared as the optimal choice on almost all impact categories, except ODP and terrestrial ecotoxicity, both of which were highly relevant to the energy profiles. The former was driven by the halon emissions during primary energy production or delivery e.g. the CBrF₃ emitted either from crude oil production or CClBrF₂ released during transporting natural gas. The latter (terrestrial eco-toxicity) was related to the emissions from fuel combustion process or electricity transmission e.g. mercury emitted from hard coal burning. Differently, other impact categories were primarily driven by the HDPE making process e.g. abiotic depletion was dominated by the fuel consumption for HDPE production. Besides, the C fate during the disposal phase played an important role in GWP100 profiles: landfill acted as a net C sink whereas the fossil C continued in HDPE released back to atmosphere during incineration. These explained the comparison results indicated in Fig. 6.3:

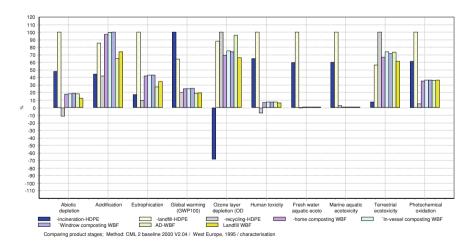


Fig. 6.3 Characterised LCIA profiles for life cycle of WBF and HDPE display board (unit per display board)

energy or plastic substitution in HDPE recycling/incineration scenarios were sufficient to offset overall environmental burdens of the HDPE life cycle and lead to a display board with negative scores on ODP, abiotic depletion or human toxicity; but HDPE recycling/incineration incurred even higher ODP and terrestrial ecotoxic impacts/GWP100 burdens than landfill due to extra energy required for recycling/GHGs released from incineration.

Generally over its whole life cycle, WBF display board delivered a better performance than HDPE with landfill scenario on most of the impact categories except acidification and terrestrial eco-toxicity. Attributable to the atmospheric emissions NH₃ from WBF biodegradation, composting led to higher acidification impacts than HDPE land filling; whilst the advantage of HDPE over WBF on terrestrial eco-toxicity was carried through from production process. However, it is not the case of the other two HDPE life cycles: HDPE incineration scenario benefited from electric and thermal energy recovery, delivering much better environmental profiles than WBF life cycle in terms of ODP, acidification eutrophication and terrestrial eco-toxicity; due to avoidance of virgin HDPE making the HDPE recycling scenario appeared as a green system with lower impacts on most of impact categories than WBF life cycles.

6.4.1.3 Normalised LCIA Results for Display Board

The normalised LCIA profiles of display board (Fig. 6.4) give interpretations of the magnitudes of each category indicator results to the reference system West Europe 1995. For a conventional HDPE display board system with landfill or incineration scenarios, aquatic eco-toxic impacts appeared relatively significant due to the vanadium ion released from the disposal stage. Besides, abiotic depletion and GWP100 indicator results were relatively significant. In comparison with these two disposal routes, HDPE recycling brought significant saving effects, causing a clear shift in significance of impact category results: acidification shifted to first place, whereas GWP100 moved to second place; in addition, its resource savings were of significance.

The superior profiles of WBF display board over HDPE on abiotic depletion, GWP100, human and aquatic ecotoxicity were suggested as significant. Marine aquatic ecotoxic impact appeared as most significant for WBF display board as well, but different from HDPE, the main causes were infrastructure involved in WBF and its feedstock (e.g. PVOH) production stage (metallic ion released from disposal of slag or ash during metal production). Acidification indicator results ranked as the second most significant for WBF display board life cycle primarily due to the acidifying emissions from wheat farming and the WBF production stage and partially attributable to gases (e.g. NH₃, SO₂) released either from WBF degradation or biogas/fuel combustion at disposal phase. For WBF, the environmental advantages of AD/landfill (energy recovery) over other biological treatments were relatively significant on acidification and eutrophication. Apart from acidification, abiotic depletion, eutrophication and GWP100 indicator results were

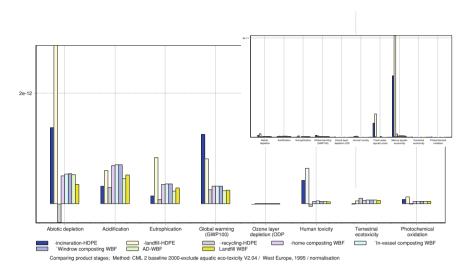


Fig. 6.4 Normalized LCIA profiles for life cycle of HDPE/WBF display board (unit: per display board). *Notes* Insert histogram includes aquatic eco-toxicities which are excluded from the main histogram due to problem of scale

suggested as relatively significant for the WBF display board life cycle as well. As analyzed in Sect. 6.4.1.1, C/N gases (CO₂/NH₃/NO_x) evolved from the WBF disposal stage were one of the primary causes for impacts on eutrophication and GWP100, which together with the acidifying emissions (NH₃/SO₂) concern major options for improvements in waste treatments. As illustrated in Fig. 6.4, across all display board case studies, impacts on terrestrial toxicity, ODP, and POCP were of little significance.

Despite the fact that normalised results discussed above offered a good insight into the relative contribution of display board life cycle to environmental problems; it only provided reference information depending on temporal and spatial scales. The influences of the reference system were considered in sensitivity analysis.

6.4.2 Coolbox Case Study

To illustrate the environmental profiles of coolbox insulated with LDPE and WBF, case studies with local distribution are given as examples.

6.4.2.1 End-of-Life Scenarios for LDPE Coolbox

Figure 6.5 gives 'cradle-to-grave' LCIA profiles for the LDPE coolbox against its environmental profiles at the distribution stage. Generally, the inclusion of end-of-

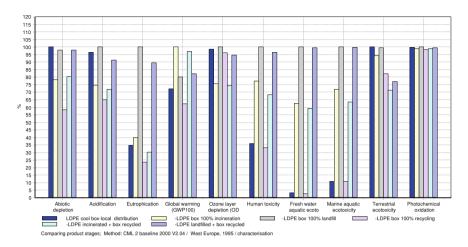


Fig. 6.5 Characterised LCIA profiles for life cycle of LDPE coolbox (unit: per box)

life (except 100 % recycling) led to an increase in environmental burdens on eutrophication, GWP100, human and aquatic eco-toxicity but not the rest of the impact categories where the 'savings' brought about by energy or virgin polymer/cardboard substitutions were sufficient to offset the extra burdens caused by waste treatment process. In contrast with recycling scenario (LDPE coolbox 100 % recycled) which represents the environmentally superior option, landfill of the whole LDPE coolbox incurred the highest burdens on almost all impact categories except GWP100 where landfill benefited from net C sink effects. End-of-life with incineration treatment delivered high GWP100 burdens due to the CO₂ generated from LDPE/cardboard combustion.

Amongst five disposal routes, two landfill-related scenarios delivered higher impacts on eutrophication, human and aquatic eco-toxicity due to the LDPE land filling, which was presented as the factor driving the environmental scores of the LDPE coolbox (over 70 %). Specifically speaking, COD release and metallic ions, especially vanadium emitted form landfill acted as main contributors (the former cause eutrophication, latter cause toxicity impacts). Although two incineration scenarios delivered better performance than landfill on human and aquatic ecotoxicity impact categories, they increased toxic impacts substantially compared with the distribution stage. It is mainly attributable to the vanadium ion released from LDPE incineration, which accounted for over 70 % of positive human and aquatic eco-toxic impacts; but these extra burdens were partially offset by the beneficial effects of energy recovery. The recovered energy not only influenced toxicity impacts, but also brought benefits to other impact categories, especially on abiotic depletion, acidification and ODP where the incineration process showed negative scores. Different from other impact categories, no significant difference was found between the POCP impact of LDPE coolbox systems with diverse disposal routes, which indicated that the production process was the dominant POCP contributor (the pentane release owing to use of pentane as a blowing agent during foam transformation).

Amongst all the scenarios assuming cardboard recycled, recycling was indicated as the best option for LDPE disposal in terms of environmental profiles except ODP and terrestrial eco-toxicity, both of which were driven by energy profiles thus incineration benefited from energy recovery delivering superior ODP and terrestrial eco-toxic profiles. Overall, a 100 % recycling scenario was suggested as a relatively optimal disposal route for the LDPE coolbox system.

6.4.2.2 End-of-Life Scenarios for WBF Coolbox

The environmental profiles for the WBF coolbox life cycle are presented in Figs. 6.6 and 6.7 in comparison with its distribution stage.

As indicated in Fig. 6.6 where the end-of-life of cardboard is identical, the comparisons of results between disposal routes for WBF component were similar to the display board: AD represented an environmentally superior choice to other disposal routes on acidification, eutrophication and GWP100 but not on the rest of impact categories where home composting and landfill were shown as better options. As interpreted in Sect. 6.4.1.1, the contribution analysis on the disposal process indicated that: emissions released either from WBF degradation or from biogas/landfill gas combustion were the dominant factors on acidification, eutrophication, GWP100 and POCP, whereas energy and infrastructure not only brought resource depletion but also played significant roles in ODP and toxicity impact categories. In addition, the renewable energy and digestate/compost during the WBF waste treatments brought environmental savings by avoidance of artificial fertilizer and energy substitution; these effects together with the benefits of

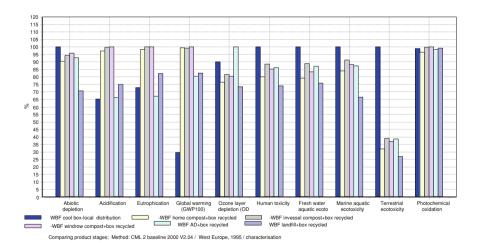


Fig. 6.6 Characterised LCIA profiles for life cycle of coolbox with box recycled and WBF biologically treated (unit: per box)

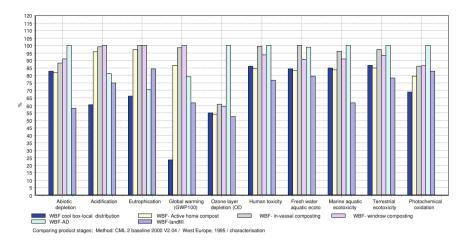


Fig. 6.7 Characterised LCIA profiles for life cycle of WBF coolbox with 100 % biological treatments/landfill scenarios (unit: per box)

cardboard recycling were sufficient to offset the burdens caused by the disposal process leading to WBF coolbox end-of-life with resource savings and negative toxic impacts (Fig. 6.6).

As suggested in Figs. 6.6 and 6.7, the disposal of the cardboard component is an important factor in 'cradle-to-grave' LCIA profiles of the WBF coolbox: the inclusion of cardboard recycling reversed comparison results between coolbox life cycle and distribution stage on most impact categories. As shown in Fig. 6.8 (irrespective of production processes) driven by infrastructure and energy inputs, home composting was indicated as a superior biological treatment option for cardboard. On the contrary, AD showed inferior profiles on most impact categories (due to the high diesel and infrastructure involved and relatively low efficiency in energy recovery). In comparison with home composting, higher toxic and ODP profiles for industrial composting and AD were found; it was caused by the emissions from crude oil production and infrastructure materials manufacturing (steel, bitumen etc.) e.g. the atmospheric emissions CBrF₃, Hg, chromium and the water emissions barite, barium, vanadium ions, nickel ions. Similarly, diesel was shown as the dominant factor in the POCP, acidification and eutrophication impacts of cardboard AD, i.e. the pollutants emitted during diesel combustion (NO_x and SO_x). Different from other impact categories, the GWP100 score was highly dependent on the cardboard degradation: industrial composting with high degradation assumptions brought greater GHGs profiles whereas cardboard landfilling was presented as a net C sink delivering the best GWP100 score. In AD scenario, besides the CO₂ released from biogas burning, combustion diesel burning was another GHG source, all of which were partially balanced by the beneficial effects of energy recovery from cardboard.

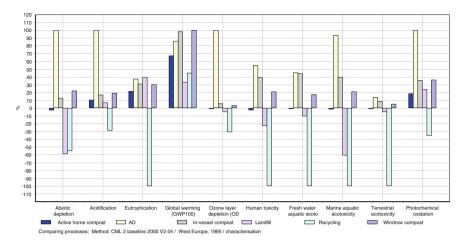


Fig. 6.8 Characterised LCIA profiles for end-of-life scenarios of cardboard (unit: kg cardboard)

In summary, either AD or active home composting was ranked as the optimum biological treatment for WBF depending on impact categories concerned. The findings for disposal of cardboard differed from WBF due to their different chemical composition. The former (cardboard) contains much lower N elements than the latter (WBF), whereas N releases (NH₃) from bio-polymer decomposition during composting was indicated as the primary driver for acidification and eutrophication scores; thus on acidification and eutrophication composting was a superior choice (to AD) for cardboard but not for WBF. Additionally, the benefits of energy recovery from cardboard digestion were not as sufficient as WBF due to the cardboard lignin barrier which inhibited the microbial access to biomass. Overall, for cardboard waste, conventional recycling was suggested as the best disposal route, followed by landfill and active home composting. Landfill appeared as an environmentally friendly choice for the WBF coolbox especially on abiotic depletion, ODP and toxic categories, which was attributable to the temporal scale modelled (100 years) and efficient energy recovery assumed.

6.4.2.3 Comparison of WBF and LDPE Coolbox

To illustrate the comparison of LDPE and WBF insulation over life cycle, the 'cradle-to-grave' LCIA profiles of coolbox systems with identical cardboard disposal (recycling) are given in Fig. 6.9. In general, the WBF coolbox system delivered better performance than the equivalent conventional coolbox insulated with LDPE on most impact categories except acidification and eutrophication, where the wheat farming and WBF production system were the main drivers. N gas flux and leachate from the wheat agro-ecosystem accounted for approx 30–50 % of impacts; besides, other major contributors to acidification and

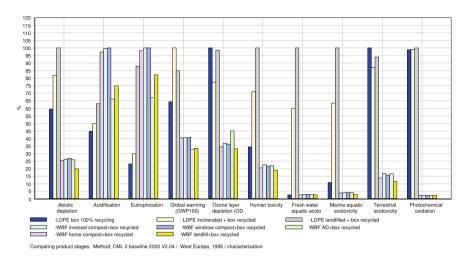


Fig. 6.9 Characterised LCIA profiles for life cycle of LDPE/WBF coolbox with cardboard recycled (unit: per coolbox)

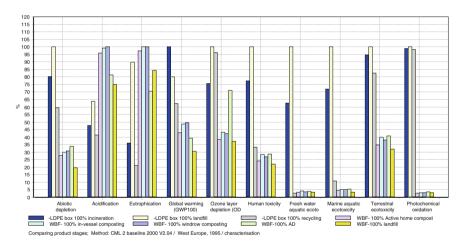


Fig. 6.10 Characterised LCIA profiles for life cycle of LDPE/WBF coolbox (unit: per coolbox)

eutrophication impacts of WBF coolbox included the NH₃ evolved from residue disposal during WBF production and processing, NO_x, SO_x, COD released from production of feedstock required for VAC (PVOH) as well as from the fuel processing/combustion involved.

Similar results were also found in Fig. 6.10 where coolbox systems with the scenarios that two components (cardboard and insulation) disposed together were compared. As analyzed in Sect. 6.4.2.1, conventional coolbox with LDPE land filled brought extra burdens on eutrophication, human and aquatic eco-toxicity due

to the COD and metallic ion release from LDPE land filling; thus landfill scenarios appeared as inferior system to other coolbox systems and moreover delivered disadvantageous eutrophication scores over the WBF coolbox AD scenario. LDPE recycling brought substantial savings on most impact categories, except ODP terrestrial eco-toxicity and POCP, which were either highly dependent on energy profiles or driven by the pentane release. Therefore, the 100 % recycling scenario partially overrides the burdens caused by LDPE coolbox production delivered similar or even better impacts than WBF coolbox on acidification, eutrophication, human and aquatic toxicity.

The findings above suggested that end-of-life scenario is not a sensitive parameter for comparison results of coolbox systems; regardless of the fate of coolbox, the environmental advantages of the WBF coolbox to equivalent conventional products on most impact categories were carried through from production stage to whole life cycle.

6.4.2.4 Normalised LCIA Results for Coolbox

The normalised LCIA profiles for coolbox systems with combined disposal routes and those with single waste treatment route (two components disposed together) are given in Figs. 6.11 and 6.12 respectively. Similar to the findings in display board case studies, impacts on aquatic eco-toxicity were indicated as most significant for the LDPE coolbox system (except 100 % recycling scenario) due to the metallic ions especially vanadium released from PE incineration and land filling.

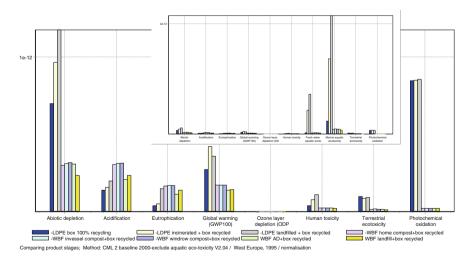


Fig. 6.11 Normalized LCIA profiles for life cycle of LDPE/WBF coolbox with cardboard recycled (unit: per coolbox). *Notes* Insert histogram includes aquatic eco-toxicities which are excluded from the main histogram due to problem of scale

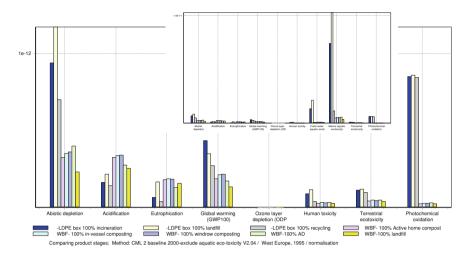


Fig. 6.12 Normalized LCIA profiles for life cycle of LDPE/WBF coolbox (unit: per coolbox). *Notes* Insert histogram includes aquatic eco-toxicities which are excluded from the main histogram due to problem of scale

Besides, abiotic depletion and POCP were relatively significant for the LDPE coolbox life cycle; LDPE recycling produced significant influences on resource depletion impacts but not on POCP scores as its driver was pentane release during the foam transformation process. The findings above suggested the options for improvements in the LDPE coolbox life cycle.

In comparison with conventional coolbox, the environmental advantages of WBF insulation was indicated as relatively significant on most impact categories, whereas, the substitution of LDPE with WBF caused a substantial shift in the magnitude of impact category results. Abiotic depletion and acidification shifted to second and third place respectively, followed by GWP100 and eutrophication. Therefore, the major contributors at the WBF disposal stage, including emissions (e.g. $CO_2/NO_x/NH_3$) from WBF biodegradation or biogas combustion were considered as relatively significant for WBF coolbox; in addition, attributable to renewable energy generation the saving effects of WBF landfill or AD scenarios over other biological treatments on GWP100, acidification and eutrophication were relatively significant for the WBF coolbox. All these concern the choices for coolbox system optimisation.

Category indicator results on ODP, human and terrestrial eco-toxicity appeared to be insignificant for both WBF and LDPE coolbox life cycle. However, normalised LCA results revealed so far only gave indicative information on the relative contributions of the coolbox to environmental problems to a specified temporal and spatial reference; other reference system could lead to different outcomes.

6.4.3 Case studies of Trough Mould and Concrete Formwork

To illustrate the comparison of WBF with different EPS grades applied in the construction sector over their life cycle, five trough mould and concrete formworks are given as examples. Their characterised LCIA results are presented below, followed by normalized profiles.

6.4.3.1 End-of-Life Scenarios for EPS Construction Products

The refractory lining is given as an example to interpret the various end-of-life scenarios for virgin EPS disposal. Generally, in comparison with the distribution stage, landfill brought extra burdens; on the contrary, the recycling scenario led to substantial savings.

For virgin EPS, the comparison results on GWP100, eutrophication, human and aquatic eco-toxicity were driven by emissions produced at the disposal phase, whereas as suggested in Fig. 6.13, the EPS refractory lining production process was the dominant parameter for impacts on other impact categories (90–95 % of impacts). For EPS land filling the COD and metal element (e.g. vanadium ion) release were considered as major environmental problems, accounting for 70–90 % of the eutrophication and aquatic eco-toxic impacts respectively, although other emissions produced from landfill site also contributed to toxic impacts, GWP100 and POCP scores, and its contribution was not significant. Different from landfill which acted as net C sink sequestrating 99 % of C contained in EPS, fossil C was utilized in incineration for energy recovery but eventually released to atmosphere as CO₂. It can explain the GWP100 indicator results where

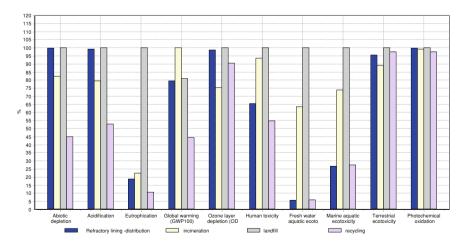


Fig. 6.13 Characterised LCIA profiles for life cycle of Filcor 70 (unit: per refractory lining)

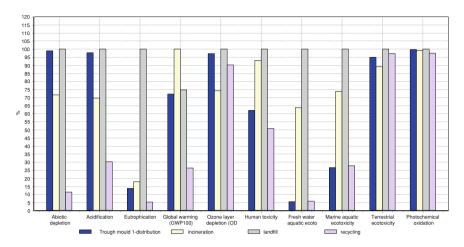


Fig. 6.14 Characterised LCIA profiles for life cycle of Filcor 20 (unit: per trough mould)

incineration was not suggested as an ideal choice. Similar to landfill, metallic ion releases were indicated as one of the major environmental concerns in incineration scenario, which caused 45 % human toxic impacts and 70–90 % of aquatic ecotoxic burdens.

As shown in Fig. 6.13, ODP, abiotic depletion, acidification and terrestrial ecotoxicity indicator results were driven by EPS refractory lining making but also sensitive to energy profiles on which incineration brought beneficial effects due to the energy substitution. Different from those impact categories on which the expandable PS making dominated and the recycling process brought dramatic savings, impacts on ODP, eco-toxicity, POCP were mainly dependent on the EPS transformation process, which is energy intensive and involves pentane as a blowing agent. During EPS transformation, the halon emissions from natural gas transport acted as the ODP score driver, emissions (e.g. vanadium, barite) from natural gas/heavy fuel burning dominated ecotoxicity burdens, whereas the pentane was the major POCP impacts trigger.

Similar results were also found in EPS construction products with recycled contents However, as indicated in Figs. 6.14 and 6.15, where trough mould cases 1 and 2 represent Filcor 20 and 45, respectively, recycling of low grade EPS showed greater saving effects than virgin EPS especially on abiotic depletion, acidification and GWP100 indicator results. As analysed in Sect. 4.4.5.1 these impact category results were driven by the expandable PS making process; thus recycled EPS content in Filcor 20, 45 was a major factor leading to environmental 'savings' and resulting in their superior environmental profiles to virgin EPS. Therefore, on abiotic depletion, acidification and GWP100, the credits brought by avoidance of virgin EPS making in the recycling scenario appeared as more sufficient to offset the burdens of low EPS grades. Overall, recycling was suggested as an optimal waste treatment for various grade EPS products.

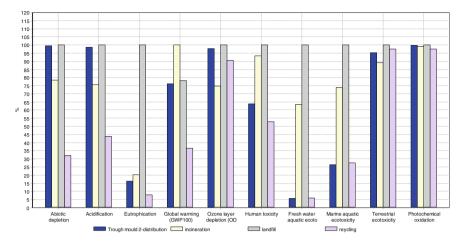


Fig. 6.15 Characterised LCIA profiles for life cycle of Filcor 45 (unit: per trough mould)

6.4.3.2 Comparison of WBF/EPS Construction Products

WBF and their equivalent EPS construction products are compared in Figs. 6.16, 6.17, 6.18, 6.19; trough mould cases 1, 2 and 3 represent the low EPS grade disposed in recycling or landfill whilst refractory lining is given to illustrate virgin EPS with various end-of-life scenarios.

Generally over its life cycle, WBF delivered better or similar environmental performance compared with virgin EPS on five impact categories (abiotic depletion, eco-toxicity and POCP) but with inferior results to virgin EPS on human toxicity, acidification and eutrophication, which were carried through from the

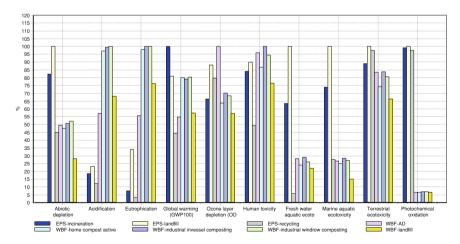


Fig. 6.16 Characterised LCIA profiles for life cycle of WBF/Filcor 70 (unit: per refractory lining)

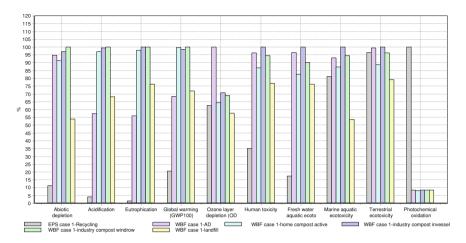


Fig. 6.17 Characterised LCIA profiles for life cycle of WBF/Filcor 20 trough mould case 1 (unit: per trough mould)

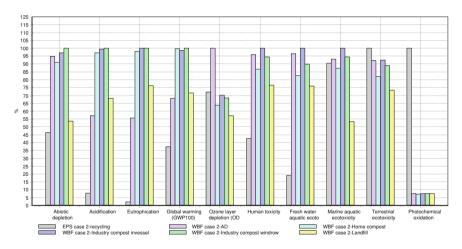


Fig. 6.18 Characterised LCIA profiles for life cycle of WBF/Filcor 45 trough mould case 2 (unit: per trough mould)

distribution stage. Furthermore, the C/N/S atmospheric emission from WBF disposal phase brought extra burdens on GWP100, acidification and eutrophication, which further reduced the environmental advantage of WBF over EPS; besides, the energy and infrastructure inputs resulted in AD and industrial composting appearing as inferior to the EPS life cycle on ODP and human toxicity.

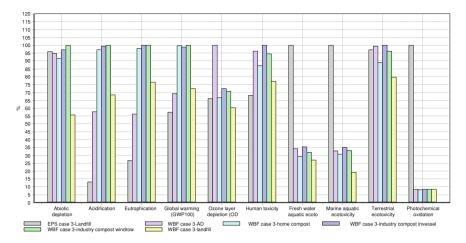


Fig. 6.19 Characterised LCIA profiles for life cycle of WBF/Filcor 20 trough mould case 3 (unit: per trough mould)

Regardless of EPS grades, EPS life cycle with recycling scenarios delivered superior or equivalent environment profiles to WBF product on most impact categories. These comparison results can be explained by the contribution analysis of the EPS life cycle (Sect. 6.4.3.1) and the comparison between WBF and EPS at the distribution stage (Sects. 4.4.5.2 and 4.4.5.3). Due to the dependency of abiotic depletion and GWP100 impacts on expandable PS making process, the recycling process reversed the comparison results i.e. EPS turning from environmentally inferior (at distribution) to superior (over life cycle) to WBF. On the contrary, recycling produced insignificant effects on ODP, ecotoxicity and POCP indicator results as they are dependent on EPS transformation process.

In contrast with recycling, EPS (irrespective of grades) with landfill and incineration only represented an advantageous system over WBF in terms of acidification, eutrophication and human toxic impacts, which was mainly driven by the production process. Besides, on GWP100, the C sink effects in EPS landfill scenarios led to its equivalent or better scores than WBF product systems. However, the metallic ion release from both EPS landfill and incineration reversed the comparison results on aquatic eco-toxicity: WBF products moved from disadvantageous (at distribution stage) to advantageous system (over life cycle) in comparison with EPS.

Interestingly, EPS grade was indicated as a significant parameter for comparison between WBF and EPS products over their life cycle. Figures 6.16–6.19 suggested that when compared with WBF life cycle, lower EPS grades (recycling scenario) showed greater advantages than virgin EPS recycling. As analysed in Sects. 6.4.3.1 and 4.4.5, it was not only attributable to the greater saving effects of recycling low grade EPS than virgin ones but also due to the various WBF

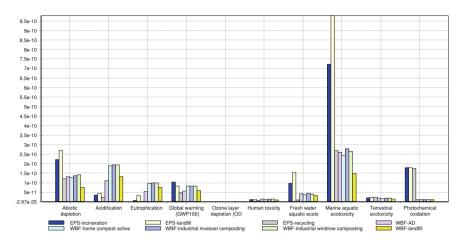


Fig. 6.20 Normalized LCIA profiles for life cycle of WBF/Filcor 70 (unit: per refractory lining)

densities modelled. Moreover, decrease in EPS grade shifted the EPS landfill scenarios from environmentally inferior to superior or equivalent systems to WBF on abiotic depletion, GWP100 and ODP.

6.4.3.3 Normalized LCIA Profiles for WBF/EPS Construction Products

Normalized LCIA comparison results are given in Figs. 6.20, 6.21, 6.22, 6.23 where marine aquatic eco-toxic indicator results appeared as most significant for all the WBF/EPS construction products whereas impacts on ODP, human toxicity

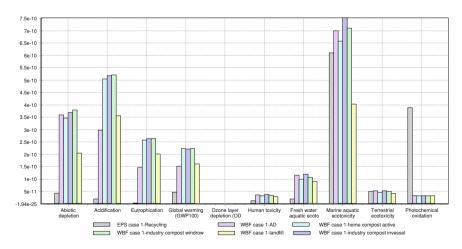


Fig. 6.21 Normalized LCIA profiles for life cycle of WBF/Filcor 20 trough mould case 1 (unit: per trough mould)

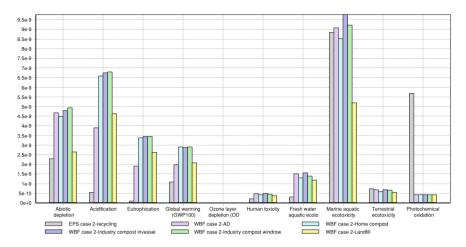


Fig. 6.22 Normalized LCIA profiles for life cycle of WBF/Filcor 45 trough mould case 2 (unit: per trough mould)

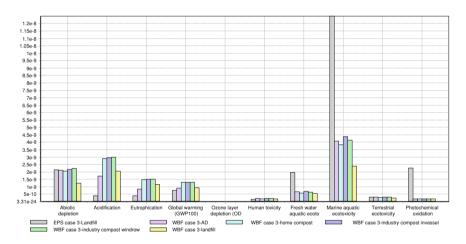


Fig. 6.23 Normalized LCIA profiles for life cycle of WBF/Filcor 20 trough mould case 3 (unit: per trough mould)

and terrestrial eco-toxicity were of relative insignificance to the reference system (West Europe, 1995).

Considering conventional EPS products, end-of-life scenario was indicated as a significant factor for magnitude of impact category results of EPS but the normalised LCIA profiles did not vary significantly with EPS grades. Besides aquatic eco-toxicity, abiotic depletion indicator results appeared as relatively significant for EPS landfill and incineration scenarios (followed by PCOP) due to the fuel consumption during expandable PS making. On the contrary, benefits of recycling

treatment caused a shift in the ranking of impact category results: compared with EPS landfill and incineration, POCP moved from third place to second, which indicated that recycling offered a choice for improvement of EPS product system.

Different from EPS, impacts on acidification or abiotic depletion were shown as the second most significant for WBF product systems, depending on the waste treatment route. Acidifying gas NH₃ emitted from WBF biodegradation was indicated as an important contributor to environmental problems of WBF system (with composting scenario) whereas the renewable energy recovered, especially in landfill scenarios, was suggested as significant savings in environmental profiles of WBF.

As illustrated in Figs. 6.20–6.23, WBF represents product systems with significant environmental advantages over EPS landfill/incineration scenarios; but the disadvantages of WBF to EPS low grade products with recycling assumptions were also of significance. In summary, both EPS grade and its end-of-life scenario were suggested as relatively significant parameters for LCIA comparison of WBF with EPS over life cycle. But it is noted that the normalised profiles revealed so far only offer the indicative information to specified temporal and spatial scales.

6.5 Comparisons of WBF with PSBF/MSBF

Apart from WBF, two alternative bio-polymers derived from starch were investigated; their overall environmental profiles throughout life cycle are presented below.

6.5.1 Comparison of WBF and PSBF/MSBF

The end-of-life scenarios for PSBF/MSBF were modelled as presented in Chap. 5; display board is given as an example to illustrate the 'cradle-to-grave' LCIA results for both biopolymers with various waste treatment routes (Fig. 6.24).

Similar to WBF, C emissions produced from PSBF/MSBF biodegradation were the dominant factor for GWP100 scores of the waste treatment process, whereas the impacts on toxicity, abiotic depletion and ODP were relevant to energy and infrastructure inputs at the disposal stage. Therefore, for MSBF/PSBF product systems, home composting was the optimum option amongst biological treatments primarily attributable to its low energy and infrastructure requirements; landfill benefited from its 'best-practice' assumptions i.e. the renewable energy recovery system; AD delivered a superior GWP100 score due to the energy recovery and lower GHGs evolved in comparison with composting where high preparation of C and a fraction of N were assumed as GHGs release; both AD and industrial composting brought extra burdens due to the intensive energy and infrastructure involved. However, differing from WBF, the acidification and eutrophication scores of PSBF/MSBF life cycle were driven by the polymer production (starch

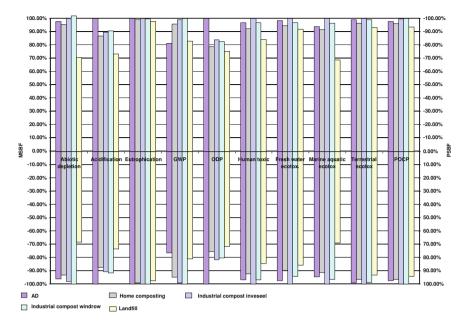


Fig. 6.24 Characterised LCIA profiles for life cycle of PSBF/MSBF display board (unit: per display board)

and PVOH making) rather than the disposal process; it can be explained by their chemical composition: negligible N/S elements contained in MSBF/PSBF. Thus clear shifts were indicated in the rankings of acidification and eutrophication scores: compared with AD, both landfill and composting moved from inferior (for WBF) to superior options (for MSBF/PSBF), whereas the emissions from the diesel combustion during AD process were major environmental concerns on acidification at disposal stage.

The characterised LCIA profiles for three biopolymers life cycle with identical waste treatment route were compared and summarised as Table 6.4. The comparison results on most impact categories were carried through from production stage (Sect. 4.4.6) to end-of-life: WBF showed great advantages over both alternative starch-based bio-polymers on resource depletion, ODP and toxicity but not on the acidification, GWP100 and POCP. Besides the contributors at the WBF production stage, i.e. NH₃ emitted from wheat farming (cause acidification) and high PVOH input (causes GWP and POCP), three indicator results were also driven by atmospheric emissions from WBF disposal stage (CO₂/NH₃/SO_x/CH₄/NO_x). In contrast with WBF, MSBF showed an inferior environmental profile to the other two biopolymers at both production and end-of-life phases because of maize farming (e.g. toxic emissions) and the intensive energy inputs to maize starch production (e.g. higher natural gas/electricity consumption than potato starch). However, at end-of-life, the difference in chemical composition (mainly N/S) of biopolymers influenced their LCIA profiles on acidification, eutrophication

	Life Cycle with diverse end-of-life									
Impact category	AD	Home compost	In-vessel compost	Windrow compost	Landfill					
Abiotic depletion										
Acidification										
Eutrophication										
GWP100										
ODP										
Human toxicity										
Ecotoxicity Fresh water										
Ecotoxicity Marine										
Ecotoxicity Terrestrial										
POCP										
Notes										

Table 6.4 Cradle-to-grave comparison of WBF with PSBF/MSBF

WBF lower impact than MSBF and PSBF

WBF higher impact than MSBF and PSBF WBF higher impacts than MSBF or PSBF

and POCP: the presence of S element in WBF led to SO₂ release in landfill scenario which further enhanced the advantages of MSBF/PSBF on POCP and acidification; protein-N released either as NH₃/leachate (from WBF biodegradation) or as NO_x (from biogas plant) not only brought extra acidification impacts but also reversed the comparison results on eutrophication, where WBF showed superior profile to PSBF at production phase (Sect. 4.4.6) but inferior over life cycle. Overall, disposal route was suggested as an insignificant parameter for comparison of WBF and MSBF/PSBF on most impact categories.

6.5.2 Comparison of PSBF/MSBF and Petrochemical Polymers

To further address the question 'is there a general environmental advantage for biopolymer over petroleum-based foams throughout "cradle-to-grave" life cycle', a range of case studies were modelled based on assumptions that PSBF/MSBF has identical thermal/compressive properties as WBF products.

As shown in Figs. 6.25 and 6.26 the disposal route for HDPE appears as a critical factor for comparison results. Similar to the findings (WBF) presented in Sect. 6.4.1.2, both PSBF/MSBF delivered better environmental performance than HDPE with landfill and incineration scenarios on most of impact categories, but

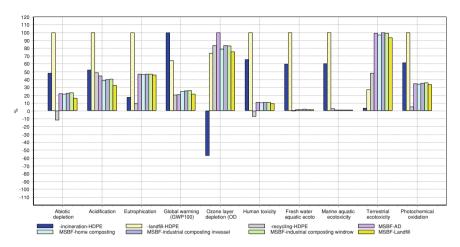


Fig. 6.25 Characterised LCIA profiles for life cycle of MSBF/HDPE display board (unit: per display board)

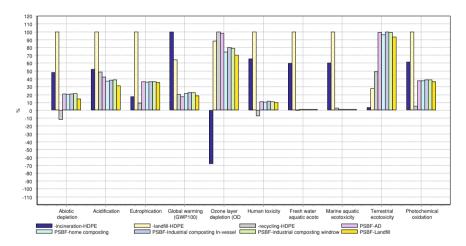


Fig. 6.26 Characterised LCIA profiles for life cycle of PSBF/HDPE display board (unit: per display board)

not HDPE recycling which benefited from avoidance of virgin HDPE making. In comparison with HDPE, the main difference between WBF and alternative starch-based foams are:

 Driven by maize or potato farming system and starch purification process, the inferior profiles of MSBF or PSBF to HDPE on ODP and terrestrial eco-toxicity were carried over from the production stage to end-of-life, which were differed from comparison results between WBF and HDPE

	Life cycle with diverse end-of-life									
				EPS T	Γrough	mould	Concrete			
Impact category	Cool-Box LDPE			Filcor 20		Filcor 45 formworl Filcor 70				
	Landfill	Incineration	Recycling	Landfill	Recycling	Recycling	Landfill	Incineration	Recycling	
Abiotic depletion										
Acidification										
Eutrophication										
GWP100										
ODP										
Human toxicity										
Ecotoxicity Fresh water										
Ecotoxicity <i>Marine</i>										
Ecotoxicity Terrestrial										
POCP										

Table 6.5 Cradle-to-grave comparison of starch foams with LDPE/EPS

Notes

- MSBF and PSBF lower impact than petrochemical polymer
- MSBF and PSBF higher impact than petrochemical polymer
- MSBF or PSBF lower impact than petrochemical polymer

 As analysed in Sect. 6.5.1, due to the different chemical composition from WBF, no significant N/S gas release assumed from PSBF/MSBF disposal thus starchbased foams remained their advantages over HDPE on acidification throughout life cycle stages.

In addition, MSBF/PSBF was also compared with LDPE and EPS; the results are summarised in Table 6.5 where the fate of petrochemical polymer was not a critical factor for comparison results. Irrespective of diverse disposal route, PSBF/MSBF was generally suggested as environmentally superior to LDPE but not to EPS on most of the impact categories. These comparison results were primarily driven by the production process rather than disposal stage, except aquatic ecotoxic and GWP100 scores. On the former, toxic compounds (mainly metallic ions e.g. vanadium) released from incineration and land filling of petrochemical were indicated as the dominant factor which reversed the ranking: PSBF/MSBF products showed inferior profiles at the distribution stage but superior to equivalent

LDPE/virgin EPS products at end-of-life. On the contrary, advantages of starch-based foams over low grade EPS at production stage on GWP100 were reversed at the disposal stage, primarily attributable to the biogenic C release during biopolymer degradation. Similar to the display board case study, the difference in the chemical composition of WBF and alternative starch-based foams drove their differed comparison results (comparison with LDPE) on acidification.

Generally the comparison results between MSBF/PSBF and petrochemical polymers (with incineration/landfill scenarios) were carried through from production stage; Overall, MSBF/PSBF was indicated as an environmentally superior choice in coolbox and display board (except recycling) case studies but not applications in construction sectors throughout the life cycle. The HDPE/EPS product with recycling was suggested as the optimum system, delivering better performance than equivalent MSBF/PSBF on most impact categories, except acidification and POCP where the extruded HDPE production process and EPS transformation process (pentane release) were the major environmental concerns respectively. However, the findings above were considered as tentative indications because the data source and modelling basis for WBF and alterative starch foams differed.

6.6 Sensitivity Analysis

The sensitivity analyses were conducted on key scenarios and parameters including N_2O modelling approach, infrastructures and disposal scenarios; their influences on 'cradle-to-grave' LCIA profiles of WBF as well as its comparison with petrochemical polymers were analyzed, where the methods and thresholds defined in Sect. 2.3.1 were applied.

6.6.1 Sensitivity Analysis on N₂O Modelling Approach

Besides the results presented in Sects. 3.6.1 and 4.5.1, analysis was also carried out on the 'cradle-to-grave' basis to investigate the sensitivity of comparison results (WBF vs. petrochemicals) to the N_2O modelling approach and system boundary definition. The coolbox is given as an example in this section.

As indicated in Figs. 6.27a and b, the WBF coolbox life cycle with diverse end-of-life scenarios are compared with LDPE. Generally, only 0.6–1.05 % of GWP100 indicator results for WBF coolbox were attributable to DNDC-simulated N₂O; whereas IPCC-derived N₂O flux shared higher GWP100 burdens (3–5 %) where above 75 % was estimated as direct emissions. In addition, GWP100 scores of WBF products derived from the six fields differed. Irrespective of modelling approach, WBF derived from Fields 1, 3, and 4 represented the best cases, showing GWP100 burdens lower than average; on the contrary, the remaining three fields

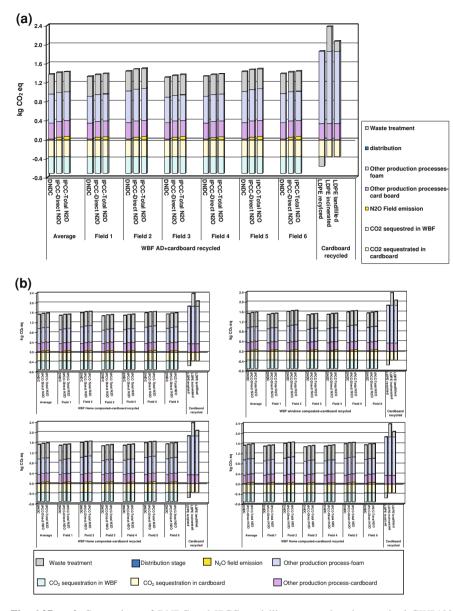


Fig. $6.27\,$ a, b Comparison of DNDC and IPCC modelling approach—characterised GWP100 profiles for life cycle of coolbox (unit: per coolbox)

delivered inferior GWP 100 profiles to average. This could be explained by their GWP100-driving factor i.e.CO₂ field emission (analyzed in Sect. 3.5.2). Although GWP100 profiles of WBF coolbox varied with modelling approach and fields, neither of them was suggested as a significant parameter for comparison of the

WBF and LDPE coolbox system: GWP100 scores of all WBF coolbox systems are superior to its equivalent LDPE products throughout the life cycle due to the biogenic C sequestration in WBF.

Similar to the coolbox case study, contribution analysis indicated that over the life cycle of display board and construction products, IPCC-simulated $\rm N_2O$ contributed higher burdens to overall GWP100 scores than DNDC modelling results (the former and the latter contributed less than 2 % and approx 4–8.5 % of GWP100 impacts respectively). Apart from it, similarities were also found in the comparison of six fields on GWP100: WBF products derived from Fields 1, 3, 4 delivered environmental advantages, showing GWP100 scores below average. However, construction products were more sensitive to the modelling approach than other WBF product systems due to greater WBF density modelled: the shift from DNDC to IPCC method brought approximately 8–14 % increase in GWP100 score of WBF construction products whereas only 6–9 % increase was observed in the case of the coolbox and display board.

The comparison between WBF life cycle and the equivalent petrochemical polymers was not only dependent on field, N_2O simulation method, but also depended on the WBF waste treatment routes which accounted for over 50 % of overall GWP100 impacts (see Sect. 6.4.1.1). Generally, the WBF products life cycle with composting scenarios appeared as inferior to EPS/HDPE recycling but superior to their landfill and incineration (except EPS Filcor 70 landfill scenario which was superior to WBF derived from Fields 2, 5, 6). However, it was not the case of WBF AD and landfill scenarios which benefited from energy recovery. As summarised in Table 6.6, the fields and N_2O modelling approach were suggested as sensitive parameters for comparison in display board but not the construction products where the EPS grade and its disposal route were indicated as critical factors.

In summary, according to the sensitivity threshold, the N_2O modelling approach was a sensitive factor for the case studies in display board and construction sectors, significantly influencing the GWP 100 scores of WBF construction products and the comparison of WBF with HDPE (with recycling scenario). Although the GWP100 score of WBF derived from different fields varied, generally it was not a critical parameter for the comparisons between WBF and petrochemical polymers over the life cycle.

6.6.2 Sensitivity Analysis on Composting Scenario

6.6.2.1 Active and Passive Home Composting

As presented in Chap. 5, two home composting operation modes were simulated, i.e. active composting (aerobically operated) and passive composting (poorly maintained).

		Life cycle with diverse end-of-life									
				EPS Trough mould			Concrete				
	Display board HDPE		Filco	Filcor 20 Filcor 45		formwork Filcor 70					
	Landfill	Incineration	Recycling	Landfill	Recycling	Recycling	Landfill	Incineration	Recycling		
WBF AD scenari	0										
WBF-Average											
WBF-Field 1											
WBF-Field 2											
WBF-Field 3											
WBF-Field 4											
WBF-Field 5											
WBF-Field 6											
WBF landfill scena	ario							•			
WBF-Average											
WBF-Field 1											
WBF-Field 2											
WBF-Field 3											
WBF-Field 4											
WBF-Field 5											
WBF-Field 6											

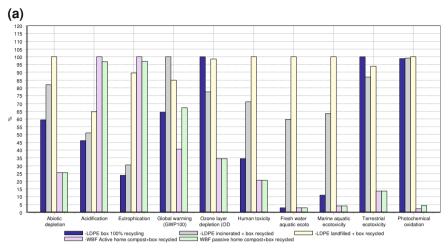
Table 6.6 Sensitivity analysis on N₂O modelling approaches

Notes

WBFs with IPCC and DNDC approach deliver lower GWP impact than petrochemical polymer

WBFs with IPCC and DNDC approach deliver higher GWP impact than petrochemical WBFs with DNDC approach deliver lower GWP impact than petrochemical but IPCC approach reverse the comparison results

Coolbox case study is given as an example (Fig. 6.28) to illustrate the sensitivity of LCIA profiles of WBF to home composting scenarios. Compared with aerobic operation, passive composting only led to an insignificant decline (less than 5 %) in acidification and eutrophication impacts but a substantial increase in GWP100 and POCP score (66–85 %) over the life cycle of WBF coolbox due to the anaerobic zone developed, which caused greater GHGs release (CH₄/N₂O) but less acidifying gas emission (NH₃). As indicated in Fig. 6.28, attributable to the differed home composting scenarios, a clear shift was caused on the GWP100



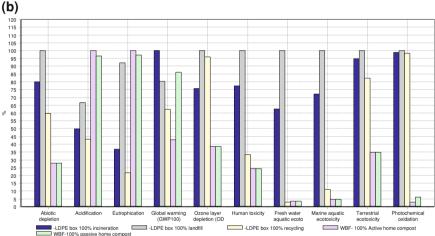


Fig. 6.28 a, b Sensitive analysis on home composting scenarios-characterised LCIA profiles for life cycle of WBF/LDPE coolbox (unit: per coolbox)

results: the rank of LDPE recycling/landfill and WBF coolbox home composting reversed. But for other impact categories, home composting scenario was suggested as a negligible factor for comparison of WBF with LDPE coolbox systems.

Similar findings were also suggested by sensitivity analysis on other case studies. As summarised in Table 6.7, the home composting scenario appeared as an insignificant parameter in the comparison between WBF and EPS/HDPE on most impact categories except GWP100 and POCP. Generally on these two impact categories, the indicator results of WBF were substantially increased (90–115 %) by assuming passive operation instead of active home composting. Besides,

	Life cycle with diverse end-of-life								
	Display board HDPE			EPS T	rough	mould	Concrete		
Impact category				Filcor 20		Filcor 45	formwork Filcor 70		
	Landfill	Incineration	Recycling	Landfill	Recycling	Recycling	Landfill	Incineration	Recycling
Abiotic depletion									
Acidification									
Eutrophication									
GWP100									
ODP									
Human toxicity									
Ecotoxicity Fresh water									
Ecotoxicity Marine									
Ecotoxicity Terrestrial									
РОСР									

Table 6.7 Sensitivity analysis on home composting scenarios

Notes

- ☐ WBF with active home composting and passive home composting lower impact than petrochemical polymer
- ☐ WBF with active home composting and passive home composting higher impact than petrochemical polymer
- ☐ WBF active home composting lower impact than petrochemical polymer, but passive home composting reverse the comparison results

impacts of WBF products on acidification and eutrophication were also influenced (decreased 5 %) by home composting scenarios, but not significantly according to the sensitivity threshold.

Apart from WBF, the other two alternative starch-based foam were also analysed. As illustrated in Fig. 6.29, home composting was neither a critical factor for comparison of PSBF/MSBF and WBF nor a sensitive parameter for their comparison with HDPE on most impact categories, except POCP where the home composting scenario shifted the MSBF/PSBF display boards from superior to inferior system to HDPE product (incineration scenario). Similar findings were also indicated in other case studies (see Table 6.7). Overall, only GWP100 and POCP indicator results were suggested as sensitive to home composting operation modes, especially the comparison between biopolymer and the equivalent petrochemical products with incineration end-of-life.

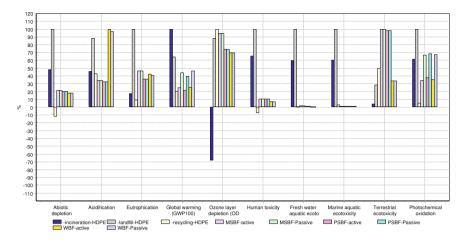


Fig. 6.29 Sensitive analysis on home composting scenarios-characterised LCIA profiles for life cycle of HDPE/WBF/PSBF/MSBF (unit: per display board)

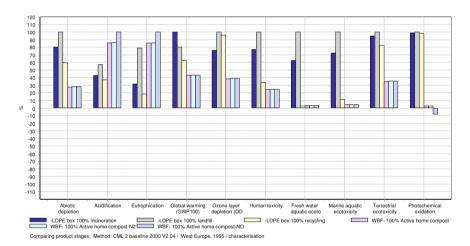


Fig. 6.30 Sensitivity analyses on N transformation assumption—characterised LCIA profiles for life cycle of WBF/LDPE (unit per coolbox)

6.6.2.2 N Transformation Assumption

As presented in Sect. 5.5, besides N_2O , NH_3 modelled in the composting scenario, two other potential emissions during N transformation, were considered in sensitivity analysis i.e. 27.8 % of initial N lost either as NO or N_2 .

Coolbox is given as an example. As shown in Fig. 6.30, N₂ loss assumed in home composting produced negligible effects (less than 1.5 % change) on

environmental impacts of WBF life cycle; differing from N_2 , the NO assumption appeared as a sensitive parameter for acidification/eutrophication/POCP scores of WBF. Approx 17 % increase in acidification and eutrophication impacts was caused due to the increasing proportion of N loss via NO and the decline in the beneficial N nutrients remained in compost; on the contrary, substantial beneficial effects on POCP were brought about by NO emission assumptions. This could be explained by the destruction of O_3 by NO under certain conditions [6, 7], which were sufficient enough to offset the environmental burdens to deliver a WBF coolbox with negative POCP value.

In addition, other WBF composting scenarios were also analyzed; the major outcomes are given in Figs. 6.31, 6.32, 6.33, where Tornado Diagrams illustrate the degree to which model output varies due to the estimated change in N gas emission. NO assumption was suggested as the more sensitive parameter for overall acidification, eutrophication, POCP scores throughout WBF coolbox life cycle, whereas the influence of N_2 scenario was insignificant. On these three impact categories, neither of the N gas assumption was concluded as critical factor for comparison of WBF with LDPE coolbox. Besides only marginal change (less than 4 % increase) was incurred by assuming NO/ N_2 emission in other category indicator results over the WBF life cycle.

Similar findings were also suggested in other case studies: impacts of WBF on acidification/eutorphication increased 15–22 % by introducing NO loss; a dramatic drop in POCP score was observed by assuming NO emission, which led to WBF life cycle with net POCP 'savings' (negative value) and reversed the POCP comparison

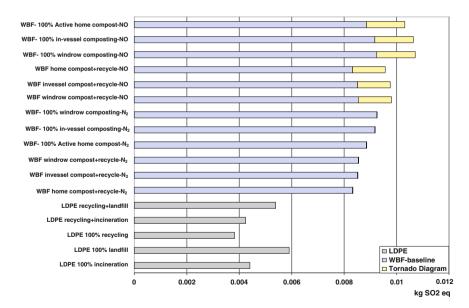


Fig. 6.31 Sensitivity analysis on N transformation assumption—characterised acidification profiles for life cycle of WBF/LDPE (unit per coolbox)

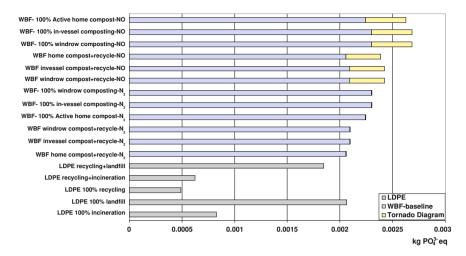


Fig. 6.32 Sensitivity analysis on N transformation assumption—characterised eutrophication profiles for life cycle of WBF/LDPE (unit per coolbox)

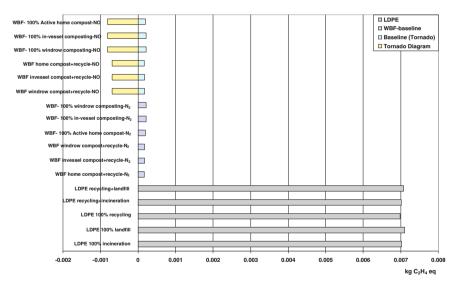


Fig. 6.33 Sensitivity analysis on N transformation assumption—characterised POCP profiles for life cycle of WBF/LDPE (unit per coolbox)

of WBF with HDPE display board (recycling scenarios). On other impact categories, N transformation scenario was neither a sensitive parameter for environmental score of WBF (less than 2.5 % change) nor a critical factor for comparison of WBF with equivalent petrochemical polymers in various applications.

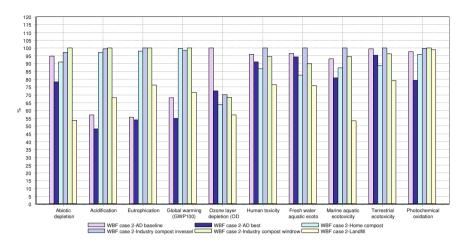


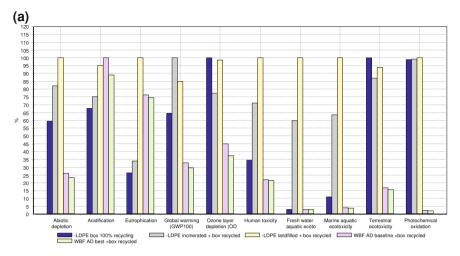
Fig. 6.34 Sensitivity analysis on AD scenario-characterised LCIA profiles for WBF life cycle with diverse end-of-life (unit: per trough mould)

6.6.3 Sensitivity Analysis on AD Scenario

As presented in Chap. 5, two AD scenarios were modelled, i.e. baseline scenario reflecting the current UK AD technology, and the model representing the optimised AD system. Their major differences are the energy flow simulated; their influences on the overall environmental impacts of biopolymers life cycle are analysed below.

Figure 6.34 gives an example to interpret the environmental saving potentials of AD scenario and its comparison with other disposal routes for WBF. With optimised system, AD best scenario appeared as a promising waste treatment offering environmentally superior profiles to industrial composting/landfill on most impact categories; especially on acidification, eutrophication, GWP100 and POCP, the AD best scenario represented the optimum option.

As illustrated in Fig. 6.35, the optimisation of AD energy utilisation brought up to 26 % of environmental savings for WBF coolbox system. Based on 10 % sensitivity threshold, abiotic depletion, acidification, GWP100, ODP, marine aquatic ecotoxicity and POCP indicator results were sensitive to AD scenario, especially on acidification, where the rank of WBF and LDPE coolbox (LDPE land filled + cardboard recycled) reversed due to the avoidance of diesel inputs by recovering thermal energy. The sensitivity analysis on other case studies reached similar conclusions to the coolbox: 10–27 % environmental savings on abiotic depletion, acidification, GWP100, ODP, marine aquatic eco-toxicity and POCP were achieved by optimising the energy utilisation in AD scenario. Moreover, on these six impact categories, AD scenario is a sensitive factor for LCIA comparison between WBF and equivalent petrochemical (Table 6.8); across all the case studies, construction applications are more sensitive to AD scenarios.



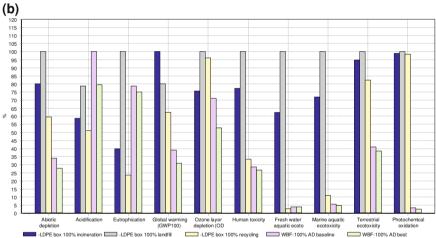


Fig. 6.35 a, b Sensitive analysis on AD scenarios-characterised LCIA profiles for life cycle of WBF/LDPE (unit: per coolbox)

As illustrated in Fig. 6.36, display board is given as an example to explain two other alternative starch-based foams. Similar to WBF, efficient renewable energy utilization in AD brought 10–20 % reduction in the environmental burdens of MSBF/PSBF on six impact categories (abiotic depletion, acidification, GWP100, ODP, marine aquatic ecotoxicity and POCP). But the AD scenario produced insignificant effects on LCIA comparison profiles between starch-based foams and HDPE. Similar findings were also suggested in other case studies. In summary, significant savings on environmental profiles of biopolymer could be expected by improving the AD energy utilization efficiency; WBF applied in construction applications ranked as the most sensitive case study to AD scenarios.

	Life cycle with diverse end-of-life									
Impact category	Display board HDPE			EPS T	rough	mould	Concrete			
				Filcor 20		Filcor 45 formwork Filcor 70				
	Landfill	Incineration	Recycling	Landfill	Recycling	Recycling	Landfill	Incineration	Recycling	
Abiotic depletion										
Acidification										
Eutrophication										
GWP100										
ODP										
Human toxicity										
Ecotoxicity Fresh water										
Ecotoxicity Marine										
Ecotoxicity Terrestrial										
POCP										

Table 6.8 Sensitivity analysis on AD scenarios

Notes

- WBF with two AD scenarios lower impact than petrochemical polymer
- WBF with two AD scenarios higher impact than petrochemical polymer
- WBF with current AD technology higher impact than petrochemical polymer, the best AD scenario reverses the comparison results

6.6.4 Sensitivity Analysis on Landfill Scenario

6.6.4.1 Temporal Boundary

Within 100 year surveyable period, zero N storage was assumed for WBF land filling, but C storage was major concern: landfill was modelled as a net C sink sequestrating 11–15 % C content of biopolymer and approximately 48 % of cardboard-C (Sect. 5.6). As discussed in Chap. 5, under infinite time frame waste could decompose until all organic matter exhausted and this organic C stored could be released to environment [1].

Thus for cardboard and biopolymers, landfill scenario with expanded time horizon was introduced, where all organic C was assumed to be released as landfill gas with a typical composition of CH₄/CO₂ (50:50 % v/v). Under infinite temporal boundary, it was assumed that landfill gas collection system was not operated

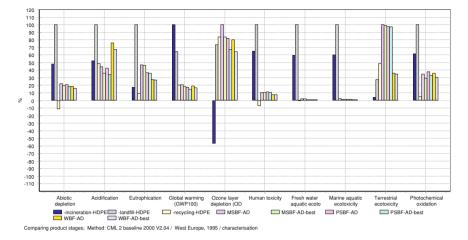


Fig. 6.36 Sensitivity analysis on AD scenarios-characterised LCIA profiles for life cycle of HDPE/WBF/PSBF/MSBF (unit: per display board)

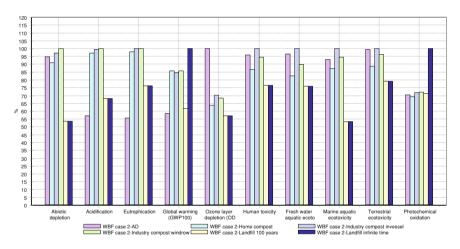
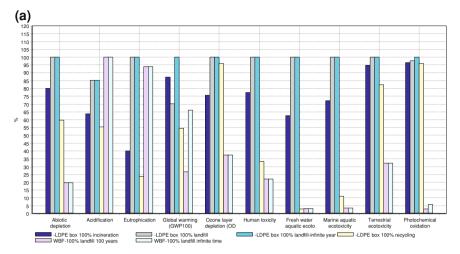


Fig. 6.37 Sensitivity analysis on landfill temporal boundary-characterised LCIA profiles for WBF life cycle with diverse end-of-life (unit: per trough mould)

whereas the cover layer still took effects with the same CH₄ oxidation efficiency (0.1) as 100 year scenario.

As illustrated in Fig. 6.37, under the 100 year time frame, landfill benefited from its 'C sink' assumption, but the inclusion of long-term CH_4/CO_2 release caused a clear shift in GWP100 and POCP profiles: the WBF with landfill scenario turned from environmentally superior to inferior system to other biological treatments. The stored C release via gas is given as an example here; however, stored chemical elements could be released to the environment via other pathways,



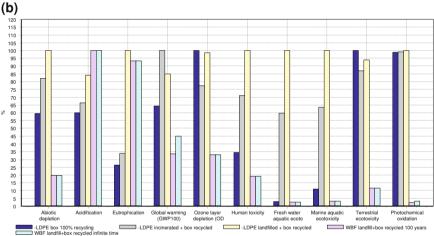


Fig. 6.38 a, b Sensitive analysis on landfill temporal boundary-characterised LCIA profiles for life cycle of WBF/LDPE (unit: per coolbox)

which are uncertain. Thus the temporal boundary was considered as a critical parameter for comparison between diverse WBF end-of-life scenarios.

Besides, comparison of WBF product systems and petrochemical polymer life cycles are given in Fig. 6.38 and Table 6.9, where default 100 year landfill models were assumed for petrochemical polymers. Generally, long-term landfill gas potentially released from WBF degradation in landfill not only substantially increased the GWP100 and POCP burdens of WBF products (30–60 %), but also reversed GWP100 comparison between WBF and virgin petrochemical polymers (recycling/landfill scenarios). In contrast with WBF, a higher proportion of cardboard-C was stored in landfill, its potential release under infinite time frame

	Life cycle with diverse end-of-life									
	Display board HDPE			EPS T	rough	mould	Concrete			
Impact category				Filcor 20		Filcor 45	formwork Filcor 70			
	Landfill	Incineration	Recycling	Landfill	Recycling	Recycling	Landfill	Incineration	Recycling	
Abiotic depletion										
Acidification										
Eutrophication										
GWP100										
ODP										
Human toxicity										
Ecotoxicity Fresh water										
Ecotoxicity Marine										
Ecotoxicity Terrestrial										
POCP										

Table 6.9 Sensitivity analysis on landfill temporal boundary

Notes

WBF with two landfill scenarios lower impact than petrochemical polymer

WBF with two landfill scenarios higher impact than petrochemical polymer

WBF with 100 year landfill lower impact than petrochemical polymer, the infinite time boundary reverses the comparison results

brought further burdens; as presented in Fig. 6.38, over doubled GWP100/POCP score is achievable in the case of WBF coolbox with 100 % landfill scenario.

The expansion of the temporal boundary in landfill scenario also caused a change in LCIA profiles of PSBF/MSBF (see example in Fig. 6.39): over 30 % increase in GWP100, POCP scores and the reversed rankings were observed (PSBF/MSBF shifted to disadvantageous systems over virgin EPS/PE). Overall, landfill temporal boundary definition was revealed as a sensitive parameter for biopolymer product systems over life cycle. However, apart from the long-term landfill gas analysed above, other pathways (leachate/gas) through which the stored C/N/S could proportionally removed in long time horizon bring great uncertainties in landfill scenarios.

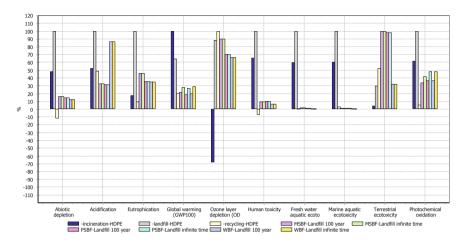


Fig. 6.39 Sensitive analysis on landfill temporal boundary-characterised LCIA profiles for life cycle of HDPE/WBF/PSBF/MSBF (unit: per display board)

6.6.4.2 Energy Recovery Efficiency

In the 100 year landfill baseline model, the 'best practice' with maximum landfill gas utilisation and high energy conversion efficiency (30 % net energy export) was assumed (Sect. 5.2.3). This assumption was tested in sensitivity analysis, where lower energy recovery was simulated.

As illustrated in Tornado diagrams (Figs. 6.40 and 6.41), the top bar (temporal boundary) represents the most sensitive parameter for WBF in terms of GWP100

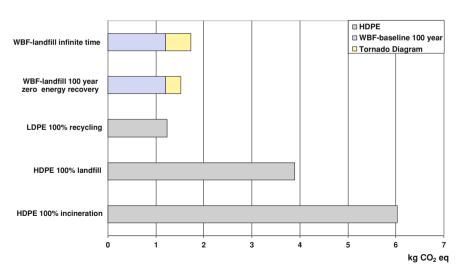


Fig. 6.40 Sensitivity analyses on landfill scenario—characterised GWP100 profiles for life cycle of WBF/HDPE (unit per display board)

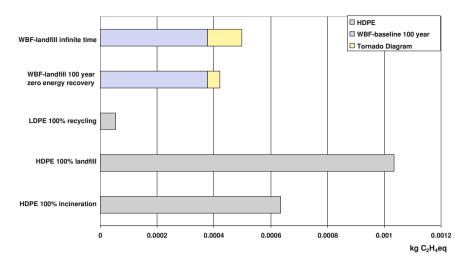


Fig. 6.41 Sensitivity analyses on landfill scenario—characterised POCP profiles for life cycle of WBF/HDPE (unit per display board)

and POCP impacts; moreover, GWP100 comparison between HDPE and WBF product systems appeared dependent on both landfill parameters (time horizon, energy recovery assumption). On other impact categories, energy recovery efficiency produced greater influences than temporal boundary, generally bringing WBF products 10–70 % extra environmental burdens. Especially for construction applications (e.g. Fig. 6.42), reduction in energy recovery in WBF landfill model not only caused up to 75 % increase in resource depletion and marine toxic scores, but also drove WBF products from superior to inferior system to equivalent EPS product life cycle on several impact categories e.g. abiotic depletion, ODP and human toxicity. Overall, energy assumption in WBF landfill scenario was considered as a sensitive parameter especially for construction case studies.

Besides, as the example shown in Fig. 6.43, comparisons between WBF waste treatment options were found to be sensitive to energy assumption in landfill scenario. Reduction in energy substitution led to a sharp increase in environmental burdens of WBF landfill scenario (approximately 10–70 % increase), which not only reversed its comparison with home composting on most of impact categories, but also drove landfill to be ranked as the environmentally inferior choice on POCP and GWP100. Thus, energy recovery assumption was considered as another source of uncertainties apart from temporal boundary in landfill scenario.

6.6.5 Sensitivity Analysis on Infrastructures

In the current LCA study, the unit processes for infrastructures were based on surrogate datasets derived from Eco-invent V2.0 or WRATE model [2], rather than

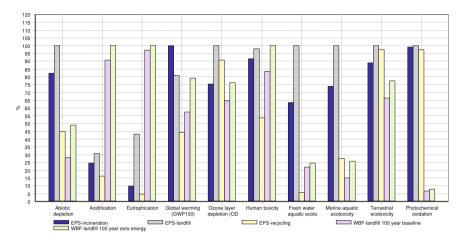


Fig. 6.42 Sensitivity analysis on landfill energy assumption—characterised LCIA profiles for life cycle of WBF/virgin EPS (unit per refractory lining)

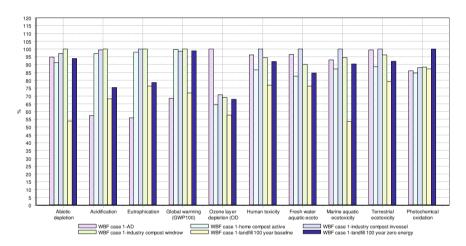


Fig. 6.43 Sensitivity analyses on landfill energy assumption—characterised LCIA profiles for WBF with diverse end-of-life (unit per trough mould)

the primary inventory due to the data unavailability. To test the influences of these datasets on LCIA results, sensitivity analyses were performed.

As indicated in Figs. 6.44, 6.45, 6.46, 6.47, 6.48, amongst petrochemical polymers, EPS especially low grade EPS applied in the construction sector appeared more sensitive to infrastructure process; generally for PE/EPS products, infrastructure accounted for the 10–80 % of overall toxic impacts but incurred marginal impacts (less than 10 %) on other impact categories. In contrast with petrochemical polymers, WBF products were more sensitive to infrastructure: the exclusion of infrastructure substantially reduced the environmental burdens of

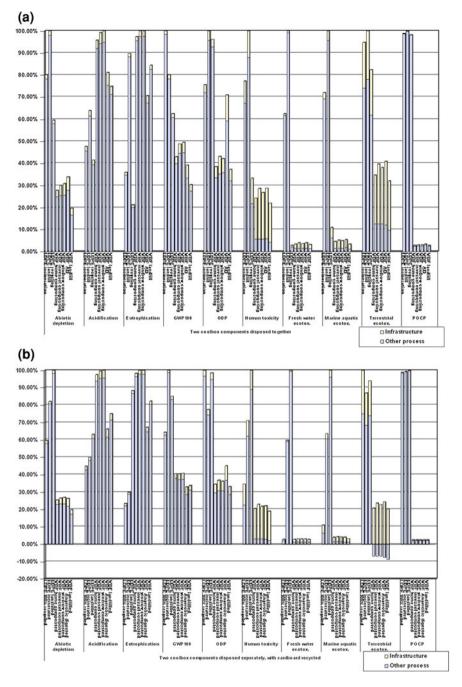


Fig. 6.44 a, b Sensitivity analysis on infrastructure—characterised LCIA profiles for life cycle of WBF/LDPE (unit per coolbox)

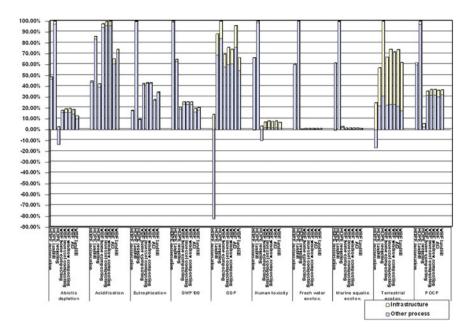


Fig. 6.45 Sensitivity analyses on infrastructure—characterised LCIA profiles for life cycle of WBF/HDPE (unit per display board)

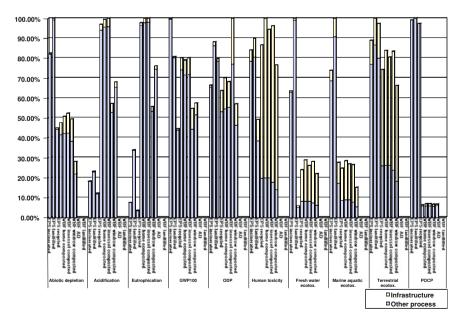


Fig. 6.46 Sensitivity analyses on infrastructure—characterised LCIA profiles for life cycle of WBF/virgin EPS (unit per refractory lining)

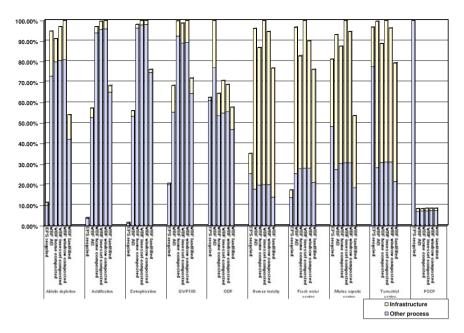


Fig. 6.47 Sensitivity analyses on infrastructure—characterised LCIA profiles for life cycle of WBF/EPS Filcor 20 (unit per trough mould)

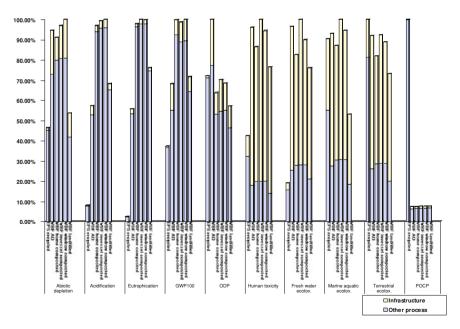


Fig. 6.48 Sensitivity analyses on infrastructure—characterised LCIA profiles for life cycle of WBF/EPS Filcor 45 (unit per trough mould)

Table 6.10 Sensitivity parameters for comparison of WBF and PE/EPS Immost cataoocias 1 ife ends with disease and of life

Impact categories Life cycle with diverse end-of-life	Life cycle	e with divers	e end-of-life									
	Coolbox LDPE	LDPE		Display	Display board HDPE		Concrete	Concrete formwork Filcor 70	lcor 70	EPS Trough mould	plnom y	
										Filcor 20		Filocr 45
	Landfill	Incineration	Recycling	Landfill	Landfill Incineration Recycling Landfill Incineration Recycling Landfill Incineration Recycling Landfill Recycling Recycling	Recycling	Landfill	Incineration	Recycling	Landfill Re	ecycling	Recycling
Abiotic depletion									D F	\mathcal{G}		
Acidification			D									
Eutrophication												
GWP100			В			A	B	В	D	D		
						E	E					
ODP				D			D	F	D	F F		
							\mathcal{G}	\mathcal{G}	\mathcal{G}	\mathcal{G}		
Human toxicity							G	F	\mathcal{G}	G		Ŋ
								\mathcal{G}				
Ecotoxicity												
Fresh water												
Ecotoxicity									\mathcal{G}	D		D
Marine										F		F
										S		Ċ5
Ecotoxicity										D D		
Terrestrial												
POCP					В							

Sensitivity parameters: A N₂O modelling approach, B active vs. passive home composting, C N transformation assumption in composting scenarios, D AD scenario, E landfill temporal boundary, F energy recovery efficiency in landfill scenario, G infrastructures

WBF: 50–90 % decreases in toxic score and 5–20 % drops in other category indicator results were observed; especially on terrestrial eco-toxicity e.g. Fig. 6.44b, the 'savings' (negative value) gained from energy substitution and cardboard recycling at the WBF coolbox waste treatment stage were overridden by the environmental burdens caused by infrastructure. Therefore, the exclusion of infrastructure favoured the WBF products: it not only drove WBF as more environmentally superior system to petrochemical polymers (e.g. Fig. 6.44), but also shifted WBF from disadvantageous to advantageous products over EPS in construction case studies (e.g. toxic impacts shown in Figs. 6.46, 6.47, 6.48). In summary, infrastructure was considered as a sensitive parameter for 'cradle-tograve' environmental profiles of both petrochemical polymers and WBF, especially their toxic score, where infrastructure was shown as a driving factor. Moreover, the discussion above indicated that the data quality of infrastructure process is critical: assumptions made or the datasets used could significantly influence the comparison between WBF and petrochemical polymers.

6.7 Discussion

The key findings in this chapter are as follows:

1. Amongst five 'baseline' disposal routes for WBF products, AD represents the optimum choice on GWP100, acidification eutrophication but not on the rest of the impact categories, where landfill or home composting was shown as better options. Contribution analysis indicated that emissions from WBF degradation were the dominant factors on acidification, eutrophication, GWP100 and POCP; but on these four impact categories, different from composting scenarios where atmospheric emissions NH₃, CO₂, CH₄ directly released from WBF decomposition were the major contributors, the impacts of AD and landfill scenarios were attributable to the SO_x, NO_x and CO₂ primarily evolved from biogas/landfill gas combustion and partially from diesel combustion. In addition, energy and infrastructure not only incurred resource depletion but also played significant roles in ODP and toxicity impact categories. The industrial composting and AD scenarios with intensive energy and infrastructure inputs delivered high ODP and toxic impacts due to the emissions from crude oil production and diesel refinery (e.g. atmospheric emission CBrF₃, vanadium mercury and the water emissions PAH, barite, barium) as well as those pollutants produced during production of infrastructure materials steel, bitumen, butyl acrylate (e.g. chromium, mercury CBrClF₂ emitted to air and the cobalt, nickel ions, vanadium ions released to water). Home composting benefited from its low energy and resource consumption, presented as the second best choice in terms of PCOP and toxic scores; the superior profiles of landfill baseline scenario on ODP, toxicity impact categories were attributable to its middle-term temporal boundary modelled, and efficient energy recovery system assumed.

In addition, at WBF disposal stage, the renewable energy and digestate/compost brought environmental savings by avoidance of artificial fertiliser and energy substitution, which partially offset the positive burdens, even leading to WBF disposal process with negative environmental scores (e.g. abiotic depletion profile for active home composting).

However, the sensitivity analysis suggested that the comparisons between WBF disposal routes were sensitive to assumptions made and parameters modelled in 'baseline' scenarios. For home composting, operation was indicated as a critical factor driving its GWP100 and POCP profiles: poorly-maintained home composting with anaerobic zone developed shifted home composting to inferior waste treatment option on GWP100 and POCP. Besides, great uncertainties in landfill scenarios were suggested via sensitivity analysis: the expansion of the temporal boundary or reduction in energy substitution led to a substantial increase in environmental burdens of landfill, especially on abiotic depletion, GWP100, POCP, human and eco-toxicity. On the contrary, as a promising biological treatment option, AD showed great environmental saving potentials: with the optimised energy utilisation system, AD best scenario offered the optimum environmental profiles on most impact categories.

- 2. Over the whole life cycle, the characterized comparison results between WBF and LDPE/HDPE/EPS varied with the case studies and their end-of-life scenarios. Generally, irrespective of end-of-life fates, the WBF cool box showed great advantages over equivalent conventional products in most impact categories (except acidification and eutrophication). But this was not the case for the display board or construction applications. WBF represented environmentally superior choices to HDPE/virgin EPS with landfill and incineration scenarios in abiotic depletion, GWP100, human and aquatic ecotoxicity and POCP; but the environmental advantages of WBF decreased with the lower EPS grade (due to the saving effects of the EPS recycled content). Whilst HDPE/EPS recycling scenario reversed the comparison with WBF: HDPE/EPS shifted to being superior systems to WBF products in most impact categories except ODP, terrestrial eco-toxicity and POCP. In the energy-driven impact categories ODP and terrestrial ecotoxicity, HDPE/EPS incineration scenarios represented the better options attributable to the energy recovery; whereas, regardless of the disposal routes, higher POCP burdens of LDPE/EPS (than WBF) were incurred due to PE/EPS transformation process. Overall, WBF was suggested as being the more environmentally friendly choice than the conventional cool box but not the display board/trough mould/concrete formwork with recycling scenarios.
- 3. Generally, for petrochemical polymers, cradle-to-grave environmental impacts on aquatic ecotoxicity, abiotic depletion, POCP and GWP100 were considered as relatively significant. The marine ecotoxicity score was relatively the most significant for WBF products, followed by acidification, abiotic depletion eutrophication and GWP100, where 40–60 % of impacts were attributable to WBF disposal process. Therefore, the major contributors at the WBF disposal

6.7 Discussion 317

stage were of relative significance including the emissions either from WBF degradation or from biogas combustion. Via normalization, it was suggested that the advantages of WBF products over equivalent petrochemical polymers with the landfill or incineration scenarios on aquatic ecotoxicity, abiotic depletion, and POCP were relatively significant. Despite that the normalized LCIA profiles gave good insight on the relative balance of the contributions of WBF products to environmental problems over their full life cycles, whilst bearing in mind that these insights are subject to the spatial and temporal reference systems used in the normalization procedure.

- 4. Over the life cycle, WBF showed great advantages over alternative starchbased foams on resource depletion, ODP and toxicity but not acidification, eutrophication, GWP100 and POCP, on which the differed chemical composition of biopolymers produced influences, e.g. SO₂ release in WBF landfill scenario due to the presence of S in WBF, protein-N released either as NH₃/ leachate (from WBF degradation) or as NOx (from biogas plant) but no significant N/S emissions evolved from PSBF/MSBF degradation. Moreover, the difference in chemical compositions of WBF and PSBF/MSBF drove their differing comparison results with PE on acidification: WBF shifted from superior (production stage) to inferior products to LDPE/HDPE (at end-of-life) but MSBF/PSBF remained their advantages over PE products on acidification throughout life cycle stages. Generally, the comparison results between PSBF/ MSBF and petrochemical polymers on most impact categories were carried through from production stage to end-of-life (except EPS/HDPE recycling). Similar findings to WBF were suggested: regardless of disposal routes, PSBF and MSBF were environmentally superior choices to the LDPE coolbox but not to conventional display board and construction products, especially HDPE/EPS products with recycling scenarios which delivered better environmental performance than equivalent MSBF/PSBF on most impact categories. However, these findings only provided tentative indication because of the different data sources and modelling basis for WBF and altenative starch foams, e.g. the secondary data for starch rather than primary inventory used for wheat flour, the assumptions on compressive/thermal characteristics of PSBF/MSBF used in the case study rather than lab-derived data used for WBF modelling.
- 5. A range of sensitivity parameters were analysed. As summarized in Table 6.10, home composting operation was considered as a sensitive factor reversing the POCP and GWP comparisons between WBF and PE/EPS because of the greater CH₄, N₂O release assumed from anaerobic zone in passive composting. Whereas the WBF life cycle with AD scenario showed great saving potentials: optimised energy utilisation in the AD scenario shifted WBF to advantageous products over conventional petrochemical polymer in various application on several impact categories (abiotic depletion, GWP, ODP and toxicity). On the contrary, the reduction in energy recovery in the landfill scenario substantially decreased the advantages of WBF over petrochemical polymers, especially moving WBF to inferior system to EPS in construction case studies on ODP and toxicity impact categories. Apart from energy recovery efficiency, temporal boundary was

considered as another critical parameter for WBF landfill scenario. Despite that comparison results appeared not sensitive to long-term WBF-C release assumed under the expanded temporal boundary, the stored chemical elements in landfill could be removed proportionally via other pathways under an infinite time horizon, which brought uncertainties in comparison outcomes.

Besides end-of-life scenarios, infrastructure also produced influences on comparison results. WBF products were indicated as more sensitive to infrastructures than petrochemical polymers: the exclusion of infrastructure not only resulted in a significant drop in WBF environmental impacts, but also drove WBF to a more environmentally superior system in comparison with conventional EPS construction products.

Overall, comparison results between WBF and petrochemical polymers on GWP100, ODP and toxicity impact categories are more sensitive; across all the case studies, construction applications were suggested as the most sensitive product systems to the parameters tested. No general advantages of WBF over petrochemical polymers were supported via our findings. This suggests that a 'case-by-case' approach is necessary when comparing the WBFs with petrochemical products in a diversity of applications.

6.7.1 Key Findings

AD represents an environmentally superior choice to other disposal routes for WBF in GWP100, acidification and eutrophication but on the rest of the impact categories landfill or home composting had lower impacts. However, this waste management hierarchy is highly influenced by uncertainties in the parameters and assumptions modelled for the various end-of-life scenarios.

The overall results do not support a statement that 'there is generic advantage of WBF over petrochemical polymers'. The comparisons not only varied between the different case studies but also were very sensitive to end-of-life scenarios. This suggests that a 'case-by-case' approach is necessary when carrying out comparative LCAs between biopolymers and their petrochemical counterparts.

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Chapter 7 Sensitivity and Uncertainty Analysis

7.1 Introduction

Standardized data quality analysis under LCA framework includes sensitivity and uncertainty analysis [15]. Sensitivity analysis has been widely used, but uncertainty analysis much less so [2, 12, 18]. Generally for LCI data, uncertainty methods can be classified as: approaches that estimate qualitative sources of uncertainties, e.g. Pedigree Matrix [12, 21] and statistical methods to quantify the data variability [20]. The pedigree Matrix has been used as a default method introduced into Ecoinvent database [8]; on but statistical methods are rarely applied [4, 6, 20]. Based on the LCI uncertainty information, a range of uncertainty analysis methods can also be applied at the LCIA phase [2]. As one of the most commonly recommended methods, Monte Carlo simulation has been applied in previous LCAs both in methodology development and in case studies [5, 7, 13, 19].

In the present work the LCI comprised from primary industrial data and DNDC-modelled outputs and meta-analysis data for end-of-life options including novel results for AD. Particularly with regard to the data quality of DNDC outputs some previous studies have performed sensitivity analysis but very few concerned uncertainty analysis [16, 17] and these have used the MSF method rather than Monte Carlo simulations. Moreover, literature review suggested that no research has yet been carried out on integrating the results of uncertainty analysis for IPCC/DNDC emissions predictions into LCA models to formally assess the uncertainty of total indicator results.

In this study, the DNDC 93 model with modified Monte Carlo simulations was applied and both sensitivity and uncertainty analysis on DNDC outputs was conducted. These results were then further incorporated into the LCA model to quantify the uncertainties in LCIA profiles for WBF products.

In the following sections, first the outcomes of sensitivity analysis are considered and then the effects of uncertainty analysis are presented.

7.2 Sensitivity Analysis

Sensitivity analysis of the basic values of certain parameters and the scenario configurations for the various case studies has already been presented in previous chapters. This section therefore focuses on the effects of sensitivity analysis for that are LCA methodology related, specifically, the characterisation and normalisation models.

7.2.1 Sensitivity Analysis on Characterisation Models

As an alternative to the mid-point method CML 2 Baseline 2000, the damageoriented method Eco-Indicator 99 H (hierarchist version) was applied to the inventories (with land use excluded). As illustrated in Fig. 7.1, the results based on EI 99 are similar to the outcomes in (Fig. 6.9) (CML method) in almost all comparable impact categories. For instance, the ranking of WBF life cycles with various end-of-life scenarios in the CML method is confirmed in the results derived from EI 99. Over its life cycle, the WBF coolbox delivered lower impacts on GWP (Climate change) human toxicity (Carcinogens in EI 99) eco-toxicity POCP (respiratory organic in EI 99) and ODP, but higher burdens on acidification/ eutrophication in comparison with LDPE coolbox. Regarding minerals in EI 99, the WBF coolbox is shown as environmentally inferior to the LDPE alternative, but in the CML approach for both coolbox systems the main contributors on abiotic depletion are fossil fuels and this result is confirmed by the Fossil Fuel comparisons in Fig. 7.1. EI 99 also accounts for the winter smog (respiratory inorganics) and the damages induced by radioactive radiation which are not included in the CML method [9, 10].

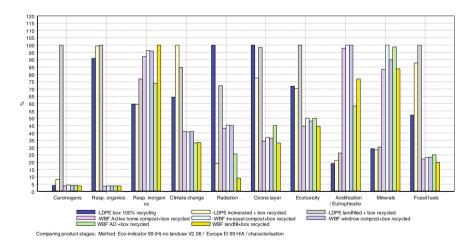


Fig. 7.1 Sensitivity analysis on characterisation model (unit per coolbox)

In the other case studies, the results derived from the CML and EI 99 methods tend to agree on most impact categories except acidification/eutrophication and eco-toxicity. Unlike the CML method, EI99 not only combines acidification with eutrophication but also aggregates ecotoxicity potential of all substances into a single indicator result. As given in Fig. 7.2, the HDPE display board systems appears to have lower impacts than WBF in the aggregated acidification/eutrophication EI 99 category and this somewhat different from the CML findings in Fig. 6.3, where HDPE in the landfill scenario incurs similar acidification scores to WBF but higher eutrophication burdens. In addition, the lower EI99 aggregated ecotoxicity impact scores for HDPE with incineration or recycling than WBF with any disposal mode in Fig. 7.2 differ from the CML outcomes (see Fig. 6.3) where both HDPE with incineration or landfill gave higher aquatic ecotoxicity impacts than WBF, and HDPE with recycling was inferior to WBF on terrestrial ecotoxicity.

Figure 7.3 is representative of both virgin and low grade EPS as similar results were found across all construction case studies. In the cases, the comparisons on toxic impact categories are sensitive to the characterisation model. EPS with landfill appears to bring substantial damage to human health in EI 99, but it is indicated as environmentally superior or equivalent to WBF in the CML method. Ecotoxicity comparisons in EI 99 can replicate the CML outcome on fresh water ecotoxicity but not on the other ecotoxic impact categories where EPS recycling delivered similar or higher burdens than WBF in CML method.

In summary, overall interpretation of the life cycles of WBFs and their comparison with petrochemical alternatives in most impact categories is not particularly sensitive to the characterization method adopted. However this generalisation is not universal and the display board and construction case studies were more sensitive to the LCIA method used than the coolbox case study. This suggests that a 'case-by-case' approach will be more secure with regard to LCIA methodological sensitivities when assessing WBFs in a diversity of applications.

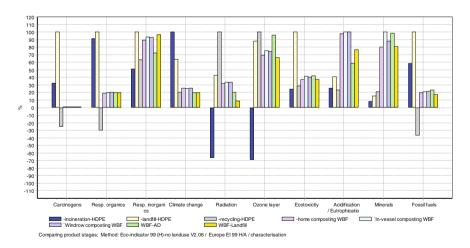


Fig. 7.2 Sensitivity analysis on characterisation model (unit per display board)

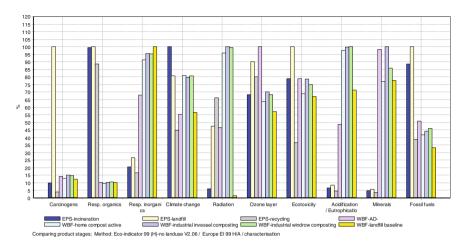


Fig. 7.3 Sensitivity analysis on characterisation model (unit per refractory lining)

7.2.2 Sensitivity Analysis on Normalization Methods

As an alternative to West Europe 1995 as a normalization reference system, World 1995 is available in CML 2 baseline 2000 v2.04. This was explored in sensitivity analysis. In World 1995 the total annual emissions or resources use in the world for the given year 1995 are chosen as the reference value, which was reported by Huijbregts et al. [11].

Comparing the normalized profiles of the coolbox shown in Fig. 6.11 and 7.4, change in normalization method produced insignificant effects on the magnitude of each category indicator result. Similar conclusions also apply to the display board case study-normalized LCIA results were not sensitive to model choice. However, this was not the case for construction product case studies. Although the marine aquatic ecotoxic impacts are still indicated as most relatively significant for construction products, the choice of reference system caused a shift in the magnitude of the other category indicator results. Impacts of WBF products on fresh water ecotoxicity appeared as more significant under the World 1995 method than under West Europe 1995, shifting from sixth (Fig. 6.21) to fourth place (Fig. 7.6). Similarly, the fresh water ecotoxicity score of EPS with landfill and incineration scenarios moved from fourth (Fig. 6.20) to second place (Fig. 7.5) with the change in normalization model. Conversely, the magnitude of impacts of WBF products on acidification, abiotic depletion, eutrophication and GWP decreased under World 1995 model (Figs. 6.21 and 7.6). The overall results suggested that amongst the case studies investigated, construction applications are more sensitive to normalization method.

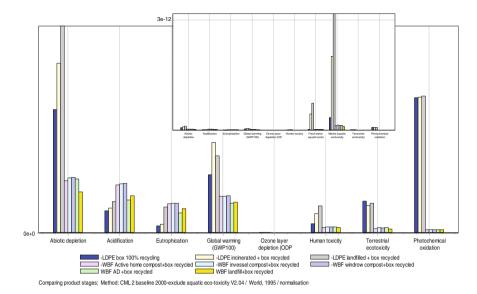


Fig. 7.4 sensitivity analysis on normalization model (unit per coolbox) *Notes* Insert histogram includes aquatic eco-toxicities which are excluded from the main histogram due to problem of scale

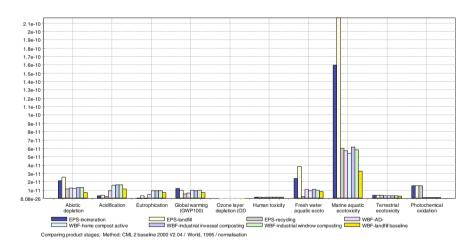


Fig. 7.5 Sensitivity analysis on normalization model (unit per refractory lining)

7.2.3 Sensitivity Analysis on Time Horizon

The time-dependency of GWP, ODP, and toxicity potential were taken into account in current study to examine the sensitivities of characterised LCIA profiles to different timeframes. The comparison results between WBF and petrochemical polymers are presented in Figs. 7.7, 7.8, 7.9, 7.10, 7.11, 7.12, 7.13, 7.14, 7.15.

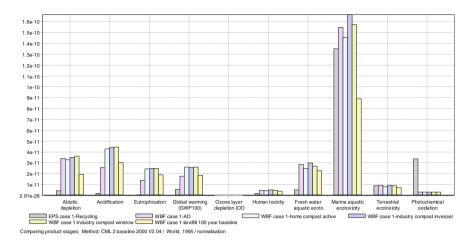


Fig. 7.6 Sensitivity analysis on normalization model (unit per trough mould)

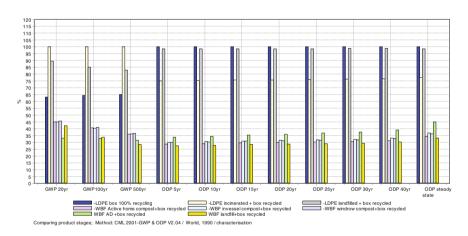


Fig. 7.7 Sensitivity analysis on time horizon-GWP and ODP (unit per coolbox)

7.2.3.1 GWP and ODP Timeframes

Expansion of time horizon not only reduced the GWP profiles of all WBF life cycles with various end-of-life scenarios but also changed both their relative ranking and their comparison with petrochemical polymers. This is attributable to differing emission profiles for the short-lived gas CH₄. The GWP of WBF with landfill and composting decreased by 40–50 %m and 30–37 %, respectively whereas only a 13–20 % decline was observed in the AD scenario when expanding the time frame from 20 to 500 years. Thus WBF with landfill shifted from being an inferior to a superior system to WBF with AD due to this timeframe perspective. Similar trends were found with the petrochemical polymers: their GWP scores

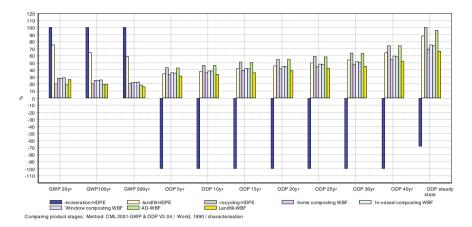


Fig. 7.8 Sensitivity analysis on time horizon-GWP and ODP (unit per display board)

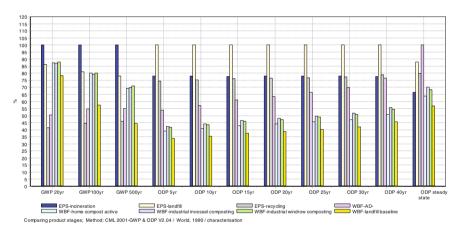


Fig. 7.9 Sensitivity analysis on time horizon-GWP and ODP (unit per refractory lining)

decreased with the expanded time horizon due to short-lived emissions, especially CH_4 and N_2O , whilst EPS/PE with landfill was more sensitive to timeframe than with the other waste treatments. Overall, the time horizon had a greater influence on WBFs due to their higher CH_4 release potentials from their life cycles than petrochemical polymers. Therefore, as shown in Figs. 7.7–7.9 the advantages of WBFs over conventional petrochemical polymers on GWP category increase with expanded timeframe.

Generally, the ODP profiles of petrochemical polymers, especially the EPS construction products were sensitive to the time horizon, but this was not so for the WBFs. The relatively stable ODP profiles of WBF products with timeframe (increase less than 10 %) were mainly derived from transportation and VAC

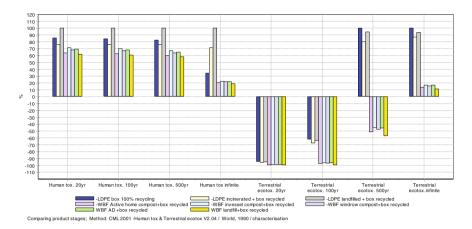


Fig. 7.10 Sensitivity analysis of timeframe-human toxicity and terrestrial ecotoxicity (unit per coolbox)

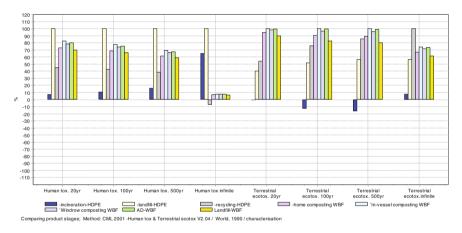


Fig. 7.11 Sensitivity analysis of timeframe-human toxicity and terrestrial ecotoxicity (unit per display board)

production. In fact, with expansion of the timeframe, ODP impacts of the short-lived gas CBrClF₂ emitted from transporting natural gas declined but were balanced by increased ODP impacts from the long-lived emission CBrF₃ released from crude oil production. Therefore, the rank between WBF various end-of-life scenarios remained stable. The ODP score of HDPE with incineration increased 60–70 % with the expanded timeframe due to a decline in saved emissions from avoided electricity (natural gas dependent) where short lived gas CBrClF₂ played an important role. The decrease in ODP scores of EPS products (decrease 40–60 %) was attributable to the short lived gas CBrClF₂ emitted from transporting natural gas, which was the dominant energy source for EPS

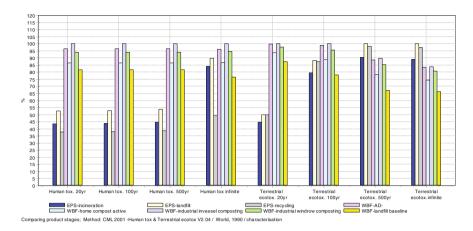


Fig. 7.12 Sensitivity analysis of timeframe-human toxicity and terrestrial ecotoxicity (unit per refractory lining)

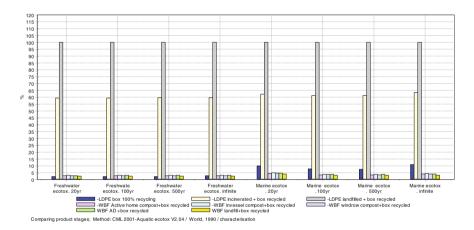


Fig. 7.13 Sensitivity analysis of timeframe-aquatic ecotoxicity (unit per coolbox)

transformation. These can explain the comparison between WBF and HDPE/EPS: the advantages of HDPE incineration over WBF decreased with the expanded timeframe, whereas inferior ODP score of EPS products (various end-of-lives) to WBF with AD reversed under the infinite timeframe. Low grade EPS showed a similar trend to virgin EPS. No significant influence of timeframe on coolbox comparison was observed.

Overall with the expansion of time horizon on ODP, the comparison of WBF and PE remained relatively stable. But the construction case studies were sensitive to expansion of timeframe, over which the advantages of WBF over EPS reduced.

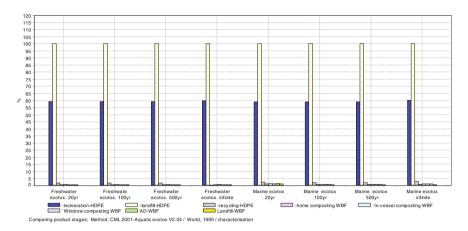


Fig. 7.14 Sensitivity analysis of timeframe-aquatic ecotoxicity (unit per display board)

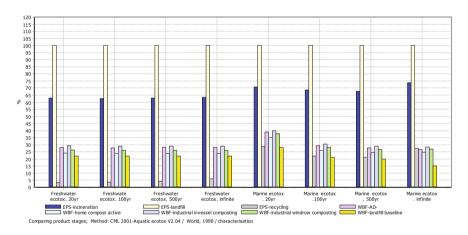


Fig. 7.15 Sensitivity analysis of timeframe-aquatic ecotoxicity (unit per refractory lining)

7.2.3.2 Human Toxicity and Eco-Toxicity Timeframes

The human and ecotoxicity impacts of WBF and its equivalent petrochemical polymers over expanded timeframes are given in Figs. 7.10–7.15. Virgin EPS is used to represent all construction case studies (low grade EPS gave similar trends).

Generally, all the toxicity impacts increased with the expanded timeframe (except HDPE with recycling or incineration), especially terrestrial and marine ecotoxicity where a substantial rise in environmental score was observed. This is due to heavy metals which are modelled as the long-term emissions producing higher toxicity impacts over longer time periods in the CML method used [10].

As analyzed in Chaps. 4 and 6, the toxicity profiles of WBF products were driven by the production of infrastructure materials involved in PVOH and WBF

production as well as by electricity generation and transmission but not the end-of-life. Thus, the relative rank of WBF life cycle with different waste treatments remained stable (Figs. 7.10–7.15).

The human toxicity and aquatic ecotoxicity impacts of the petrochemical product life cycles with landfill or incineration were driven by metallic ions (e.g. vanadium, nickel) released from waste disposal. The petrochemical products with recycling are different, depending on the balance between 'avoided' PE/EPS manufacture and burdens caused by polymer production or transformation. Across all petrochemical polymers, terrestrial ecotoxicity scores were driven by emissions from fuel combustion or energy transmission. These factors help to explain the results observed in Figs. 7.10–7.15.

The effect of expanding the timeframe on human toxicity scores of petrochemical polymers with landfill or incineration either shifted to being inferior to WBFs or showed increasing disadvantage over WBFs. Petrochemicals with recycling remained equivalent or superior to WBFs on human toxicity. HDPE with incineration showed increasing advantages over WBF on terrestrial exotoxicity over the 500-year timeframe due to the increasing beneficial effects of 'avoided' mercury emission from hard coal combustion. However, the overall toxic impacts of petrochemical polymers are more sensitive to the timeframe than WBF. Thus on the toxicity impact categories, WBFs either strengthened their advantages over petrochemical polymers (Figs. 7.10, 7.13–7.15) or moved towards superior or equivalent system to petrochemical products (Figs. 7.11, 7.12).

7.3 Uncertainty Analysis

7.3.1 Uncertainty Analysis of LCI

The uncertainty introduced into the LCI results was quantified by the methods defined in Chap. 2. In the case of industry-based or computer-simulated inventory data that contained information on data variability the statistical methods were applied. For other primary or secondary data only represented by a single measurement values, the Pedigree Matrix (expert judgement) approach was used.

7.3.1.1 Uncertainty of N₂O Field Emissions

Two approaches were applied to simulate N_2O field emission, i.e. IPCC approach and DNDC model, in both of which the combined uncertainty for model-derived N_2O was estimated by running Monte Carlo simulation with 5,000 iterations.

As presented in Sect. 2.2.2.4, a set of DNDC-generated N₂O fluxes (based on randomized sensitive soil parameters) were further compared with various hypothesized standard distributions by applying non-parametric methods Chi

hypothesized distributions	Chi square test	a	K–S test ^b	
	Statistic χ ²	H ₀ ^c	Statistic d_{max}	H_0^d
Normal	500.384	Reject	0.073	Reject
Lognormal	420.060	Reject	0.058	Reject
Uniform	1020.097	Reject	0.248	Reject
Triangle	802.023	Reject	0.187	Reject
Weibull	507.572	Reject	0.076	Reject
Raylaigh	1358.673	Reject	0.323	Reject
Beta	418.099	Reject	0.065	Reject
GEV^a	423.496	Reject	0.060	Reject
Gamma	420.275	Reject	0.063	Reject

Table 7.1 GOF results for DNDC-simulated N2O field emissions (Field 1)

Notes

square and K-S tests. For each hypothesized distribution, the characteristic parameters were estimated by MLE. Below, field 1 is given as an example to interpret the statistical analysis results where pH and field capacity were identified as the most sensitive soil parameters. As shown in Table 7.1, both test statistics γ^2 and d_{max} were used as measures of how far the observed samples (N₂O) deviated from the hypothesized distribution. Although the null hypothesis that the observed frequency distribution is consistent with expected theoretical distribution was rejected, the rank of χ^2 and d_{max} still indicated the best representative of the observed samples: the larger disagreement between the observed and the expected frequency, the greater was the χ^2 and d_{max} value obtained. In most cases, the bestfitted distributions identified by the two non-parametric methods were consistent, however, when discrepancy occurred results obtained from Chi square test took priority as it is more suitable for the large sample size (except average data for 6 fields). Thus, in the case of field 1, Beta distribution was identified as the best-fitted one; its PDF is plotted in Fig. 7.16, where the observed frequency for N₂O is illustrated as a bar chart (expressed as frequency/sample size).

In addition, uncertainties for IPCC-derived N₂O emissions were estimated by statistical analysis software RiskAMP Monte Carlo Add-In Library version 2.97 (Structured Data, LLC), where the uncertainty range of EFs (emission factors) given in the IPCC Guideliness (2006) were used. The sets of IPCC-simulated data were further analyzed by statistical methods (MLE, GOF) and compared with DNDC in Table 7.2 where apart from the best-fitted distribution identified, the CV is also given as a normalized measure of dispersion of the N₂O data. Generally the sample size for N₂O emission is 5,000, except for average N₂O derived from DNDC (sample size less than 500) as this was obtained by averaging the six-fields data which were based on identical randomized soil parameters (field capacity and soil pH).

 $^{^{}a}$ GEV = generalized extreme value

^b Number of bin = 50; significance level $\alpha = 0.05$

^c H_0 null hypothesis (no difference) is rejected if $p < \alpha$

^d H_0 null hypothesis (no difference) is rejected if d_{max} is greater than critical value

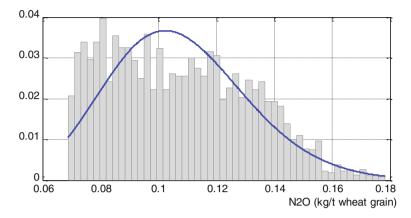


Fig. 7.16 PDF of Beta Distribution—best-fitted distribution for DNDC-simulated Field 1 N_2O emissions

Table 7.2 Uncertainty analysis results for DNDC vs. IPCC. (The statistics χ^2 and d_{max} are indicated in the bracket)

	IPCC			DNDC		
	Best-fitted distril	oution	CV	Best-fitted distribu	ıtion	CV
	Chi square	K-S test	- (%)	Chi square	K-S test	- (%)
Field 1	Weibull (101.519)	Weibull (0.022)	36.4	Beta (418.099)	Lognormal (0.058)	22.7
Field 2	Weibull (111.981)	Weibull (0.024)	36.7	Lognormal (662.417)	Lognormal (0.068)	27.1
Field 3	Weibull (118.664)	Weibull (0.026)	36.7	GEV ^a (698.953)	Lognormal (0.066)	18.9
Field 4	Weibull (99.448)	Weibull (0.019)	36.9	Beta (472.146)	Lognormal (0.054)	22.6
Field 5	Weibull (99.76)	Weibull (0.018)	36.5	Lognormal (571.693)	Lognormal (0.066)	25.0
Field 6	Weibull (152.928)	Weibull (0.028)	37.4	GEV (418.971) ^a	Lognormal (0.060)	19.2
Average	Weibull (103.979)	Weibull (0.025)	36.4	GEV (67.837) ^a	Lognormal (0.099)	22.6

Notes

As illustrated in Table 7.2, for IPCC-estimated N_2O , the best-fitted distribution identified by Chi square agreed with K–S test outcomes i.e. the Weibull distribution as presented in Fig. 7.17 where the observed frequency distribution was plotted as bar chart. However, discrepancy occurred in the case of DNDC-simulated N_2O : for each individual field (large sample size), Chi square results took priority whereas for average DNDC-estimated N_2O data, K–S tests were considered as more reliable because the latter is more powerful for the smaller sample

^a GEV = generalized extreme value

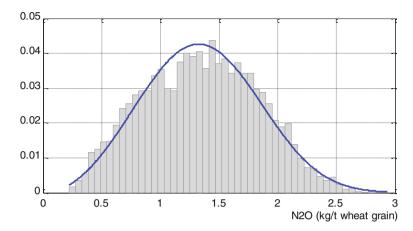


Fig. 7.17 Probability density function of Weibull Distribution—best-fitted distribution for DNDC-simulated Field 1 N_2O emission

size [22]. The CV shown in Table 7.2 indicated that the sets of IPCC-simulated data were more statistically dispersed than the DNDC results, attributable to the wide uncertainty range of EFs given in IPCC Tier 1 approach. Furthermore, uncertainty analysis on IPCC-derived N_2O suggested the result calculated based on default EFs deviated far from the mean of the hypothesized distribution. These findings further confirm that in comparison with the DNDC model, a larger degree of uncertainty is introduced into the LCIA results by applying the IPCC Tier 1 approach which is developed for national GHGs inventory reporting purposes and is intended to be broadly applicable. Therefore, the development of regional EFs for the IPCC Tier 1 together with their PDFs would be useful.

7.3.1.2 Uncertainty of DNDC-Simulated Results

The results for uncertainty analyses of DNDC-simulated N emissions are given in Table 7.3 where the number of bin is 50. Unlike N_2O and NO_3^- , for which the most sensitive soil parameters were consistent in the six fields (field capacity, pH for N_2O and bulk density porosity for NO_3^-), it was not possible to obtain sets of average data for NO and NH_3 due to a lack of comparability of their sensitive soil parameters between the six fields. Therefore, the uKingncertainty range of average NO and NH_3 were estimated by Pedigree Matrix method.

7.3.1.3 Uncertainty of Other LCI Inventory

Uncertainty were introduced into the LCIA results due to the variability of AD data where the energy recovery efficiency and energy consumption were the major

	NO		NH_3		NO_3^-	
	Distribution	SD σ^a	Distribution	SD σ^a	Distribution	$\mathrm{SD}\sigma^{\mathrm{a}}$
Field 1 ^b	Lognormal	3.251E - 04	GEV	8.377E - 04	GEV	8.286E - 05
Field 2 ^b	GEV ^e	2.568E - 04	GEV	2.457E - 03	GEV	1.00E - 03
Field 3 ^b	GEV	3.146E - 04	GEV	1.080E - 03	Gamma	3.208E - 05
Field 4 ^b	GEV	2.966E - 04	GEV	7.174E - 04	GEV	8.464E - 04
Field 5 ^b	GEV	4.589E - 03	Lognormal	2.211E - 03	GEV	8.957E - 04
Field 6 ^b	GEV	3.817E - 04	GEV	1.110E - 03	GEV	8.574E - 04
Average ^c	NA^d	NA ^d	NA ^d	NA^d	GEV	5.958E - 04

Table 7.3 Uncertainty analysis for DNDC-modelled N emissions

Notes

concerns in the AD scenarios for WBF products. As illustrated in Table 7.4, the observed sample i.e. daily data collected from AD plant over a three-month period (Jan–March 2009) were analyzed to derive statistical dispersions and best-fitted distributions where the K–S test values (more appropriate for small sample size) took priority.

The uncertainties for the GHGs emitted from diesel combustion in agriculture and waste treatment stages were estimated based on the uncertainty ranges of EFs recommended in the IPCC Guidelines [14]; the statistical methods MLE and GOF were applied.

In addition, for other LCI inventories represented by a mean value and without information on data variability, statistical methods MLE and GOF were not applicable. Thus, their uncertainties were quantified by the expert judgement-based approach Pedigree Matrix, where lognormal was introduced as the default probability distribution and data quality were characterised by six indicators [data reliability, completeness, representativeness, temporal geographical and technological coverage (defined in Sect. 2.3.2.1)].

7.3.1.4 Limitation in LCI Uncertainty Analysis

However, some of the best-fitted distributions identified above were not applicable in Simapro due to the limitations of software where only four probability distributions are included (normal, lognormal, uniform and triangular distribution). Therefore, via the rank of statistics χ^2 or $d_{\rm max}$ the best-fitted one amongst four "Simapro-built-in" distributions was actually used when aggregating uncertainty: for instance, in Table 7.1 lognormal was indicated as best-fitted 'Simapro-built-in' distribution.

^a SD σ of model-derived data (unit: kg/t wheat grain)

^b For large sample size, Chi square results took priority

^c For smaller sample size, K-S test took priority

^d NA = not applicable by GOF, as the sensitive soil parameters varied between 6 fields

^e GEV = generalized extreme value

	Best-fitted distribution		SD $\sigma^{\rm b}$
	Chi square test ^a	K-S test ^a	
Energy recovery ^c	Lognormal	Lognormal	0.334
Energy consumption ^d	GEV	GEV	6.064

Table 7.4 GOF results for AD data

Notes

- ^a Number of bin = 10; significance level $\alpha = 0.05$
- ^b SD of observed samples
- ^c Unit kWh electricity/per m³ biogas
- ^d Unit % electricity generated

Sample size is an important factor for the statistical methods applied—it affects the robustness of MLE, where the larger the sample size, the smaller the bias in parameter estimates [1]. In the current LCA, due to limitations in industrial data accessibility, only sets of data collected from limited time-periods were used in statistical analysis. In further research, better representativeness of the industrial data variability could be achieved via increasing sample size and including a wider temporal range.

In addition, there are certain limitations in the Pedigree Matrix method, where the uncertainties are estimated by expert judgement. Inappropriate technical and statistical judgements and misunderstanding between the inventory compiler and experts can introduce unintentional bias.

7.3.2 Uncertainty of LCIA Results

The uncertainty results were computed via Monte Carlo simulation in Simapro 7.0 software where the LCA model with the method CML 2 Baseline 2000 v2.04 was applied running 1000 iterations to reach multiple estimates of LCIA outputs.

7.3.2.1 Uncertainty in LCIA Profiles of WBF

Based on the probability distribution of the computed category indicator results *e.g.* Fig. 7.18 (number of bin = 50), the uncertainty ranges for the characterised LCIA profiles were derived. As illustrated in Fig. 7.19, the blue error bars represent the uncertainty ranges in terms of the ratio of the 2.5th and 97.5th percentile U, V to mean value (see results in Table 7.5). The 95 % confidence interval given in Table 7.5 indicated that by repetition, 95 % of the cases the characterised result would fall within the range (U, V). Moreover, the CV was considered as the normalized indicator of dispersion in the category indicator results. Thus the CVs presented in Table 7.5 suggested that larger degree of uncertainty was introduced

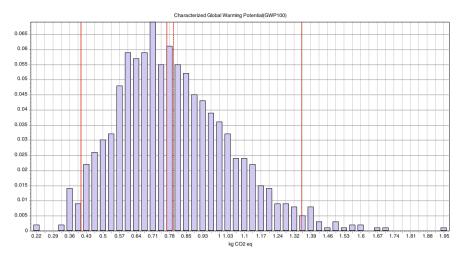


Fig. 7.18 Probability distribution of characterised GWP100 profiles for WBF AD scenario (unit: per coolbox)

in toxic impacts of the WBF coolbox with AD especially its aquatic eco-toxicity results due to the large uncertainties in the major toxic drivers such as heavy metal emissions. Conversely, abiotic depletion, GWP100, acidification and eutrophication scores for WBF coolbox showed low variance. Similar results were also observed in other WBF case studies with diverse end-of-life scenarios.

7.3.2.2 Uncertainty in LCIA Comparisons

TheMonte Carlo simulation was run with 1,000 iterations at the 95 % confidence level to estimate the uncertainties in the LCA comparisons between WBF and equivalent petrochemical polymers. As illustrated in Fig. 7.20 where the coolbox is used as an example, the uncertainty analysis reveals that there is a better than 85 % probability that the WBF option delivers better cradle-to-grave LCIA results than LDPE product on most impact categories. As an identical end-of-life scenarios (recycling) were modelled for the cardboard components, the results indicate that it is quite certain that the WBF coolbox with AD scenario in general would be an environmentally superior choice than the LDPE coolbox even with 100 % recycling. However, within the specific acidification and eutrophication categories, there is only a very low probability (0–17 %) that the WBF with AD option incurs lower impacts than LDPE with recycling. For fresh water ecotoxic impacts the uncertainty analysis also reveals that no clear statement can be given about which polymer would offer the more environmentally friendly choice.

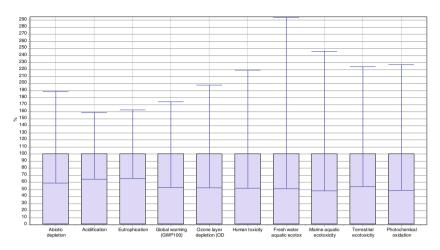


Fig. 7.19 Uncertainties for characterised LCIA profiles of WBF AD scenario (unit: per coolbox)

Table 7.5 Uncertainty analysis for WBF with AD. (Unit per coolbox, method: CML 2 baseline 2000 v 2.04)

Impact category	Mean	Median	SD^a	CV	U^a	V^a
				(%) ^a	(2.50 %)	(97.50 %)
Abiotic depletion (kg Sb eq)	5.86E - 03	5.49E - 03	1.85E - 03	31.50	3.21E - 03	1.04E - 02
Acidification (kg SO ₂ eq)	7.46E – 03	7.25E – 03	1.73E - 03	23.20	4.66E – 03	1.16E - 02
Eutrophication (kg PO ₄ ³⁻ eq)	1.62E - 03	1.57E - 03	4.35E – 04	26.80	1.03E - 03	2.55E - 03
GWP100 (kg CO ₂ eq)	8.03E - 01	7.73E - 01	2.43E - 01	30.30	4.06E - 01	1.35E + 00
ODP(kg CFC-11 eq)	8.14E - 08	7.59E - 08	3.10E - 08	38.00	3.97E - 08	1.50E - 07
Human tox (kg 1,4-DB eq)	2.45E - 01	2.24E - 01	9.87E – 02	40.30	1.16E – 01	4.92E - 01
Fresh water ecotox (kg 1,4-DB eq)	6.12E – 02	5.27E - 02	3.29E - 02	53.80	2.67E - 02	1.55E - 01
Marine ecotox (kg 1,4-DB eq)	8.84E + 01	7.74E + 01	4.30E + 01	48.70	3.70E + 01	1.90E + 02
Terrestrial ecotox (kg 1,4-DB eq)	2.30E - 03	2.10E - 03	8.88E - 04	38.60	1.14E - 03	4.72E - 03
POCP (kg C ₂ H ₄)	2.49E - 04	2.26E - 04	1.03E - 04	41.30	1.09E - 04	5.13E - 04

Notes

Selected examples of uncertainty analysis results are presented in Tables 7.6 and 7.7, where WBFs are compared with petrochemical polymers in best (recycling) and worst (landfill) cases. Generally, there are over 85 % probabilities that WBF is environmentally superior to LDPE and HDPE (except HDPE recycling) in most impact categories. In construction product cases, the advantages

^a U: 2.5th percentile V 97.5th percentile

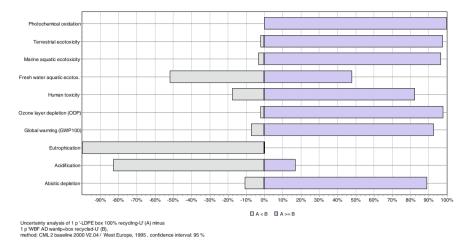


Fig. 7.20 Monte-Carlo simulation results of characterised LCIA comparison between WBF and LDPE coolbox (unit: per coolbox) *Notes* A = LDPE coolbox with 100 % recycling; B = WBF coolbox with AD + recycling scenario

of WBF over all EPS products on POCP is certain whereas there are high probabilities that WBF delivers better aquatic ecotoxic scores than EPS with landfill. However, on other impact categories the uncertainty analysis indicated considerable variation with the different end-of-life scenarios and with the EPS grades. Across all the case studies, WBF consistently showed high probabilities of incurring higher acidification and eutrophication impacts than the petrochemical polymers.

7.3.2.3 Influence of N₂O Modelling Approach on LCIA Uncertainties

The influence of different N_2O modelling approaches on uncertainties in the GWP100 comparisons were investigated by running Monte Carlo simulation with 1,000 iterations at the 95 % confidence level. The comparisons of WBF with AD scenario with HDPE with landfill or recycling are given as examples to illustrate the major findings (Table 7.8).

The uncertainty analysis supported the results presented in Sect. 6.6.1. It was quite certain that neither the N_2O modelling approach nor different fields produced significant influences on the comparison between WBF and petrochemical polymers (except HDPE with recycling). Although WBFs based on IPCC and DNDC showed opposing outcomes in the comparisons with HDPE with recycling on GWP100, the probabilities (50–60 %) suggested the comparisons were not certain.

The CV shown in Table 7.8 indicates the normalized dispersion of data points i.e. the differences in GWP profiles of HDPE and WBF. However, the CVs derived

	Coolbox	X	Display HDPE	board	Trough Filcor 2		Concret formwork Filcor 70	rk
Impact category	Landfill	Recycling	Landfill	Recycling	Landfill	Recycling	Landfill	Recycling
Abiotic depletion	99.9%	89.2%	99.4%	73.2%	58.3%	94%	89%	52.9%
Acidification	60.1%	82.9%	68.5%	69.3%	99.5%	99.8%	93.8%	97.9%
Eutrophication	62.2%	99.8%	95.8%	93.9%	87.6%	100%	78.3%	100%
GWP100	99.1%	92.8%	95.7%	51.5%	58.2%	93.1%	80.8%	57.8%
ODP	97.5%	98%	50.5%	54.6%	71.3%	75.1%	51%	55.1%
Human toxicity	98.4%	82.5%	97.5%	68.1%	62.3%	89.1%	56.3%	75.9%
Ecotoxicity Fresh water	100%	51.8%	100%	53.5%	88.5%	98.5%	91.9%	97%
Ecotoxicity Marine	100%	96.7%	100 %	91.5%	92.4%	52.5%	94.9%	56.7%
Ecotoxicity Terrestrial	95.1%	97.8%	58.5%	70.8%	51.4%	51.4%	59.4%	59.1%
POCP	100%	100%	91.7%	72%	99.8%	100%	100%	100%

Table 7.6 Uncertainty analysis for LCIA comparison of WBF with AD vs, petrochemical polymer life cycle (indicated by probability)

Notes:

Over 50% probability that WBFAD scenario lower impacts than petrochemical polymer

= Over50% probability that WBF AD scenario higher impact than petrochemical polymer

from comparison between HDPE with recycling and WBF with AD were not considered as valid indicators because:-

- 1. CV is designed for non-zero mean and is more suitable for variables with positive values
- 2. Either positive or negative values were derived by subtracting GWP score of WBF with AD from that of HDPE with recycling due to the great uncertainties in their GWP100 comparison.

The 'valid' CVs in Table 7.8 indicate that the IPCC method led to slightly more widely dispersed comparison results than the DNDC method (comparison between HDPE with landfill and WBF with AD).

The other case studies gave similar findings to those above. Overall, although larger degrees of uncertainty were introduced into the GWP profiles of WBF by using IPCC-estimated N_2O , the choice of the N_2O modelling approach was not suggested as a critical factor for the uncertainty analysis of GWP comparisons between WBF and the petrochemical polymers.

	Coolbox	.	Display HDPE	board	EPS To mould Filcor 2		Concrete formwork Filcor 70	rk
Impact category	Landfill	Recycling	Landfill	Recycling	Landfill	Recycling	Landfill	Recycling
Abiotic depletion	99.8%	90.2%	99.5%	74.8%	60.3%	93.8%	90.2%	51.2%
Acidification	86.8%	94.6%	57.6%	85%	99.9%	99.9%	99.3%	99.8%
Eutrophication	64.1%	100%	85.9%	98.5%	97.3%	100%	95.1%	100%
GWP100	96.5%	84.4%	92.9%	56.6%	79.4%	99%	55.7%	81.2%
ODP	99%	99.9%	66.6%	76.0%	58.0%	53.7%	75.0%	72.2%
Human toxicity	99.1%	85.7%	98%	64.3%	54.2%	85.1%	59.9%	73.4%
Ecotoxicity Fresh water	99.9%	55.6%	100%	52.3%	92.1%	97.3%	94.6%	95%
Ecotoxicity Marine	100%	97.3%	100%	93.3%	93.8%	51.7%	95.8%	59.1%
Ecotoxity	97.9%	97.6%	5/1 3%	78.1%	56 1%	53 4%	65.1%	63.2%

Table 7.7 Uncertainty analysis for LCIA comparison of WBF with home composting verses petrochemical polymer life cycle (indicated by probability)

Notes:

POCP

Terrestrial

= Over 50% probability that WBF home composting scenario lower impacts than petrochemical polymer = Over50% probability that WBF home composting scenario higher impact than petrochemical polymer

78.1%

72.8%

56.4%

100%

53.4%

99.9%

65.1%

100%

63.2%

99.9%

54.3%

92.1%

Table 7.8 Influence of N₂O modelling approach on uncertainties of GWP100 comparison

Impact	HDPE I	andfill			HDPE 1	recycling		
category	IPCC		DNDC		IPCC		DNDC	
curegory	P	CV	P	CV	P	CV	P	CV
Field 1	97.4%	64.6%	97.0%	68.3%	53.2%	44.7%	54.2%	8.0%
Field 2	93.0%	75.5%	94.8%	69.1%	59.6%	-5.5%	50.4%	6.4%
Field 3	95.4%	66.4%	96.6%	64.3%	51.8%	-22.6%	55.8%	9.3%
Field 4	96.8%	65.3%	96.8%	64%	52.4%	23.2%	51.8%	18.7%
Field 5	91.8%	80.5%	95.0%	71.4%	50.8%	-471%	59.4%	-7.0%
Field 6	95.8%	76.2%	95.0%	69.8%	54.6%	-10.6%	50.6%	-69.5%
Average	94.8%	72.1%	95.7 %	69.4%	52%	-23.6%	51.5%	24.7%

Notes

Over 50% probability that WBF AD scenario lower impacts than HDPE

 \Box = Over50% probability that WBF AD scenario higher impact than HDPE

 \overline{p} =probability; CV=coefficient of variation of HDPE-WBF

97.9%

100%

97.6%

100%

7.4 Discussion

Overall neither the characterisation nor the normalization models were indicated to be sensitive parameters for comparison of WBF with LDPE in the coolbox cases. However, the display board and construction applications were more sensitive to the characterization methods adopted; especially in the comparison of WBF with HDPE or EPS with landfill or recycling scenarios using the EI 99 aggregated impact categories (acidification/eutrophication and eco-toxicity). Application of the CML method led to WBFs being indicated as more environmentally superior to EPS/HDPE with landfill/recycling scenarios than under EI 99.

Amongst the LCA case studies, construction products were also more sensitive to normalization method. The results suggested that normalized LCIA profiles only provided indicative information on the relative contributions of WBF products to environmental problems and are subject to variation depending upon the spatial reference used—in this case Western Europe or World. However, only one alternative reference region was examined in the sensitivity analysis and other reference systems should be examined in order to confirm this observation.

The timeframe was identified as a sensitive parameter for the LCIA comparisons between WBF and petrochemical polymers with the latter being more sensitive to timeframe than the former (except on GWP). Overall, with the expanded time horizon, WBF either strengthened its advantages over petrochemical polymers or shifted towards being a superior or equivalent system to conventional products on GWP and toxicity impact categories. Although on ODP, inferior profiles of EPS products to WBF AD scenario reversed under infinite time-frame, the advantages of WBF over PE (except HDPE incineration) remained relatively stable. These results suggest that the LCIA results assessed under single timeframe should be interpreted with care and sensitivity analysis on varying timeframe should be included as a measure of robustness for LCAs, especially comparative LCAs. Generally 100-year is recognized as a valid and important timeframe for GWP e.g. timeframe of GWP specified in PAS 2050 [3]; infinite time is the commonly applied time horizon for ODP and toxicity impact categories (see Sect. 1.3.2.3). But any single timeframe should not be defined as a rigid or definitive parameter as the methodological rigidity of characterization models could introduce inadvertent bias into the LCA outcomes. Therefore, time horizon varying from 20-years to infinite-time for impact categories like GWP, ODP, toxicity should be examined to deliver unbiased information for policy makers.

The results in current study indicated the limitations in the current LCI uncertainty analysis methods *e.g.* bias introduced by Pedigree Matrix method, limitations in Simapro 7 software, thus the improvements in the methodological aspects could be further explored. In current study, the level of uncertainty in LCIA comparisons (WBF vs. petrochemical polymers) varied between the case studies, which indicate a case-by-case comparison is needed when carrying out comparative LCAs on biopolymers. Moreover, these results suggest that the LCAs

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without interpretations of the degree of uncertainties should not be used as robust evidence as those biased findings can mislead the policy makers.

In comparison with DNDC, IPCC-simulated N_2O results were more statistically dispersed, attributable to the wide uncertainty range of EF given in the IPCC Tier 1 approach. Therefore, for IPCC approach, it is necessary to develop region-specific EFs as well as their uncertainty estimations. Moreover, for field-specific LCAs, the process-oriented model investigated here (DNDC) was considered to be superior to the IPCC Tier 1 approach, as the former not only expand the LCA system boundary by including more factors involved in the agricultural C/N cycles, but also can provide improved LCI data quality and reduce or, at least allow for better calibration of the uncertainties in the LCI inventory.

7.4.1 Key Findings

The WBF case studies indicate that, the parameters and assumptions in the database as well as the characterization and normalization methods need to be addressed in sensitivity analysis in order to draw robust LCA conclusions.

This research has demonstrated the introduction of statistical methods into uncertainty analysis in the LCA model. Combined with the findings from previous chapters, a conclusion can be drawn that DNDC is a preferred method to IPCC Tier 1 approach when conducting site-specific LCAs as the former allows the LCA system boundary to be expanded for the agricultural emissions and provides for a better calibration of uncertainty in the LCI.

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Chapter 8 General Discussion and Conclusions

The initial task of this research was to investigate the cradle-to-grave environmental profiles of novel WBFs and address the question 'is there a general environmental advantage for WBFs over petrochemical polymers?' This topic was addressed by developing an LCA model and case studies based on pilot manufacturing of WBFs that was focussed on addressing a number of central issues in conducting LCAs on bio-based materials. During the course of this research, a number of important issues concerning the application of LCA to bio-based materials and for LCA in general emerged as expected. These are essentially 'lessons learnt from the journey'. These are presented below in parallel with the overall findings, followed by the recommendations for future work and the conclusions from this study.

8.1 Discussions

8.1.1 Cradle-to-Grave LCIA Profiles of WBFs

WBFs (and two starch-based alternatives examined) are probably best considered as a group of starch-PVOH blended 'biopolymers'. Their environmental profiles have been examined in detail in this thesis with the following key points emerging.

Biogenic C sequestered into starch-based biopolymers during crop growth brings GWP100 'savings' though these are not sufficiently enough to completely offset the GWP 100 burdens caused by farming and PVOH production. Atmospheric emissions and N leaching from the agro-ecosystem also causes impact in terms of acidification and eutrophication and the emissions evolved during production of PVOH (especially its fossil feedstock C_2H_4 , and $C_2H_4O_2$) cause POCP burdens. Throughout the life cycle, the energy utilization and infrastructure involved in biopolymer and PVOH production not only dominate abiotic depletion but also act as driving factors on ODP and toxicity. Moreover, biopolymer waste treatments cause burden

especially on GWP 100, acidification, eutrophication and POCP due to emissions resulting from biopolymer biodegradation. The current study also suggests that the choice of starch source (wheat flour or purified starch) is critical: it not only influences the environmental scores at the production stage but also affects the emission profiles at end-of-life which depend on the chemical composition of biopolymers.

Amongst the diverse disposal routes available for starch-PVOH blends, AD is a promising choice with fewer GHGs evolved and high energy recovery. For N-containing biopolymers like WBFs, AD can be an optimum option in terms of minimising acidification and eutrophication impacts than other biological treatments. With the optimized energy utilization system, AD even can offer better environmental performances. Active home composting is another good end-of-life disposal option benefiting from its low infrastructure and energy inputs thus delivering low abiotic depletion, ODP and toxicity impacts. However, low quality ('passive') operation of home composting needs to be avoided as this shifts home composting to being an inferior system for GWP100 and POCP due to CH₄ emissions. Although landfill appears to fare well on the abiotic depletion, ODP and toxicity impact categories, great uncertainty exists over how robust this is due to high sensitivity to the energy recovery efficiency assumed and the temporal boundaries applied.

8.1.2 Environmental Advantages for WBFs Over Petrochemical Polymers?

The results summarized in Table 8.1 give the answer to this question. At the production stage WBF shows environmental advantages over petrochemical polymers in four impact categories (abiotic depletion, ODP, GWP100 and POCP), but incurs higher acidification and eutrophication burdens due to the N emission and leaching from the wheat agro-ecosystem. For the remaining impact categories (except terrestrial eocoticity), WBF delivers better or equivalent scores to PE but causes higher impacts than EPS. This cradle-to-gate comparison profile is carried through from the production phase to the full cradle-to-grave life cycle incorporating end-oflife in the cool box application. In the case of the display board and the construction cases the perspective is more mixed—WBFs are environmentally superior to HDPE or virgin EPS with landfill or incineration scenarios in the abiotic depletion, GWP100 ecotoxicity and POCP impact categories but were equivalent or inferior to EPS or HDPE with a recycling scenario in most impact categories. If taking recycled content into account, EPS even gains more environmental advantages, with which WBF can hardly compete. These can be explained by the following facts: The performance of HDPE and EPS in these cases benefits greatly from recycling by the avoidance of virgin polymer manufacture; PE/EPS landfill acts as net fossil-C sink, effectively reducing GWP100 burdens; attributable to fossil energy recovery, PE/EPS incinerations deliver low ODP and terrestrial ecotoxic score; moreover, high density of WBF was modelled to deliver the equivalent compressive characteristics to various EPS grades.

Table 8.1 Summary of LCIA comparisons and sensitivity parameters^b

		olbox	ζ.				oard			crete			EPS	Trou	ıgh me	ould
Impact	LD	PE			HDI	PE				nworl or 70	k		oduction	Landfill Filcor 20		Filocr 45
categories	Production	Landfill	Incineration	Recycling	Production	Landfill	Incineration	Recycling	Production	Landfill	Incineration	Recycling	Filcor 20/45 production	Landfill	Recycling	Recycling Filocr 45
Abiotic depletion												D F	H I	G		
AP a				D		J										
EP a						J										
GWP100				В				A E		B E	В	D K		D		
										K						
ODP						D				D G	F G	D G	H I	F G	F G	K
										K	K	K		K	K	
Human toxicity							K		G	G J	F G	G	G	G J	G	G
										K	K					
Ecotox Fresh water	G						J							J		
							J	J	H I			G J	G H	J	D F	D F
Ecotox									1			K	11		G	G
Marine															J	J
															K	K
						J		J		K	K	J	Н	D	D	J
Ecotox								K				K	I	G	G	K
Terrestrial														J	J	
														K	K	
POCP							В									

Notes:

⁼ WBFs lower impact than petrochemical polymer at production/end-of-life = WBFs higher impact than petrochemical polymer at production /end-of-life = WBF similar impacts to petrochemical polymer at production; over life cycle, their comparison depends on WBF end-of-life scenarios

a. AP=acidification potential; EP=eutrophication potential

b. Sensitivity parameters: A=N₂O modelling approach; B=active vs. passive home composting; C=N transformation assumption in composting scenarios; D=AD scenario; E=landfill temporal boundary; F=energy recovery efficiency in landfill scenario; G=infrastructure; H=PVOH model; I=conversion process in display board/construction case studies; J=characterisation model choice; K=time horizon of impact category

However, as shown in Table 8.1, the comparison results should be considered as indicative information, especially for the construction products in GWP100, ODP and the toxicity impact categories. The comparisons results are sensitive not only to the parameters modelled for the WBF end-of-life scenarios, but also to uncertainties in the datasets (*e.g.* infrastructure, PVOH) and to the characterization methodologies. Furthermore, the LCIA profile of the WBFs relative to alternative petrochemical foams was variable depending upon the particular case study in question. Perhaps the clearest result has emerged in the case of the coolbox where throughout the life cycle WBF offers an overall environmentally superior choice over the conventional product. But its advantages over HDPE/EPS at production stage can reverse at end-of-life, depending on waste treatment option examined and the EPS grade.

8.1.3 Generic Environmental Advantages of Starch-PVOH Blends Over Petrochemical Polymers?

Generally the LCIA results of PSBF/MSBF agreed with most of findings on WBF above. However, PSBF/MSBF showed high impacts on abiotic depletion, ODP, terrestrial ecotoxicity where energy-intensive starch purification steps plus maize/ potato farming shifted MSBF/PSBF towards being less environmentally beneficial systems. On acidification, PSBF/MSBF was superior to PE throughout the life cycle stages due to their negligible N and S contents.

Overall, from environmental perspectives, the group of starch-PVOH blended biopolymers examined can offer optimum options compared with petrochemical polymers in thermal packaging applications. For applications where compressive properties take effect, starch-PVOH blended biopolymers can hardly compete on environmental grounds with the petrochemical products with close-loop recycling. However, these LCA results are based on current technology and in comparison with the well developed petrochemical industry biopolymers are still at the development stage. Thus, from the dynamic perspective, the further optimization in biopolymer technologies could bring WBF (starch-PVOH blends) great potential to deliver even better environmental profiles than petrochemical polymers, driven by more efficient bio-energy/material-crop farming systems, optimization in the biopolymer composition and properties, improvement in production processes, bio-ethanol instead of fossil feedstock for PVOH production etc.

8.1.4 LCA System Boundary

Although neither the agricultural system boundary nor the landfill temporal boundary appeared as a highly sensitive parameter for most of the LCIA comparisons of WBF and petrochemical products (Table 8.1), an important LCA

8.1 Discussions 349

scoping issue was explored in the present work: system boundary definition. Actually, in most of previous LCAs, a steady state of soil quality was considered as 'general rule' and neither atmospheric deposition nor the crop rotation was included into system boundary. Under this boundary definition, empirical modelling approaches and default EFs were most commonly applied methods to estimate field emissions. The current study has discussed two N₂O modelling approaches. Although IPCC Tier 1 approach indirectly reflects climatic/soil conditions via crop production, it fails to account for regional agro-ecosystem differences and site-specific farming practices. It is acknowledged that the IPCC Tier 1 approach is designed for national GHG inventory reporting, thus worldwide applicable EFs could introduce bias into regional N₂O estimations. On the contrary, DNDC simulates field emissions under expanded system boundary by directly taking into account factors like climatic condition, soil fertility change, interactions between crops within rotation etc. Thus, sensitivity analysis carried out on N₂O is not only to examine the influences of modelling approach but more importantly to investigate the effects of system boundary definition on the GWP100 score for the WBFs. The results suggest that the environmental profiles of agricultural products can be sensitive to the system boundary definition at this level. Therefore, by following 'general rules' in LCA practice, c.

Apart from this, the temporal boundary is considered to be a critical parameter and uncertainty source for the landfill model [6, 8]. Infinite time period is suggested as first choice [9], but most of LCAs incorporate a surveyable time e.g.100 years, under which, landfill is normally modelled as a net C sink. However, as stated by Barlaz [4] refuse could decompose until all organic matter exhausted. Thus, the temporal boundary is insignificant for biopolymers which can be biodegraded within surveyable years but is critical for materials that will undergo long-term degradation, especially when their different waste treatments are examined [8]. In the present study the baseline scenario of a 100 year timeframe was compared in sensitivity analysis with an infinite timeframe for WBF carbon release via landfill gas; neither other potential pathways for carbon release nor the releases of other chemical elements under an infinite timeframes were investigated. Thus no general conclusion can be produced here. The level of uncertainties introduced into landfill scenario by temporal boundary definition worth further exploring. But our findings indicate the inclusion of expanded temporal boundary into landfill scenario should be considered in the LCAs on materials with slow biodegradation process to avoid the misleading LCIA outcomes.

8.1.5 Data Quality Analysis of LCA Model

Sensitivity analysis indicates that data qualities for infrastructure and PVOH are critical: they affect comparisons between WBF and conventional products (see Table 8.1). But, in fact, great uncertainties were introduced into infrastructure and PVOH models that were established due to the use of surrogate datasets or expert

estimations for inventory development. Serious data gaps for petrochemical products exist even for widely applied polymers like PVOH [10]; in previous LCAs on biopolymers, infrastructure was generally excluded and PVOH was stated as missing data [7, 13]. This LCA practice is not appropriate as our findings suggest the exclusion of such datasets can introduce bias into LCIA results which can further mislead policy makers. Therefore, more efforts should be put into generic LCI database developments.

Apart from PVOH, there is a lack of data on waste treatment processes. In fact, only limited LCAs have compared biological treatments with recycling, incineration and landfill and amongst biological treatments, home composting and AD have only rarely been modelled in LCAs of solid waste (see introduction 1.4.3.4). Therefore, in the current study a substantial research effort was made to fill these data gaps, which not only covered the anaerobic degradation of WBFs and other components of the coolbox but also included industrial data collection on the AD process. Sensitivity analysis suggests that parameters modelled in other end-of-life scenarios are also critical such as the operation mode of home composting, element flows within landfill and composting scenarios, energy recovery efficiency in landfill. Thus, more research efforts are needed to develop reliable LCA inventories for waste treatments.

LCIA results are not only sensitive to LCI data and scenarios but also to the LCIA methods. In the current study the expansion of the time horizon in the characterization model led to the WBF profile shifting towards lower impact. Applying a midpoint LCIA approach (CML 2 baseline) the WBF profile also appeared to generate a more advantageous profile over petrochemicals than under the end-point approach (EI 99). The magnitude of the category indicator results also varied with the normalization reference systems. Thus, it is necessary to carry out sensitivity analysis at the level of the LCIA methodology to gain a deeper understanding of the reliability of the LCA results.

Uncertainty analysis at both the LCI and LCIA levels was specifically explored in the current study and several limitations in the LCI uncertainty analysis methods were found. Firstly, in the well recognized Pedigree Matrix method, bias can be introduced into uncertainty estimation by inappropriate technical and statistical judgements. Secondly, four standard Simapro built-in probability distributions cannot represent some of the observed frequency in this study, which can lead to bias in uncertainty estimation of LCIA profiles. Therefore, statistical methods are suggested instead of expert judgement-based approaches for analyzing both industrial and model-simulated datasets. However, almost all publicly available LCA databases, *e.g.* Eco-profiles [5] only provide average inventory data with no uncertainty information. In the case of industrial data, information on data variability is rarely provided. Further exploration of the effects of data uncertainty on reporting aspects of LCAs is needed in order to develop scientific analysis defining how representative and reliable information can be integrated into LCA models and provide acceptable quality evidence for decision makers.

Uncertainty analysis carried out on IPCC and DNDC outputs indicated that both the EFs and their uncertainty ranges given in IPCC Tier 1 introduce higher levels 8.1 Discussions 351

of uncertainties into the LCI than the process-based DNDC model (see results in Chap. 7). This finding further confirms that for field-specific LCA studies, process-oriented models are a superior choice to empirical models for LCI data quality.

Overall, the present study has attempted to deal with a number of aspects of uncertainty in LCA. This has led to an increase in the confidence of LCA findings, at the same time it has indicated the areas where improvements in data or methods are needed in order for robust conclusions to be drawn *e.g.* improvement in IPCC Tier 1 EF uncertainty range. Accommodately, uncertainty in the application of scientific and technical data is not only an issue for LCA, but also it attracts increased attentions in wider scientific and political communities [1].

8.2 Further Observations

A number of issues in addition to the main foci of the work emerged during this research. They are regarded as useful insights and contributions to analyses of the environmental impact of bio-based materials.

A number of previous studies have attempted to generalise answers to the question 'is there a generic environmental advantage for biopolymers over petrochemical polymers' by comparing different LCA studies [11]. However, such comparisons are usually hampered by between-study variation in factors like LCA methodological choice, data quality and assumptions of individual study. The current study eliminated the influences of such factors and was able to address the question via multiple case studies based on the same sets of parameters and methodological background for the WBF/MSB/PSBF biopolymers. The finding that a case-by-case approach is necessary for investigating the environmental profiles for WBF-like biopolymers is thus arrived at free of the between-study limitations referred to above although as noted below a number of improvements to the comparative basis can still be made.

During this research, serious data gaps (e.g. waste treatment and starch-PVOH polymer production process) were found in publically available sources and previous LCA studies. Thus, the present study has developed complete LCI inventories for WBF in a transparent manner by using primary data collected from industrial sources combined with new data from laboratory experiments supplemented with secondary data. The developed datasets have contributed to filling important data gaps and, through transparent presentation in this thesis, are available for use by other LCA practitioners. For instance, one of the data gaps was inventory data for the production process of PVOH. This is surprising as it is a commonly used polymer but no datasets were found in the public domain over the three and half years of this PhD program. The dataset developed here is considered to be a reasonable estimation of the generic production process and represents a publically available data source for PVOH via this thesis.

Comparison of the environmental profiles of WBF, PSBF and MSBF suggests that their environmental performance is broadly similar and therefore, conceptually,

these materials can be regarded as a "class" of starch-PVOH based biopolymers. This representation is based therefore not only on the similarities in structure and composition but on a functional attribute—their environmental performance. Further analysis would be required to determine whether additional starch based foams can be added to this class on the basis of both composition and environmental profile.

The LCA contribution analysis indicated for this group of biopolymers that the emissions evolved from the agro-ecosystem and PVOH production, together with the energy and infrastructure involved in biopolymer production were the major contributors to the environmental burdens of the their life cycle in most impact categories. The atmospheric emissions resulting from biopolymer degradation at the end-of-life were considered as another important contributor to environmental impact on GWP, acidification and eutrophication.

Through the combination of laboratory research and LCA modelling, this thesis supports the contention that AD is a highly suitable waste management option for biopolymer products. There are very few published studies on the performance of biopolymers in AD systems and this work therefore represents novel comparative findings in which AD is compared with a number of potential waste disposal routes. It should be noted that the comparison was based on a particular UK industrial AD system. This is a specific commercial facility which enphasizes the practical nature of the modelling but may reflect specific plant attributes. Further analyses of the type presented here are recommended, ideally based on modelling/experimentation reflecting a wider array of AD technologies.

Amongst the diverse 'end-of-life' scenarios examined, AD and/or home composting were suggested to be the optimum waste management choices for the class of starch-PVOH biopolymers investigated. AD offered superior GWP scores to both home and industrial composting; AD could hardly compete with home composing in terms of ODP and toxic impacts due to its high infrastructure and thermal energy inputs. When interpreting the hierarchy of waste management options for WBF/PSBF/MSBF, the following should be noted:-

- The data quality and representativeness of LCA inventory. The AD system
 modelled in the current study presented a site-specific case whereas the
 inventories for other waste management options were based on meta-analysis
 rather than primary data as AD.
- 2. The composition of biopolymers (*e.g.* the S, N content) could play an important role in their environmental impacts on GWP, acidification and eutrophication.
- 3. The environmental profiles of diverse waste management options depended on the parameters modelled in end-of-life scenarios such as the element flows, the operation mode of home composting and the temporal boundary of landfill.

These findings also suggested that the site-specific data combined with experimental results are needed to provide scientific evidence defining how representative and reliable information can be integrated into LCA models of waste treatments.

The current study has explored aspects of the methodology for application in LCA of crop-derived products—specifically, system boundary definition and data quality issues were investigated. Case studies on WBF suggested that the

8.2 Further Observations 353

'generic rules' of LCA system boundary definition *e.g.* a steady state of soil quality over crop cycle [3] and a 'standard' 100-year temporal boundary for the landfill model exert particular influences on the outcomes. Applying different rules, *e.g.* site specific DNDC rather than the commonly applied IPCC Tier 1 generic approach, can influence the scales of the agricultural emission results substantially. The current study presented a method to expand the system boundary by integrating the process-oriented agro-ecosystem model DNDC for field emissions into the life cycle inventory. The uncertainty analysis further confirmed that for site-specific LCAs, the process-oriented model is preferred to IPCC Tier 1 approach, as the former provides improved LCI data quality and reduces, or at least allows for better calibration of the uncertainties in the LCI inventory.

A further significant methodological issue lies in the analysis of data quality. The current study not only carried out sensitivity analyses on the life cycle inventory data *e.g.* inclusion/exclusion of infrastructure, production process variables but also examined the effects of variation in the characterisation and normalisation models. These sensitivity analyses, combined with uncertainty analyses, not only led to an increase in confidence in the current LCA findings but also suggest that LCAs lacking explicit interpretation of the degree of uncertainty and/or sensitivities should not be used as robust evidence for policy or comparative assertions.

8.3 Future Work

There are several research opportunities raised by the current study:

LCIA results presented in current study should be considered as indicative information because

- Although the coolbox underwent laboratory tests and industrial trials, other WBF case studies were modelled as concept products based only on their labderived mechanical performance.
- In comparison with the primary data used for the wheat flour inventory and the WBF properties, secondary databases and assumptions were applied to the MSBF/PSBF modelling.

Thus one potential research area would be to integrate further results to be derived from lab tests or industrial trials into the LCA model to provide more precise LCIA results of WBF construction products and other applications. Furthermore, databases should be extended to include inventory data for PVOH and starch production.

Under current study, lab research mainly focused on biodegradability of WBF/PSBF/MSBF and energy recovery potential under anaerobic digestion, but their biodegradation under aerobic condition or in landfill needs further exploration. Therefore, to fill this data gap, it would be beneficial to run lab-scale reactors to simulate home/industrial composting as well as landfill systems. Not only the biodegradation behaviour of the three biopolymers should be investigated but also

the fate of chemical elements should be traced. Process-oriented models such as GasSim [2] and LandSim [12] could be extended to simulate the specific pathways via which each chemical element is removed. In addition, further efforts would be worthwhile to generate primary inventory data for industrial composting and landfill processes to further improve the LCA model accuracy.

The system boundary issues have been addressed in current study by comparing DNDC and IPCC, but other process-oriented models are also available. It could be interesting to compare different process-oriented models (e.g. Daycent, RothPC-1) under an LCA framework to explore the effects of variations in the system boundary defined in the different models and to analyze the sensitivities of LCIA profiles to the choice of modelling approach and boundary definitions. It should also be noted that the DNDC modelling did not include indirect emissions which are included in the IPCC Tier 1 approach—it will be beneficial to have such indirect emissions modelled within the DNDC context or, at the very least, to explore the significance of this current limitation of the model.

Further exploration of the methods to quantify the robustness for LCAs is needed in order to provide unbiased information for decision-making. Specifically, it could be beneficial to investigate the influences of characterization models, timeframe on the LCA findings. The methodologies for uncertainty analysis could be further developed, which include industrial data reporting, uncertainty estimation methods, and modification in LCA software. Furthermore, it will be useful and indeed essential to fully quantify the uncertainty and confidence in LCA outcomes by developing complete inventory, in which statistical variability is available for all inventory components.

Only ALCA approach was applied in the current study. The approach of CLCA should be considered in future research to investigate the environmentally relevant flows caused by potential development and market penetration of the WBF product system. Issues such as land use and land use change, substitution effects with petrochemical polymers, influences on the waste management infrastructure would be appropriate and amenable to CLCA. Impact categories such as land use (despite methodological uncertainties) and, particularly due to increasing recent interest, water consumption would be interesting to incorporate into future LCA research on biopolymers such as the ones investigated in this study.

8.4 Conclusions

Overall, the results of this study do not support a general statement that "there is a generic environmental advantage for WBFs (starch-PVOH blended biopolymers) over petrochemical polymers". It is the use in this research of multiple case studies of different WBF applications and conducting these under the same modelling parameter backgorund with consistent datasets and assumptions for the WBFs that makes it possible to arrive at this conclusion with some confidence. As with most LCAs the findings need to be tempered by the understanding that, the comparisons

8.4 Conclusions 355

made in the case studies are affected by assumptions and methodological choices concerning specific parameters.

In providing an answer to the question posed at the inception of this study, a number of key aspects of this comparative LCA perspective can be recognized. The following attributes can be recognised from the work as critical to the comparisons undertaken and, in a sense, these represent a sequence of priority issues as a potential hierarchy for decision-making based on the LCA 'evidence' in this work:

- 1. The specific applications of the WBFs affect the comparative outcomes verses petrochemical polymers.
- 2. The End-of-life scenarios for the WBFs and petrochemical polymers are influential on the comparisons.
- 3. The presence of recycled content in the petrochemical polymers is a significant factor in comparisons with WBFs.
- 4. The specific source of starch feedstock is a significant factor for the environmental profile of the biopolymer products.

Amongst diverse end-of-life scenarios, AD and home composting offer promising waste treatment choices for starch-PVOH biopolymers. The former offers lower GHG emissions and energy recovery whereas the latter benefits from low energy/infrastructure consumption. In order to define an appropriate waste management hierarchy for WBF-like biopolymers, the following factors need considering (not in order of priority):

- The composition of biopolymer examined, especially N, S contents
- The temporal boundary of landfill scenarios
- The energy recovery efficiency in landfill
- The energy utilization efficiency in AD
- The operation mode of home composting

An expanded system boundary should be considered in the LCA study on cropbased bio-products. Relevant system boundary expansion can be achieved by integrating process-oriented agro-ecosystem models into the overall LCA model. This approach has been demonstrated in the WBF case studies in which comparison of the output from the IPCC Tier 1 emissions approach with that of the DNDC model showed that the latter not only allowed for system boundary expansion but also provided improved LCI data quality and better calibration of the uncertainties in the LCI inventory.

When conducting LCA on crop-based products, data and methodological quality analyses are necessary to encompass sensitivity analysis on the model parameters, effects of key assumptions and the characterization methods and, importantly, to encompass formal uncertainty analysis. LCAs of bio-based polymers (and other products) without interpretation of the degree of uncertainty and sensitivities of outcomes should not be used as robust evidences for policy makers.

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Appendix A Pedigree Matrix Method

In pedigree matrix, data quality is assessed according to six characteristics (U_1 – U_6). Each characteristic is divided into five quality levels with an indicator score between 1 and 5 (Table A.2) and an uncertainty factor expressed as the contribution to the square of the geometric standard deviation is attributed to each score of the six characteristics (Table A.3). In addition, for the different input and output a basic uncertainty factor is introduced into uncertainty analysis of data (Table A.1).

Table A.1 Basic uncertainty factors for inputs and outputs [38]

Input/output group	c	p	a
Demand of:			
Thermal energy, electricity, semi-finished products, working material, waste treatment services	1.05	1.05	1.05
Transport services (tkm)	2.00	2.00	2.00
Infrastructure	3.00	3.00	3.00
Resources:			
Primary energy carriers, metals, salts	1.05	1.05	1.05
Land use, occupation	1.50	1.50	1.50
Land use, transformation	2.00	2.00	2.00
Pollutants emitted to water:			
BOD, COD, DOC, TOC, inorganic compounds (NH ₄ , PO ₄ , NO ₃ , Cl ₂ , Na etc.)		1.50	
Individual hydrocarbons, PAH		3.00	
Heavy metals		5.00	1.80
Pesticides			1.50
NO ₃ , PO ₄			1.50
Pollutants emitted to soil:			
Oil, hydrocarbon total		1.50	
Heavy metals		1.50	1.50
Pesticides			1.20
Pollutants emitted to air:			
CO_2	1.05	1.05	
SO_2	1.05		
NMVOC total	1.50		
NO_X , N_2O	1.50		1.40
CH ₄ , NH ₃	1.50		1.20
Individual hydrocarbons	1.50	2.00	
PM > 10	1.50	1.50	
PM10	2.00	2.00	
PM2.5	3.00	3.00	
Polycyclic aromatic hydrocarbons (PAH)	3.00		
CO, heavy metals	5.00		
Inorganic emission, others		1.50	
Radionuclides (e.g. Radon-222)		3.00	

Notes

C combustion emissions, P process emissions, a agricultural emissions

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	matrix
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Table A.2 Feuigree maury [50]	utx [56]				
Indicator score	1	2	3	4	5
Reliability	Verified data based on measurement	Verified¹ data partly based Non-verified data partly on assumptions or non-based on qualified verified data based on estimates measurements	Non-verified data partly based on qualified estimates	Qualified estimate (e.g. by industrial expert); data derived from theoretical information (stoichiometry)	Non-qualified estimate
Completeness	Representative data from site relevant for the market considered over an adequate period to even out normal fluctuations	Representative data from >50 % of the sites relevant for the market considered over an adequate period to even out normal fluctuations	Representative data from some sites (\$\infty\$50 %) relevant for the market considered or >50 % of sites but from shorter period	Representative data from only one site relevant for the market considered or some sites but from shorter periods	Representativeness unknown or data from a small number of sites and from shorter periods
Temporal correlation	Less than 3 years of difference to reference year (2006–2008)	Less than 6 years of difference prior to reference year (2006– 2008)	Less than 10 years difference prior to reference year (2006– 2008)	Less than 15 years difference prior to reference year (2006– 2008)	Age of data unknown or more than 15 years difference prior to reference year (2006– 2008)
Geographical correlation	Data from area under study Average data from larger area in which the studied area is include	Average data from larger area in which the studied area is included	Data from smaller area than NA ³ area under study or from similar area ²	NA^3	Data from unknown or distinctly different area
Technological correlation	Data from enterprises, processes and materials under study (i.e. identical technology)	NA³	Data on related processes or materials, but same technology. Or data from processes and material under study but from different technology	Data on related processes or materials but different technology, data on laboratory scale processes and same technology	Data on related processes or materials but on laboratory scale of different technology
Sample size	>100, continuous measurement	>20	>10 aggregated figure in environmental report	>=3	Unknown

I Verified = published in public environmental reports of companies, official statistics 2 Area grouping: North America, Australia; EU, Japan, South Africa; South America, North and Central Africa and Middle East; Russia, China Far East Asia 3 NA no available

Table A.3 Uncertainty factors for pedigree matrix [38]

	1 0				
Indicator score	1	2	3	4	5
Reliability	1.00	1.05	1.10	1.20	1.50
Completeness	1.00	1.02	1.05	1.10	1.20
Temporal correlation	1.00	1.03	1.10	1.20	1.50
Geographical correlation	1.00	1.01	1.02	NA	1.10
Technological correlation	1.00	NA	1.20	1.50	2.00
Sample size	1.00	1.02	1.05	1.10	1.20

Notes

¹ NA not available

² Uncertainty factors are expresses as the contribution to the square of the geometric standard deviation

Appendix B Inventory for Crop Rotation

B.1 Crops Rotation and Nutrients Application

The crop rotations of six different crops were on six fields during the five-year period, are summarized on Tables B.1 and B.2.

To evaluate the representativeness, these site-specific data were compared with the 2007 British Fertilizer Survey [22]. According to this survey, amongst tillage crops in GB, oilseed rape and winter wheat are the most N-demanding, for both of which the majority of N fertilizer is applied in straight form, (accounting for over 90 % of N fertilizer for both crops). In the farm studied, N application rates for these two crops are consistent with generic practice, but N fertilizer composition was different from the GB generic case—for oilseed rape, only 53–54 % of N applied was in straight form.

In the survey, potatoes together with winter barley ranked as the second most N-demanding crops (vary between 131 and 166 kg N/ha during 5 years), but their N nutrient composition are different. Over 70 % of N applied on potato was in compound form while straight N accounted for over 85 % of N fertilizer applied on winter barley.

Table B.1 Crop rotation

	2003	2004	2005	2006	2007
Field 1	Sugar beet	Winter wheat	Set-aside	Soisson	Oilseed rape
Field 2	Spring barley	Spring barley	Potatoes	Soisson	Sugarbeet
Field 3	Spring barley	Spring barley	Sugar beet	Soisson	Oilseed rape
Field 4	Potatos	Winter wheat	Set-aside	Soisson	Oilseed rape
Field 5	Sugar beet	Winter barley	Potatoes	Soisson	Potatoes
Field 6	Potatoes	Winter wheat	Sugar beet	Soisson	Spring barley

Table B.2 Summary for crop rotation and fertilizer overall application rate

Crop year 2002	for crop rotation ar	iu ieitilizei overali a	application rate	
Crop year 2003	Sugar beet	Spring barley		Potato
Aron (%)	26.975	44.361		28.664
Area (%) N (t/ha)	1.268E-01	1.377E-01		28.004 1.710E-01
	3.630E-02	2.339E-02		1.710E-01 1.285E-01
P_2O_5 (t/ha)				
K_2O (t/ha)	1.683E-01 8.004E-02	4.680E-02 5.772E-03		2.690E-01 1.290E-02
MgO (t/ha)				0.000E+00
SO ₃ (t/ha) Na ₂ O (t/ha)	1.043E-02 2.595E-01	7.413E-02 0.000E+00		0.000E+00 0.000E+00
2 , ,				0.000E+00 0.000E+00
Limestone (t/ha)	5.126E-03	4.056E-03		0.000E+00
Crop year 2004	Winter wheat	Spring barley		Winter barley
Area (%)	35.734	44.361		19.905
N (t/ha)	2.150E-01	1.176E-01		2.154E-01
P_2O_5 (t/ha)	7.299E-03	2.335E-02		0.000E+00
K_2O (t/ha)	1.460E-02	4.671E-02		0.000E+00 0.000E+00
MgO (t/ha)	1.801E-03	5.761E-03		0.000E+00 0.000E+00
SO ₃ (t/ha)	4.809E-02	5.607E-02		4.455E-02
Na ₂ O (t/ha)	0.000E+00	0.000E+00		0.000E+00
Limestone (t/ha)	1.266E-03	4.048E-03		0.000E+00
Crop year 2005	1.200E-03	4.046E=03		0.000E+00
Crop year 2003	Set-aside	Potato		Sugar beet
Area (%)	23.246	49.304		27.450
N (t/ha)	0.000E+00	2.065E-01		7.874E-02
P_2O_5 (t/ha)	0.000E+00	1.967E-01		4.929E-02
K_2O (t/ha)	0.000E+00	2.972E-01		6.949E-02
MgO (t/ha)	0.000E+00	6.725E-02		6.357E-02
SO_3 (t/ha)	0.000E+00	0.000E+00		0.000E+00
Na ₂ O (t/ha)	0.000E+00	0.000E+00		1.995E-01
Limestone (t/ha)	0.000E+00	0.000E+00		0.000E+00
Crop year 2006 winte		0.0002.00		0.0002.00
Crop year 2007				
crop year 2007	Spring barley	Oilseed rape	Sugar beet	Potato
Area (%)	13.596	35.096	31.869	19.439
N (t/ha)	9.855E-02	2.237E-01	1.034E-01	2.743E-01
P_2O_5 (t/ha)	2.084E-02	3.680E-02	4.765E-02	8.979E-02
K_2O (t/ha)	3.775E-02	3.681E-02	9.461E-02	2.696E-01
MgO (t/ha)	8.562E-03	0.000E+00	5.770E-02	3.476E-02
SO ₃ (t/ha)	7.134E-02	8.933E-02	0.000E+00	0.000E+00
Na ₂ O (t/ha)	0.000E+00	0.000E+00	1.402E-01	0.000E+00
Limestone (t/ha)	2.945E-03	4.397E-02	0.000E+00	0.000E+00

A similar practice was also found in our site-specific study, except for N fertilizer composition for potato where more N fertilizer was supplied in straight form.

The same as the survey, sugarbeet and spring barley were found to be requiring less N; for spring barley around 60~% of N comes from straight N nutrients. In the

case of sugarbeet, Swaffham showed the same practice as generic GB straightform accounting for 90 % of N applied.

The farm practice for K/P nutrients at Swaffham was the same as the GB fertilizer survey. Potato was the most nutrient-demanding crop, application rates of phosphate and potash for potato are higher than the other five crops by at least three or four times, except sugarbeet which received over double the amount of potash than barley/wheat/oilseed rape.

Generally, sulphur nutrients are less commonly applied compared with NPK nutrients. According to the British fertilizer survey [22], only winter wheat, winter/spring barley and oilseed rape were sulphur-receiver, in GB, oilseed rape received the highest SO₃ dressing compared with the rest three crops. This trend is consistent with the record at Swaffham farm.

B.2 Field Operation

Table B.3 gives the data on field operation, which were checked for the representativeness by reference to the UK Farming survey [78] and the crop database used in UK-DNDC (Cardenas L, 2008, UK DNDC model, "personal communication").

As shown in Table B.4, in Swaffham farm, fungicide and herbicides were applied to all crops. Amongst six crops, potato is most fungicide-demanding, over 10 times and the majority of fungicide treatment occurred between June and Aug. Herbicide was used to control weeds, especially as a pre-drilling clean up and pre-harvest desiccant, such as sugarbeet, for which, early herbicide application was recorded in March prior to drilling. In addition, the herbicide formulation glyphosate was also applied on the fields in set-aside. In the case of insecticides, they were used less regularly than herbicide/fungicide still applied for several crops for beetle control etc. All the chemical spraying practice was agreed with the GB pesticide survey [40] thus was used as validated data for LCA study.

Crop	Planting date	Harvesting date	Tillage date	Tillage methods
Sugar beet	28th April	17th Nov	15th March	Plough (20 cm)
Spring barley	1st Mar	17th Aug	15th Feb	Plough (20 cm)
			20th Feb	Power Harrowing (20 cm)
Winter barley	15th Dec	17th Aug	20th Nov	Plough (20 cm)
			10th Dec	Power Harrowing(20 cm)
Potato	5th April	3rd Oct	20th Mar	Ploughing (30 cm)
Oilseed rape	30th Aug	17th Aug	20th Aug	Plough (20 cm)
			25th Aug	Power harrowing (20 cm)
Winter wheat	30th Sep	17th Aug	15th Sep	Plough (20 cm)

Table B.3 Field operation-cultivation and harvesting

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	Sugar beet	Spring barley	ugar beet Spring barley Winter barley Potato Oilseed rape	Potato	Oilseed rape	Wheat	Set-aside
Number of spray around applied on the crop	und applied on	the crop					
Spraying fungicide	0-1	2–3	33	12–16	3	3	0
Spraying herbicide	9	2–3	2	2–3	4	3-4	1
Spraying insecticide	1	0-1	0	2		1	0
Growth regulator	0	0	1	0	0	2	0
Adjuvant	3.4	0	1	0-2	0	1–2	0
Application time during one crop season	ing one crop se	ason					
Spraying fungicide	July	May-June	April-May	May-Aug	May-Aug Oct and April	April-June	ı
Spraying herbicide	March-June May	May	April and Aug	May	Pre-drilling and pre-harvest Oct/Nov and April Autumn or April	Oct/Nov and April	Autumn or April
Spraying insecticide	March	June	I	June	May	Nov	ı
Growth regulator	1	1	March	ı	I	March-May	ı
Adjuvant	April-June	ı	March	May-June	ı	March-April	I

Table B.5 Crop yields

	Moisture content (%)	Yield on wet basis (kg/ha)	Yield on dry matter basis (kg/ha)	Straw/crop residue (kg/ha)	Incorporation of crop residue (%)
Crop year 2003	3/2004/2005/200)7			
Spring barley	14.5	5,400	4,617	NA	100
Winter wheat	14.5	8,600	7,353	4,000	100
Winter barley	14.5	5,400	4,617	NA	100
Potato	80	58,000	11,600	NA	100
Sugar beet	90	60,000	6,000	NA	100
Oilseed rape	9	4,200	3,822	NA	100
Crop year 2006	5-Soisson winter	r wheat			
Field 1	14.5	8,800	7,524	4,000	100
Field 2	14.5	8,600	7,353	4,000	100
Field 3	14.5	8,800	7,524	4,000	100
Field 4	14.5	8,500	7267.5	4,000	100
Field 5	14.5	8,300	7096.5	4,000	100
Field 6	14.5	8,600	7,353	4,000	100

Notes

NA not available

B.3 Crop Yield and Other Parameters

Average yield for each crop provided by the farm was representative of crops grown in crop years 2003/2004/2005/2007, while for crop year 2006 field-specific data for Soisson were used in the calculation. As indicated in Table B.5, crop yield on wet basis was converted to dry matter basis primarily based on moisture content recorded in Swaffham farm and in the UK National Statistics (2009, 2008, 2007). In statistical data, moisture contents of UK cereal crops (wheat/barley) and oilseed rape were adjusted in 2008, however, considering the crop years studied are 2003–2007, the standardized value before 2008 was preferred (14.5 and 9 % for cereal and oilseed rape, respectively). Moisture content for potato and sugar beet was derived from a previous study carried out by Williams et al. [103].

In addition, Table B.5 gives the yield of crop residues and the proportion of residues incorporated into the field. This information was used to calculate the changes in residual soil fertility in crop rotation due to incorporation of previous crop residues. As for other crop parameters including the proportion of crop grain/leaves/stem/root, C content and C/N ratio in crop, the UK DNDC crop database was used (Cardenas L, 2008, UK DNDC model, "personal communication").

Appendix C Inventory for Composting Model

Composting waste treatment was simulated, where multiple-input inventory approaches were introduced [79]. In addition to UK site-specific composting parameters derived from the WRATE model [35], lab-determined initial waste compositions were correlated with emission factors of chemical elements developed by literature data-mining to estimate the theoretical potential fate of each chemical element. The methodologies and calculation procedures are given below.

C.1 Composting Model of BFMSW

As shown in Table C.1, data recalculated based on the WRATE model were used to represent the operations of UK composting sites [35]. In the home composting scenarios, the compost bin was the only input, additional water was assumed to be insignificant. In comparison with home composting, industrial composting, either in-vessel or windrow, brought extra energy consumption but produced less compost output which was caused by the rejection of non-organic fractions assumed to be present in the feedstock. Comparing the two industrial composting representations, higher water and electrical energy consumption but lower diesel inputs were found for the in-vessel than windrow composting process, confirming previous studies [14]. However, the total energy data recorded in the WRATE model was lower than the energy requirements reported in previous studies, where energy consumption fell into the range of 35–95 kWh electricity and 2–3.6 L diesel/tBFMSW for in-vessel composting and 21–65 kWh electricity and approx 9 L diesel/tBFMSW for windrow composting [44, 75, 14]. This difference could be attributable to the different efficiency as well as the technology modelled.

Based on the dataset described above, composting models were established where 100 % of the waste stream was assumed as WBF/PSBF/MSBF or

	Home composting	In-vessel	Windrow
Input			
Organic waste	Green/kitchen/paper	Green/kitchen	Green
Annual capacity(kg)	1.000E+03	1.430E+07	1.974E+07
Electricity (MJ/kg waste)	0.000E+00	6.168E-03	1.831E-03
Diesel (kg/kg waste)	0.000E+00	8.083E-04	3.074E-03
Additional Water ^a (L/kg)	0.000E+00	2.098E-04	0.000E+00
Facility ^c	HDPE bin	Composting plant	Plant
Output			
Compost (kg/kg waste)	7.460E-01	5.101E-01	5.712E-01
Rejected waste ^b (kg/kg waste)	0.000E+00	5.000E-03	7.577E-04
Liquid-to sewage treatment	0.000E+00	0.000E+00	8.307E-03

Table C.1 Home composting and industrial composting

Notes

cardboard. Therefore, the same amount of energy and infrastructures inputs as for BFMSW were assumed to be required for composting of foam or cardboard waste but with specific modelling of the waste-specific outputs. The rejected wastes are not considered to be by-products of composting foam/cardboard waste, thus, they were excluded form the inventory.

C.2 Decomposition and Mineralization Estimation

A biodegradability test based on mass loss was carried out in-house [76]. The material was incubated at 25 °C for over 20 days in a lab-scale aerobic composting system, which gave an indication of biodegradability of test material under a home composting system. Based on the composition analysis as well as the degradation of carbohydrate fraction derived from literatures, the biodegradability of studied material under composting was predicted.

According to in-house lab data [76], WBF was biodegraded rapidly, reaching approx 85–90 % mass loss in simulated aerobic home composting within 20 days; after which, no further degradation occurred. This may be explained by the limited biodegradation of PVOH-component in WBF under aerobic condition: the biodegradability of PVOH in composting found in literature fell into a range of 7–12 % over 30 days or more [15, 55]. As for the starch component, a 100 % of mineralization of starch (released as CO₂) was observed under controlled composting condition (58 °C, aeration) after 45 days [26]. In comparison with WBF, a similar biodegradability was observed in the decomposition profiles of MSBF, but a slower degradation was found at initial stage (first 15 days) [76], which could be attributable to the different C/N ratio present in WBF and MSBF. The starch and protein component of WBF had an initial C/N ratio of 34.2 which

^a Excluding the rainfall and self-contained water in organic waste

^b Rejected waste to be landfilled

^c Construction materials derived from WRATE model [35] are not presented here

fell into the standard-recommended C/N range (10–40) [66] and moreover was close to the optimum C/N ratio (30) for composting found by Hamoda et al. [46]; thus WBF provided and ideal balance to favour microbial activity and accelerate the composting process.

In accordance with the in-house test, during 20 day period cardboard appeared less biodegradable than WBF/MSBF, but still showed nearly 60 % mass loss over 21 days under a controlled composting system [76] which was comparable to the results reported in other studies: 51.7 % of cardboard degradation in composting (58 °C) for 45 days [66]. This difference could be mainly caused by the different organic fractions of the studied materials: theoretical biodegradable fractions of cardboard determined in current study and reported by Lopez Alvarez et al. [66] were 84 % of TS and 63 % of TS respectively.

Three components of cardboard were involved: lignin, a aromatic polymer synthesized from phenylpropanoid precursors, and other two macromolecules constructed from sugars i.e. cellulose, hemicellulose [90]. Amongst them, lignin was found as resistant to biodegradation and its decomposition showed a lag phase in composting [37]. It is acknowledged that the most effective lignin-degrading microorganisms in nature are white rot fungi which cannot survive under thermophilic conditions; while other bacteria genera can solubilize and modify lignin structure but the ability to mineralize it are limited [100]. According to Tuomela et al. [97], the most frequently occurring lignin-degraders in composting are thermophilic fungi, for which optimum growth condition is 40-50 °C. This confirmed the results observed in previous studies, under temperature of 35–50 °C more lignin was decomposed, mineralization reached 23-24 % within 45-48 days [98] but more lignin was bound to humic substances than oxidized to CO₂ [98, 100]. According to a review [97], irrespective of lignin-source, generally less than 30 % of lignin degradation occurs within a period of less than 50 days at 25-50 °C. However, with a sufficient duration of composting at optimum temperature, a higher degradation levels can be achieved: 50 % lignin decomposition was reported for a paper mixture within 590 days composting at ambient temperature 17-23 °C [32]; even a higher lignin biodegradation (70 %) within a 35 day incubation period at 50 °C has been reported [97].

Besides, lignin is associated with cellulose/hemicellulose to form a cross-linked three-dimensional structure which can inhibit microbial access to biodegradable fractions [68]. However, the cellulose present in cardboard/paper is less resistant than cellulose of wood due to changes induced in the paper manufacturing [32]. As for hemicellulose, although the types of enzymes involved in its degradation are similar to cellulose, more enzymes are required for its complete degradation due to its greater complexity in comparison with the linear polymer cellulose [68, 90]. Therefore cellulose can be expected to show higher decomposition rate, followed by hemicellulose. This is verified in previous publications: composted at 17–23 °C cellulose and hemicellulose were reported to show a similar decomposition rate but, over longer digestion period (590 days), the former was decomposed to a greater extent [32]. This conclusion was confirmed by research carried out by Francou et al. [37]; they found within an 84 day incubation at 28 ± 1 °C

averagely 55–85 % of cellulose and around 40–65 % of the hemicellulose fraction was degraded with lignin recalcitrant to degradation, only reaching 13–25 % degradation. Similar biodegradation of cellulose was also reported by other authors [83]. But a high degradation rate of carbohydrate is achievable when not associated with lignin. Over 95 % of pure cellulose was decomposed and mineralized to $\rm CO_2$ during a 45 day composting period at thermophilic temperature (58 °C) was observed by Degli-Innocenti et al. [26]. It indicated that pre-treatment such as ball milling could enhance degradation of cellulose/hemicellulose.

Actually majority of the studies discussed above especially those concerning starch, PVOH, cellulose and hemi-cellulose were conducted according to standard testing method [52], i.e. the biodegradation was determined by the ratio of the CO₂ evolved from the test material to the maximum theoretical CO₂ estimated based on total organic C content. This approach does not take into account the C converted to new cell biomass, which is not mineralized to CO₂ during the test [52]. Thus most of the biodegradability results reported primarily represented the mineralization of test material; whereas via literature review, it was found that the most of the studies on lignin degradation used biochemical composition analysis methodology but C gaseous release was rarely concerned [97]: such as studies carried out by Eklind and Kirchmann [32] and Francou et al. [37]. Only limited studies analyzed both decomposing material and evolution of CO₂ [98, 37].

Based on the data derived from literature, the assumptions on biodegradation of each component are given in Table C.2 where decomposition and mineralization rate indicate the estimated potential mass loss of components and the potential C gas evolution respectively. A more effective degradation of foams/cardboard could be expected in industrial composting where longer thermophilic stage and more optimum C: N ratio than home composting could be achieved. Thus the results derived from tests carried out at optimum conditions were selected to represent the centralized composting scenarios whereas those obtained from studies carried out at a mesophilic ambient temperature was assumed as representative of home composting scenario. As shown in Table C.2 the main component of foam, i.e. starch, was assumed to reach 100 % mineralization according to Degli-Innocenti et al. [26]; for another fraction PVOH, a biodegradation range of 7–12 % derived from literature was preferred [15, 55], where the max and min value was assumed as the case of industrial and home composting respectively.

As for cardboard, cellulose and hemicellulose fractions were assumed as highly decomposed and mineralized [37]. The decomposition of lignin was assumed as 50 and 70 % respectively in home and industrial composting scenarios [32, 98], but in both scenarios, only 23–50 % of lignin was assumed to be released as CO₂, which meant the rest decomposed lignin was bound to humic substances [98]. Therefore, the estimated biodegradation of WBF/MSBF/PSBF ranged between 86 and 90 %; whereas, 60–70 % of cardboard were assumed to be mineralized, most of the remaining fractions were bound to humus, where the lignin was the primary precursor [98].

	Home-compostin	Home-composting		sting
	Decomposition (%)	Mineralization (%)	Decomposition (%)	Mineralization (%)
Components (a	lry weight basis)			
Starch	100.000 ^a	100.000 ^a	100.000 ^a	100.000^{a}
Wheat protein	100.000	100.000	100.000	100.000
PVOH/dry	7.000	7.000^{b}	12.000	12.000 ^b
Soya flour	100.000	100.000	100.000	100.000
Cellulose	70.000^{c}	70.000	95.000 ^a	95.000^{a}
Hemicellulose	60.000^{c}	60.000	95.000	95.000
Lignin	50.000^{d}	23.000 ^e	$70.000^{\rm e}$	50.000 ^e
Products (dry	weight basis)			
WBF	86.418	86.418	87.152	87.152
PSBF	86.758	86.758	87.483	87.483
MSBF	90.269	90.269	90.802	90.802
Cardboard	63.909	60.398	89.573	69.051

Table C.2 Biodegradability assumed in composting scenarios

Notes

C.3 Element Flow and Trace Gas Emissions

Composting can be sources of atmospheric CH₄ [95] and N can be lost as NH₃ or N₂O during this process [93]. Researches were carried out on C/N dynamics under different composting methods with various operation parameters. It was found that even with optimal operation the anaerobic zone development and subsequent CH₄/ N₂O production was unavoidable in systems like windrow composting (dominant composting system in UK) due to the compaction and reduction in aeration in composting piles [49]. To estimate the gases released from test material (foams or cardboard) under composting system studied, a multi-input inventory approach described by Obersteiner et al. [79] was applied, which takes into account the laboratory-determined elements embodied in the waste and release factors for each element developed from literature-based data. Only data from experimental tests carried out under conditions similar to those defined in composting scenarios were applied. This approach directly associates the waste composition with resulting emissions, gives estimation of element flow in a waste-specific manner; under this methodology specific composting condition and process are considered but for those emissions highly process-dependent it is difficult to predict. The methodologies and calculation procedures are given below.

^a [26]

^b [15, 55]

c [37]

^d [32]

e [97, 98]

Limited data have been reported on trace gas emissions from composting of BFMSW [53]. As summarized in Table C.3, mainly the data concerning organic household waste were included, except two studies [81, 93] which explored animal waste; however their C/N ratio was close with other studies thus they gave good indication of C/N dynamics of organic household waste. According to composting volume, studies were divided into full scale (over 2,000 L), pilot scale (100–2,000 L) and lab scale (less than 100 L) [72]. As represented in the table, the data derived from different studies varied widely. For example, much lower total gaseous N attributable to the low temperature profile and high C loss during composting of green waste was reported by Hellebrand [47]; N₂O-N emission Figure reported by Szanto et al. [93] is greater than other studies due to anaerobic regions occurring in static pile. Despite the varying process conditions and the lack of complete information, same trend emerges in most of studies: sum total of NH₃ and N₂O ranged between 10 and 62 % of the initial N, except pure green or paper waste; cumulative N gaseous losses presented in most studies mainly consist of NH₃, and majority of the initial C mass is transformed into CO₂ in composting of house-hold waste.

As shown in Table C.3, N₂O and NH₃ were considered to represent total N gaseous losses during composting in most studies reviewed, but actually besides these dominant gases NO and N₂ could be also generated via denitrification or aerobic/anaerobic ammonia oxidation [62], which were only concerned in few studies. Szanto et al. [93] traced the fate of N(NH₄⁺, NO₂⁻, NO₃⁻, N₂O, NH₃), found that under active composting system, there was a ineligible N loss present as unknown form, which was supposed as N₂. Fukumoto and Inubushi [39] also reported similar results: difference between total N gaseous loss and sum of NH₃ N₂O was significant; but differently, NO was considered as the most likely other N gas (except N₂O) induced by NO₂⁻ accumulation. However, both studies focused on manure, no publications on household waste concerning NO was available; due to the data gap, only NH₃ and N₂O were taken into account in LCA model, while other N gas emissions were studied in sensitivity analysis.

In addition to N gaseous, N losses also include leachate which was discussed in previous studies. Barrington et al. [8] reviewed studies on total N losses (including leachate) from composting of manure found that total N loss ranged between 16 and 72 %, which was agreed with their own investigation. Amongst these total N losses, generally only small proportion was observed as leachate while gaseous loss dominated. As reported by Martins and Dewes [71], only 9.6–19.6 % of initial N was lost as leachate where NH₄⁺–N accounted for 77–98 %; if under the optimal moisture content, the leachate N loss could reach as low as 1 % of total N loss [8]. The same as N leachate, Barrington et al. [8] concluded a negligible proportion of C was lost via seepage(less than 1 % of C loss). Therefore, in LCA model, an optimal condition minimizing leachate was assumed, only C/N gaseous losses were taken into account.

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Studies	Scale and condition	Compost material	Period	C loss (% of initial total C)	otal C)	N loss (% of initial total N)	(N)
				CO ₂ -C	CH₄−C	N ₂ O-N	NH ₃ -N
[59]	Full scale	Organic household wastes 168 days	168 days	NA	NA	Total gaseous N loss is 51.6 %	51.6 %
	Full scale	Household and green waste 168 days	168 days	NA	NA	Total gaseous N loss is 26.2 %	26.2 %
[6]	Pilot scale (constant $16 \% O_2$)	Household waste and wheat 31 days straw (C:N = 22)	31 days	65 %	Nearly 0 %	0.4 %	33 %
	Pilot scale (constant $16\% 0_2$)	Household waste and wheat 22 days straw (C:N = 22)	22 days	% 19	Nearly 1 %	% 9.0	23 %
[47]	Full scale (aeration channel)	Green waste	During composting	81 %	1.7 %	0.5 %	1.2 %
[81]	Pilot scale (forced aeration 25 °C)	Animal waste + wheat straw (C:N = $17-29$)	56 days	36.4-44.8 % 0-0.06 %	0-0.06 %	0.71–1.2 %	16.5–48.9 %
[93] ^a	Pilot scale (static pile ambient temperature)	Animal waste + straw (C:N = 13)	118 days	NA	$25.2 \pm 1.2 \% 9.8 \pm 0.1 \%$	9.8 ± 0.1 %	$2.4 \pm 0.1 \%$
	Pilot scale (turned pile ambient temperature)	Animal waste + straw (C:N = 7)		NA	% 8.0	2.5 ± 0.4 %	$4.0 \pm 0.4 \%$
							(continued)

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Studies	Scale and condition	Compost material	Period	C loss (% of initial total C)	al total C)	N loss (% of initial total N)	al total N)
				CO ₂ -C	CH ₄ –C	N ₂ O-N	NH ₃ -N
[61]	Lab scale 52 ± 2 °C	Food waste (C:N = 8.4)	58 days	76.5 %	NA	NA	61 %
	inoculated forced	Green waste (C: $N = 18$)	77 days	58.2 %	NA	NA	22 %
	aeration	Paper waste (C: $N = 120$)	198 days	35.7 %	NA	NA	11 %
		Mixed waste (C:N = 47)	170 days	63.8 %	NA	NA	3 %
[33]	Pilot scale (natural ventilation 17–23 °C)	Organic household waste + paper	590 days	NA	NA	62 % N loss	
[49]	Full scale in-vessel (20 °C)	Kitchen and green waste	7 days	% 8		24.6 %	
[34]	Pilot scale (forced aeration, 40/55/67 °C)	Organic household waste (C:N = 22)	24 days	55.5–65.1 % NA	% NA	NA	3.4–31.6 %
[50]°	Default value			NA	1.5–3 %	1.91 %	NA
	Range			NA	0.01–6 %	0.64-5.09 %	NA

 a Szanto et al. [93] assumed that 50 % of VS is C b NA not available c Composition of biowaste assumed: 2 %N of dry matter and 25–50 % organic C of dry matter

C.3.1 N Gas Emissions Factors

Despite the varying process conditions and emission data recorded in literatures, by analysing the key parameters influencing N dynamics during composting, appropriate release factor ranges for N gas were identified to represent the different composting scenarios.

C.3.1.1 Key Parameters Affecting N flow

In this section mainly NH₃ and N₂O are discussed. Both of them are products of N turnover, mainly concerning four pathways: ammonia oxidation, nitrification, denitrification, volatilization [62], but depending on various factors.

As reported by Paillat et al. [81] and Szanto et al. [93] NH₃ was mainly influenced by temperature, C/N ratio, initial micro-flora, pH, N and C biodegradability and highly related to three ammonium consumptive fluxes, i.e. nitrification, immobilization and volatilization. Specifically speaking, due to the sensitivity of nitrifying bacteria to high temperature and the dependence of nitrification on O_2 , [48] low O_2 concentration as well as high temperatures reduce nitrification, which increases NH_4^+ accumulation further enhancing volatilization of NH_3 ; higher biodegradable C can remove NH_4^+ by immobilization and reducing NH_3 emission. The pH, conditioned by production of NH_4^+ , VFA and emission of NH_3 and CO_2 [82], also shifts the NH_4^+ : NH_3 equilibrium (an alkaline pH enhances volatilization of NH_3).

 N_2O is an intermediate product during nitrification and denitrification processes [81]. According to previous research [48], high temperatures lead to lower nitrification processes, reducing N_2O emission. This could explain why N_2O is mainly emitted during the mesophilic phase [81] although NH_4^+ can be oxidized under thermophilic condition by methanotrophs [53, 93]. In addition, it was reported that O_2 plays a key role in N_2O emission, the absence of O_2 results in anaerobic zones developing a main cause of higher production of N_2O [93]. Another factor affecting N_2O emission is available C, Szanto et al. [93] showed N_2O emission increased with the depletion of readily biodegradable C.

In summary, all these parameters were classified into two categories: (1) properties of waste, and (2) operation and management of composting. They were considered as the criteria for literature screening.

C.3.1.2 N Emission Factors

Literature review led to two general conclusions: theoretically up to 85 % of initial N is available for volatilization [8] no N gas release above this range was reported; food waste or mixed household waste showed greater N emissions than green waste or paper waste (see Table C.3).

To develop N emission factors, studies on source-separated waste were preferred in review, where the material properties as well as the composting operations were the main considerations. In addition, to avoid overestimation of N gaseous loss, the results obtained from total N analysis which included both gas and leachate loss were rejected e.g. [8]. Specifically, composting with turning operation or forced aeration were considered to represent active home composting, but data derived from tests operated at less turning frequency were used in the passive composting scenario. In the case of WBF, results derived from composting of starch (food) like waste materials at optimal C/N ratios (approx 30) were preferred; whereas literature on ligno-cellulose material was used to indicate N fate during composing of cardboard.

Generally, a consistent proportion of N gases were recorded in most studies: over 95 % of N emissions were released in the form of NH_3 –N, the remaining less than 5 % of N gas was N_2O –N [8, 9, 71, 81]. This ratio was assumed to represent the split of NH_3 and N_2O in industrial composting scenarios. As observed by Amlinger et al. [1] similar total N gaseous losses but a greater proportion of N_2O emissions can be expected during home composting than in industrial composting. In current home composting scenarios, the same total N gaseous loss as industrial composting but less turning frequency was assumed. Thus an upper range of N_2O (5.09 % of initial N) suggested by IPCC [50]was applied in the active home scenario; while for the passive home composting scenario, a N_2O factor derived from a static composting test was used (approx 10 % of initial N) [93]. Although this study mainly explored animal waste, it still gave good indication of N_2O emission as its C/N ratio as well as emission factors under active composting was consistent with those for household waste (see Table C.3).

As presented in Table C.4 the N_2O emission estimated for WBF in active composting systems was within the IPCC range (0.2–1.6 g N_2O/kg dry waste) [50]; however, in the case of cardboard it was lower than IPCC range which could be explained by the different N content between cardboard (0.2 % in dry matter) and bio-waste assumed in IPCC Guidelines (2 % N in dry matter).

As for other potential N gaseous losses, as discussed before, only few publications are available [93, 39] but no precisely measured results are indicated. As Fukumoto and Inubushi [39] showd, the difference between the total N loss and the sum of NH₃, N₂O ranged between 13.3 and 27.8 % of initial N, depending on NO_2^- accumulation; the latter (27.8 %) which was derived from tests without addition of mature compost was considered as more representative and was applied in LCA sensitivity analysis in the present study, where both N₂ and NO gases were taken into account as potential emissions.

C.3.2 C Gas Emission Factors

Besides N emissions, the same multiple-inventory approach was applied to estimation of gaseous C releases. In this section, the associated parameters were

Per kg received waste		WBF	PSBF	MSBF	Cardboard
Active home composting	CO ₂ (kg)	1.317E+00	1.283E+00	1.342E+00	9.396E-01
	CH ₄ (kg)	1.228E-02	1.196E-02	1.251E-02	8.761E-03
	$N_2O(kg)$	1.024E - 03			1.711E-04
	NH_3 (kg)	9.190E-03			4.694E-04
Passive home composting	$CO_2(kg)$	1.013E+00	9.870E-01	1.032E+00	7.228E-01
	CH ₄ (kg)	1.228E-01	1.196E-01	1.251E-01	8.761E-02
	$N_2O(kg)$	2.012E-03			3.362E-04
	NH_3 (kg)	8.426E-03			3.418E-04
Industrial composting	$CO_2(kg)$	1.330E+00	1.296E+00	1.351E+00	1.367E+00
	CH ₄ (kg)	1.240E - 02	1.209E-02	1.260E-02	1.274E-02
	$N_2O(kg)$	6.458E-04			3.893E-05
	NH_3 (kg)	9.482E-03			5.716E-04

Table C.4 Assumption of N/C gaseous emission factors

analyzed and the representative C emission factors were developed by data screening.

C.3.2.1 Key Parameters

The dynamics of CH₄ emission have been recorded as similar to those of NH₃ [81], both being primarily emitted during the thermophilic phase [95]. As observed by Smith et al. (2006) and Szanto et al. [93], in compost (especially in static compost), there were gradients in CH₄ concentration with depth. Actually, this phenomenon indicated that net CH₄ emission from a compost pile depends on the balance between production and oxidation of CH₄. The production of CH₄ is the result of complete mineralization of organic matter under anaerobic condition through methanogenic fermentation [94]; CH₄ was found to be mainly oxidized by methanotrophs [64]. It is believed that microbial oxidation of CH₄ only happened in the presence of O₂ or SO₄⁺, so O₂ availability was assumed as the major factor limiting activity of methanotrophs. However, according to Raghoebarsing et al. [85], anaerobic oxidation of CH₄ coupled with denitrification of NO₃⁻ is possible where CH₄ and NO₃⁻ are the electon-donor and acceptor pair.

Therefore, multiple factors influence CH₄ production and oxidation including pH, organic matter and temperature. A review [64] presented relationships between these factors and CH₄ production/oxidation: a positive correlation was shown between methanogenesis and organic matter content; the optimal pH for methanogens is around neutrality or slightly alkaline; in contrast, methanotrophs are more tolerant to pH variations but sensitive to acidification. Similar result was also observed in previous studies [95]: increase in CH₄ release was accompanied by increase in pH. CH₄ oxidation was reported to be negatively correlated with water content, which indicates higher moisture may lead to higher CH₄ emission from compost [67]. As indicated above, higher temperatures may also enhance CH₄ release to a certain extent. This can be explained by the optimum temperature

for methanogens (30–40 °C) [64]. However, methanotrophs was found active under a wider range of temperature [64]; thus, under either mesophilic or thermophilic conditions, CH₄ oxidation potential is high enough to assume an effective reduction in the potential for CH₄ emissions from compost. This was confirmed by various researchers (although compost is still assumed to be an important source of CH₄ [53]) and over 90 % of CH₄ produced is usually assumed to be oxidized to CO₂ in the compost before it reaches the atmosphere [45, 53, 95].

Besides the CO_2 generated from oxidation of CH_4 , it is also produced directly by complete mineralization of organic C under aerobic conditions. CO_2 production is related to temperature, its peak emission was observed at the change between mesophilic and thermophilic phases [9, 34]; in addition, CO_2 emissions was considered as highly influenced by the initial microbial flora, C availability [81] and O_2 concentration [92].

C.3.2.2 C Emission Factors

Based on all the parameters analyzed above, the composting operations and degradable C constituents were the main criteria for determination of C emission factors. Therefore, composting systems designed to simulate aerobically operation and mismanagement were selected to represent active and passive home composting respectively. Previous studies on starch-like feedstocks gave good indications of the C emission factors for foam waste; whereas publications on ligno-cellulose materials were assumed to represent C fate in cardboard composting. In addition, those studies presenting total C loss only by mass loss of the substrate were rejected as although these results do include the C gas release but not the breakdown of C present in the surrounding matrix (e.g. microbial cellular constitute). This matrix effect may be significant: 30–40 % of C input was estimated to be incorporated by microbes as cellular component [8].

Following these criteria, the mineralization rates (Table C.2) were used to calculate total C emission factors. As shown in Table C.3, the major proportion of C gas emission was CO₂ with only trace amounts as CH₄. As reported by Amlinger et al. [1] who compared different waste and composting systems, decomposition of household waste led to higher CH₄ generation than green waste and greater CH₄ could be detected from home composters than windrow composting piles. However, as indicated in previous studies and IPCC guidelines, the CH₄ generated is assumed to be oxidized to a large extent in composting [45, 50, 95]. Via literature review, the CH₄ emission factor concluded by Amlinger et al. [1] (no greater than 2.5 % of total C emitted) was selected as an appropriate estimation for the active composting scenarios as it was representative of aerated composting systems [47, 81] and consistent with the range recommended by IPCC [50]. For the passive home composting model where a low CH₄ oxidation rate can be expected due to low O₂ levels, the higher CH₄ emission factor derived from a study carried out on static composting was preferred [93].

Per kg received waste		WBF	PSBF	MSBF	Cardboard
Active home composting	C(kg)	6.947E-02	6.817E-02	5.036E-02	1.763E-01
	N(kg)	4.581E-03			1.644E-03
	S(kg)	8.740E - 04			8.974E-04
Passive home composting	C(kg)	6.947E - 02	6.817E-02	5.036E-02	1.763E-01
	N(kg)	4.581E-03			1.644E-03
	S(kg)	8.740E - 04			8.974E-04
Industrial composting	C(kg)	6.574E - 02	6.451E-02	4.766E - 02	5.682E-02
	N(kg)	4.581E-03			1.644E-03
	S(kg)	8.740E-04			8.974E-04

Table C.5 Chemical properties of mature compost assumed

The calculated C emission factors are given in Table C.4. The CH_4 loss fell the range of 9.1–13.4 g/kg dry waste for active composting scenarios, which are consistent with the emission range suggested in IPCC Tier 1 approach (0.08–20 g CH_4 /kg dry waste) [50].

C.3.3 Mature Compost

Besides gasified C/N, the remained fractions were assumed to be contained in mature compost and applied as fertilizer and soil improver, including undecomposed organic C components (lignin cellulose/hemicellulose), and other elements (e.g. NO₃⁻-N, NH₄⁺-N, S). As indicated in Table C.5, the C:N ratios calculated on WBF-derived compost varied between 14.4 and 15.2 which was consistent with the results reported by Dimambro et al. [29]. The C:N ratio assumed for cardboard-derived compost in home-composting scenarios appeared above the C:N range found in previous literatures (10–40) [29, 99, 13, 18, 36].

Appendix D Landfill Model

In addition to biological waste treatments, landfill was modelled as a conventional disposal route where methods like multi-input inventory approaches [79] were applied. In addition to the landfill site-specific parameters, initial waste compositions were associated with release factors to estimate the potential fate of chemical elements contained in foams and cardboard in a landfill situation.

D.1 Infrastructure and System Modelled

Selective previous landfill models established on the empirically based inventory are presented in Table D.1 where the parameters applied in the current study are given. Typically, a 100 year time horizon was modelled, which included operation and the post-closure monitoring period. In all the previous studies, it was assumed that throughout the first 30 years leachate was collected and treated, as it is an obligatory operation [79]; whereas gas collection was assumed to run during the monitoring period. But the system efficiency modelled varied, generally a 80-90 and 90-100 % efficiency were assumed for landfill gas and leachate collection respectively except in one study where a much lower gas capture efficiency (45 %) was modelled [73, 79, 69]. The high gas collection efficiency agrees with UK survey-based data [43]. Landfill gas for a well-managed landfill site—was determined as triangle PDF of between 90 and 97.5 % with a mean of 95 %. Regarding the combustion of collected gas, IPCC guidelines indicated the energy recovery rate can vary widely depending on the operation system [50]. For a covered well-managed landfill site, a high energy recovery efficiency (over 85 %) and a split between recovered thermal to electrical energy (3:2–3:1) are connon in previous research [69, 79, 77]. As for leachate treatment, it was found that both TOC (total organic C) and NH₄⁺ removal efficiency depended on technology and

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	Study 1 [73]	Study2 [79]	Study 3 [69]	Current model
Waste stream	MSW	MSW	Household waste	Foam/cardboard
Temporal boundary	102 years	100 years	100 years	100 years
Bulkdensity (kg/m ³)	800	1,000	1,000	1,000
Liner	Clay liner HDPE, PP Year 0–32 efficiency 99.99 %	30 years 100 % efficiency	Clay liner	Clay liner 30 years 100 %
Cover layer	Sand organic soil geomembrane	CH ₄ oxidation layer	Clay and soil cover	Clay cover
Landfillgas collection	30 year collection	25 year collection	38 year collection	100 years collection
Landfill gas treatment	Flare		CHP and energy recovery	Combustion energy
				recovery
Lechate collection	Year 2-32 leachate	Year 0–30,100 % of	Year 0-20 95 % leachate	Year 0-30 100 %
	collection	leachate collection	collected	collection ^a
		efficiency	Year 21–40 70 % of leachate collected	
	Year 31–102 none	Year 31-100 none	Year 41–100 none	Year 31–100 none
Leachate treatment	Treatment in aeration pond	Biological treatment then discharge	Leachate treatment plant with removal 98 % of N leachate	Treatment with 99.5 % of NH ₄ ⁺ removal and 80 % of TOC removal ^{a,b}

Notes

a Uncollected lechate discharge to ground water; leachate treated prior to discharge to surface water [69]

b [87, 35]

operation conditions, but generally 85–99 and 60–80 % was achievable for $\mathrm{NH_4}^+$ and TOC respectively [87]. Therefore in the r landfill scenarios, a highly efficient gas and leachate collection system (90 and 100 % efficiency respectively) were modelled, where assumptions of energy recovery and leachate treatment were mainly obtained from results presented by Manfredi and Christensen [69] and Renou et al. [87] as well as the WRATE model [35].

In addition, technical barriers are also modelled. Clay bottom liner and cover layer were generally accepted as representative and applied in models, such as the UK-based model Gassim [43], Landsim [91], and WRATE [35]. Liner efficiency normally was assumed as nearly 100 % up to the end of post-closure monitoring period [73, 79]. This assumption was agreed by field data from operating landfills, where the average efficiency for liners is 99 % [7]. Therefore, in the current LCA model, and engineered clay bottom liner and a clay cap together with daily soil cover were modelled; 100 % efficiency for bottom liner was assumed for the first 30 year, after which, deterioration of the barrier was taken into account.

A top biological CH₄ oxidation layer was simulated, which reduces the fugitive CH₄ emission. The oxidation efficiency of 90 % or above has been assumed in previous studies [79, 69], but a much lower oxidation factor for covered well-managed landfill (0.1) was recommended by IPCC [50] and Gassim model [43]. As pointed out in the IPCC approach, in real landfill sites a proportion of CH₄ escapes though cracks/fissures as well as besides the fractions diffusing through the a homogeneous daily cover soil, thus the lab-determined oxidation factors for uniform and homogeneous soil cannot be applied directly [43]. Therefore, in the present model for the landfill model, a CH₄ oxidation efficiency factor of 0.1 was applied which took into account both CH₄ diffusion through the cap and escape via cracks/fissures.

D.2 Biodegradability Estimation

D.2.1 WBF/PSBF/MSBF Biodegradability

To estimate the biodegradation levels in foams, the biodegradability of their main components (starch, PVOH) were analyzed individually as given in Table D.2, where decomposition and mineralization was defined as estimated potential mass loss and the potential gas evolution respectively. The former took into account the degraded fraction present in the matrix such as aqueous intermediates or microbial biomass, whereas the latter was based on literature-data derived from lab-scale gas emission tests.

As a highly biodegradable component, starch was reported to be completely mineralized and 100 % of the theoretical CO₂ was evolved within 45 days as found under controlled composting tests [26]. Thus, in landfill scenario complete biodegradation of starch and 100 % C conversion efficiency into gas were assumed.

Table D.2 Biodegradability assumed in landfill

% dry weight basis	Decomposition (%)	Mineralization
Starch	100.000	100.000
Wheat protein	100.000	100.000
PVOH	10.000^{a}	9.000^{a}
Soya flour	100.000	100.000
Cellulose	64.000 ^b	50.000^{c}
Hemicellulose	62.000 ^b	50.000^{c}
Lignin	$0.000^{\rm d}$	0.000^{d}
WBF	86.859	86.859
PSBF	87.193	87.193
MSBF	90.589	90.589
Cardboard	53.834	42.352

Notes

As for PVOH, previous study indicated that either aerobic or anaerobic landfill conditions did not enhance the biodegradability of PVOH/starch composites significantly and PVOH remained as a main residue component [51]. This conclusion was also confirmed by Tudorachi et al. [96] who found that after 18 day inoculation with micro-organisms isolated from landfill, starch and the amorphous part of PVOH was degraded but the crystalline regions of PVOH remained. Therefore, in the present LCA landfill scenario, aeration was assumed as an insignificant parameter for the PVOH biodegradation profile. Via literature review, no quantified degradability data derived from landfill simulation test s were available so, instead, simulated soil burial tests results were considered as reasonable indications of PVOH biodegradation under landfill condition. Irrespective of the PVOH physical state (either film or powder) the extent of mineralization under soil burial observed was 8–9 % within 74 days [15]; interestingly, incubation with 18 different soils within prolonged test periods (2 years), PVOH showed similar biodegradability (less than 10 %) via weight loss tests [17]. This indicated that the extent of PVOH degradation can be independent of soil composition and was stable within certain burial periods. The PVOH modelled in the current study has a low hydrolysis degree. Although PVOH with lower hydrolysis degrees were found to have slightly larger propensity to microbial assimilation, no mineralization higher than 12 % has been reported [17] and according to Chiellini et al. [16] this was attributed to the absorption of PVOH by inorganic or organic components present in soil, which inhibited the biodegradation of PVOH. In the current landfill scenarios, the inhibition effect of soil absorption was assumed to be present and the biodegradation of PVOH was estimated as shown in Table D.2; potential further biodegradation as indicated by Chiellini et al. [16] was not taken into account due to the lack of evidences.

^a [15, 17]

^b [6]

^c [50]

^d [74, 104]

As indicated in Table D.2, the biodegradation rate of the WBF/PSBF/MSBF was estimated to vary between 86.9 and 90.6 % with the of PVOH residual fractions remaining as inactive solid mass.

D.2.2 Cardboard Biodegradability

Only in the presence of O_2 does fungal decay of wood or paper occurs thus during burial in an anaerobic landfill, biodegradation of wood products results only from bacterial activity which is known to degrade lignocellulose material at a slower rate than fungi [104]. Therefore, an overall lower biodegradation profile for cardboard in landfill was modelled than was modelled for the aerobic composting scenarios.

Amongst three components of cardboard, lignin was considered as recalcitrant under anaerobic conditions [5, 101] thus was not assumed to significantly decompose in landfill [19, 74, 104]. Based on this, in this current landfill scenarios the degradation of lignin was assumed to be negligible. For cellulose and hemicellulose, generally they can be metabolized by landfill bacteria [41, 74] but their decomposition in landfill depends on many factors including environmental conditions (such as moisture, pH), landfill management, waste composition as well as bioavailability [4, 74]. In addition, the extent of their biodegradation can vary with their association with lignin [74], as lignin has been demonstrated to form both physical and chemical barriers to microbial attack and further inhibit decomposition of cellulose/hemicellulose [11, 74, 101, 4].

Generally methods applied in previous studies to estimate the biodegradability of these three fractions were either composition analysis or gas measurements. The former is refereed as to total C loss-indicated by the decline of cellulose and hemicellulose content—which was normally, determined under actual landfill conditions in field studies. This method takes into account the breakdown fraction present in the matrix but could lead to overestimation of the C gas loss from landfill [74, 104]. The latter concerns mineralization rates determined by the ratio of measured landfill gas emissions to theoretical C gas potential, which were normally carried out at lab-scale such as in simulated landfill reactors [6]. A comprehensive review of field studies was conducted by Barlaz [4] and, despite lack of uniform data across those studies, the same trends were demonstrated i.e. the depletion of cellulose and hemicellulose and the decline in the ratio of cellulose: lignin with landfill depth and age [4]. This indicates the limitations of the data presented in some field studies: they only demonstrate the material biodegradability for given temporal periods (generally less than 100 years). In contrast, due to controlled conditions at lab-scale, the latter method can give ultimate biodegradability [4]. Therefore, for landfill scenarios with a 100 year time frame, the data derived from lab-scale reactors was preferred for biodegradation assumptions in the current LCA study.

As shown in Table D.2, mineralization rates of cellulose and hemicellulose were derived from IPCC guidelines. According to the IPCC method [50] two factors were concerned to estimate the extent of material decomposition in anaerobic landfill: the total degradable organic C (DOC) and fraction of DOC decomposed in landfill (DOCf). In the IPCC approach, the DOCf was defined as the fraction of C ultimately degraded and released from landfill, whereas DOC loss as leachate was considered as less than 1 % and is thus negligible [50]. Therefore, the default values recommended by IPCC [50] for dry cardboard: 0.44 (DOC with lignin considered as degradable) and 0.5 (DOCf), led to an estimation of 50 % loss of original C via gas emissions. This assumption is agreed by mineralization rates reported by Ress et al. [88] and Barlaz [4] where 55 % of waste cellulose was converted to CO₂ and CH₄ in landfill and 54.4 % of theoretical CH₄ from cellulose/hemicellulose components was yielded during the degradation of cardboard.

As for the decomposition rate, the mass loss results derived from field study on landfill sites with limited time periods were rejected, such as the low decomposition rate reported by Ximenes et al. [104] which was due to age limitation (30-46 years) of the landfill investigated. Instead, mass loss results derived from lab studies were selected: as given in Table D.2, the results revealed by Barlaz et al. [6] were chosen as they were cardboard-specific and consistent with most other studies: irrespective of lignin. In most published studies 50-60 % of cellulose/hemicellulose was estimated to be decomposed in landfill [104]. Actually, higher decomposition rates of cellulose are reachable under optimized lab studies: 77–80 and 71–77 % decomposition rate was recorded for cellulose and hemicellulose [74, 88]. In addition, after de-lignification e.g. ball mill pretreatment, cellulose was observed to decompose nearly to the extent of filter paper (95–97 %) [74, 4]. These results were rejected because: (1) they were not cardboard-specific, and (2) results derived from optimized experimental condition were considered unrepresentative of real landfill condition where larger particle size, low moisture, poor mixing can be expected.

As given in Table D.2, the overall biodegradation rate of cardboard was assumed to be 53 %, with 42 % of the original C lost via $\rm CO_2/CH_4$, which meant approx 10 % of degraded cellulose and hemicellulose could accumulate as an aqueous intermediate and ultimately microbial biomass. This estimation was slightly higher than the range of paper mineralization agreed in previous studies (26–40 % of total C released as landfill gas) [74] and the biodegradation rate of cardboard assumed in the Eco-invent v 2.0 dataset (32.44 %).

D.3 Element Flow in Landfill Scenarios

Based on the biodegradation profiles assumed, the potential fate of each chemical element embodied in waste material was analyzed, where the multi-input inventory approach was introduced [79]. As presented in Table D.3, studies

providing empirically based life cycle inventory for sanitary landfill were analyzed. Based on fundamental biochemical processes in landfill as well as literature-derived data, assumptions were made for the current landfill scenarios, which are given in Table D.4.

D.3.1 C Transformation in Landfill

As described by previous authors [4, 74, 94], generally, waste undergoes complex four-phase decomposition in landfill. In the first phase of aerobic decomposition large quantity of CO₂ are produced; with O₂ depletion, anaerobic degradation is triggered, where the metabolic steps are similar to AD. In the second anaerobic acid stage the polymers are hydrolyzed to sugars, long-chain carboxylic acids etc., and then metabolized by fermentative bacteria to form short-chain organic acids, and alcohols etc. [74]. The C existing in the forms of organic acids and their accumulation is characteristic of phase 2. C conversion to CH₄/CO₂ is the feature of the third and fourth phases where simple molecules are further utilized by acetogenic and methanogenic bacteria. Similar to AD, CH₄ and CO₂ gases are the main output from C flows in landfill, but differently a higher proportion of CO₂ can be expected from landfill gas [86] due to the initial aerobic decomposition stage. As shown in Table D.4, average landfill gas composition with 50 %v/v CH₄ recommended by IPCC [50] was applied in current model. This estimation was within the range of 50-60 % CH₄ (v/v) modelled in other studies (Table D.3) [73, 79], and agreed by the lab-derived results in literature [88]. Based on this assumption and mineralization rate listed in Table D.2, the total C gas production was estimated as Table D.5. Uncollected landfill gases are also assumed to diffuse through the landfill cover, during which CH₄ is partially oxidized to CO₂, but with the majority released to atmosphere. The collected landfill gas was assumed to be combusted in a biogas plant.

In addition to C gaseous loss, remaining C in landfill could accumulate as aqueous intermediates, microbial biomass and recalcitrant solids [74]. Data on leachate recorded in previous studies varied: 10 % of C loss was estimated as leachate by Manfredi and Christensen [69]; whereas, other authors [77, 88] concluded that leachate loss only accounted for about 1 % of C, which is also the assumption in the IPCC guidelines (2006). However, the C leachate rates highly depend on precipitation, landfill management and waste composition etc.; significant leachate even above 10 % of total Chave bene found [50]. In order to better evaluate the potential environmental impacts of C leachate, a relatively high factor was chosen: decomposed but not gasified C was estimated as TOC leachate where a constant concentration over 100 years was assumed. Considering the removal efficiency given in Table D.1, TOC were partially removed but over 50 % was assumed to be discharged to either ground or surface water.

The remaining C fractions were assumed as recalcitrant solid. As estimated in Table D.5 approx 40 % of inactive solid C for cardboard was derived from lignin

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		Study 1 [73]		Study 2 [79]		Study 3 [69]	
C flow							
Landfill gas composition	CH ₄ (vol %)	50 %		% 09		5-60 % ^a	
	CO_2 (vol %)			40 %		30–70 % ^a	
Landfill gas potential (m ³ /ton fresh matter)	ter)			120		170	
Landfill gas emission (% total C gases)		NA^{c}		Year 0-5	22 %	Year 0-2	2 %
				Year 6–30	75 %	Year 3-5	% 8
				Year 31-100	3 %	Year 6-40	20 %
						Year 41–100	16 %
C distribution (% converted organic C) C gas	C gas	NA^c		% 06		% 8.68	
	Leachate			10 %		10.2 %	
Landfill gas collection efficiency (%)		Year 0-1	% 0	Year 0-5	% 0	Year 0-2	% 0
		Year 1–2	20 %	Year 6-30	45 %	Year 3-5	% 06
		Year 2–32	% 08	Year 31–100 0 %	% 0	Year 6-40	% 06
		After 32 years	% 0			Year 41–100	% 0
Landfill gas energy recovery efficiency		Combustion engine (electricity) 23 % ^b	ne (electricity)	NA^{c}		85 % recovery (hear ratio = $3/2$)	85 % recovery (heat: electricity energy ratio = 3/2)
		Boiler (heat) 70 % ^b	₄ %				
CH ₄ oxidation rate (%)		Year 1–2	50 %	Year 0-5	% 0	Year 0-1	% 0
		Year 2–32	% 66	Year 6–100	% 06	Year 2–100	% 06
N flow		rear 33-100	-0.01/yr				
N distribution (% total N)	N gas	NA^{c}		NA^c		% 0	
	Leachate					13.7 %	
	Stored					86.3 %	
N leachate generated (mm/yr)		NA^c		Year 0-5	650	Year 0-2	500
				Year 6–30	390	Year 3-10	250
				Year 31-100	390	Year 11–40	200
						Year 41–100	180
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		Study 1 [73]	Study 2 [79]		Study 2 [79] Study 3 [69]	
% total N leachate released to ground and surface water NAc	d surface water	NA^{c}	Year 0–5 1.2 % Year 0–2	1.2 %	Year 0-2	1.3 %
			Year 6-30 5.2 % Year 3-10	5.2 %	Year 3-10	1.9 %
			Year 31-100 93.7 % Year 11-40	93.7 %	Year 11-40	13.4 %
					Year 41–100	83.4 %
N leachate distribution (%sub-total N NH ₄ ⁺ -N	NH_4^+N	NA^c	Year 0-5	73.2 %	73.2 % 100 % NH ₄ ⁺	
leachate at each phase)			Year 6–30	49.6 %		
			Year 31-100 91.7 %	91.7 %		
	NO_2^N	NA^c	Year 0–5	0.4 %	NA^c	
			Year 6–30	3.3 %		
			Year 31–100 0.6 %	% 9.0		
	NO_3^N	NA^c	Year 0-5	26.4 % NA ^c	NA^c	
			Year 6–30	47.1 %		
			Year 31–100 7.6 %	7.6 %		

^a Landfill gas composition differed at four stages (CH₄ occupied 25, 40, 60, 5 % of landfill gas at phase 1, 2, 3, and 4 respectively) ^b Bioreactor scenario CHP ^c NA data not available

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		Assumptions				References
		WBF/PSBF/MSBF	ΙΉ	Cardboard		
С Яом						
Landfill gas composition	CH_4 (vol %)	50 %		50 %		[50, 73]
	CO_2 (vol %)	50 %		50 %		
Landfill gas emission (% total emissions)		Year 0-5	100 %	Year 0-5	22 %	[79]
				Year 6-30	75 %	
				Year 31-100	3 %	
C distribution (% degraded C)	C gas	100 %		% 06		[79, 69]
	Leachate	% 0		10 %		
Landfill gas collection efficiency (%)		Year 0-30	% 06	Year 0-30	% 06	[69, 43]
		Year 31-100	% 0	Year 31-100	% 0	
Energy recovery efficiency		Total 85 % recov	ery (heat: ele	Total 85 % recovery (heat: electricity energy ratio = 3/2)	io = 3/2)	[69, 42]
		30 % net electric energy (wi plant energy considered)	energy (with considered)	30 % net electric energy (without heat recovered and with in- plant energy considered)	l and with in-	
CH ₄ oxidation rate (%)		Year 1-100	10 %	Year 1–100	10 %	[50, 43]
N $flow$						
N distribution (% total N)	NH ₃ -N gas	10 %		5.4 %		[7]
	Leachate + N_2O/N_2 90 %	% 06		48.5 %		Estimation
	Stored N			46.2 %		

Table D.4 (continued)

		Assumptions				References
		WBF/PSBF/MSBF	BF	Cardboard		
% of total liberated N		Year 0–5	100 %	Year 0–5	15.7 %	[69]
		Year 6-30	% 0	Year 6-30	29.6 %	
		Year 31-100	% 0	Year 31-100	54.7 %	
N leachate composition	NH ₄ ⁺ -N	Year 0-5	73.2 %	Year 0-5	73.2 %	[62]
(% sub-total N leachate at each phase)		Year 6–30	% 0	Year 6–30	49.6 %	
		Year 31-100	% 0	Year 31-100	91.7 %	
	NO_2^N	Year 0–5	0.4 %	Year 0-5	0.4 %	
		Year 6–30	% 0	Year 6–30	3.3 %	
		Year 31-100	% 0	Year 31-100	0.6 %	
	NO_3^N	Year 0–5	26.4 %	Year 0–5	26.4 %	
		Year 6–30	% 0	Year 6–30	47.1 %	
		Year 31-100	% 0	Year 31-100	7.6 %	
NO ₃ ⁻ -N conversion (%)	Year 0-30	100 % (including 95 $\%N_2$ and 5 % N_2O)	ig 95 %N ₂ ar	$10.5\% N_2O$		Estimation based on [84]
	Year 31-100	90 % (including 88 % N_2 and 2 % N_2O)	88 %N ₂ and	$12\% N_2O)$		
% total N leathate released		Year 0-5	100 %	Year 0-5	0.2 %	Estimation
(ground and surface water)		Year 6-30	% 0	Year 6–30	2.0 %	
		Year 31-100	% 0	Year 31–100	% L'L6	

% total C	CO ₂ –C (%)	CH ₄ –C (%)	C leaching (%)	Non-active solid C (%)
Starch	50.07	49.93	0.00	0.00
Wheat protein	50.07	49.93	0.00	0.00
PVOH/dry	4.51	4.49	1.00	90.00
Soya flour	50.07	49.93	0.00	0.00
Cellulose	25.03	24.97	14.00	36.00
Hemicellulose	25.03	24.97	12.00	38.00
Lignin	0.00	0.00	0.00	100.00

Table D.5 Assumptions of C fate

with the rest originated from cellulose and hemicellulose fractions resistant to degradation. This estimation differs from the finding of Bogner and Spokas [12]: most of the non-active solid C is originated from lignin. For the fate of this non-active solid C, there are two assumptions depending on the temporal boundary. Firstly, for the infinite time horizon, Barlaz [4] declared that refuse will decompose until all organic matter is exhausted, this organic C stored could therefore be released to the environment in the long-term. An alternative assumption for a surveyable time frame is that landfill presents a net C sink [3], which means not only fossil C in PVOH but also a fractions of biogenic C e.g. those contained in lignin are sequestrated in landfill. As addressed by Barlaz [3], the C not degrading under optimal lab-simulated landfill reactors can be estimated as C storage in landfill. Because the decomposition estimation in the present study was based on lab-scale landfill studies and a surveyable period 100 year was defined as the temporal horizon, in the current LCA model the second assumption (i.e.a net C sink) was adopted.

D.3.2 N Transformation in Landfill

Concerning N fate, processes in soil or in AD treatment such as ammonification, volatilization, nitrification, denitrification, etc. may all occur during the landfill process [10]. Firstly, the major N source in landfill waste—protein—undergoes a two-step ammonification, which includes hydrolysis to amino acids and the further conversion to $\rm CO_2$, $\rm NH_3/NH_4^+$, and VFA via subsequent deamination or fermentation [56]. The majority of N release is present in the form of $\rm NH_4^+$ as the landfill pH level is generally less than 8 [10]. As described by Berge et al. [10], the liberated $\rm NH_4^+$ –N could either be leached from the waste, bound to organic/inorganic compounds or volatilized as atmospheric emissions; or instead, $\rm NH_4^+$ –N could be converted to other forms via biochemical process including nitrification, denitirification, anommox etc.

Via aerobic process nitrification, NH_4^+ –N is oxidized to NO_3^- and NO_2^- , due to its dependency on dissolved O_2 concentration, this process is more restricted to the upper portions of the landfill cell or the cover where air may infiltrate into the landfill system [10]. In addition, mesophilic temperatures more favour nitrification

which is inhibited at temperatures above 54 °C [102]. However, even under unfavourable conditions, other pathways could take place to oxidize NH_4^+ such as anaerobic process anommox with NO_3^- and N_2 produced, thermophilic oxidation pathway by methanotrophs [53, 93]. The NO_3^- could be further reduced by denitrifiers under either anaerobic or anoxic environments. With a high C: N ratio, a rapid denitrification occurs where mainly hetertrophic and facultative microbes are involved and NO_2^- , NO, N_2O or N_2 are produced, but for the aged landfills with lower C:N ratios but high S concentrations, antotrophic denitrification may occur with N_2 as only product [10].

Landfill is heterogeneous and can support different microenvironments (aerobic anaerobic anoxic zones) which allow several N transformation processes to be present simultaneously [10]. In the current LCA model, NH₄⁺ sorption was not taken into account as it was assumed that within 100 years, all NH₄⁺ bound to other compounds are released. Thus, the most likely metabolic steps are firstly ammonification, nitrification, followed by either denitrification or ANAMMOX; but these multiple processes occur in different sections of the landfill simultaneously depending on the distribution of aerobic/anaerobic regions and the leachate flows. However, NH₄⁺ is present as the dominant liberated N form due to the accumulation of NH₄⁺ but with fewer pathways for its degradation [80, 10]. The long-term N leachate composition was investigated by Kulikowska and Klimiuk [63] who indicated that NH₄⁺ concentration increased with the age of landfill and remained high without decreasing trend; this result was also concluded by Kjeldsen et al. [60] and Renou et al. [87] who carried out comprehensive reviews on leachate composition and treatment. These conclusions were generally applied in previous landfill models (Table D.3), amongst which, the N transformation modelled by Obersteiner et al. [79] was the most representative agreeing with the theoretical N dynamic pattern. In their model, NH₄⁺ was the dominant N leachate component in phase 1 with 26 % NO₃⁻, which represented the occurrence of ammonification and partial nitrification; in phase 2, NO₃⁻ and NH₄⁺ were present as the major N leachate (nearly 50 % each), which indicated the occurrence of subsequent nitrification or possible ANAMMOX; with the removal of NO₃⁻ via denitrification, NH₄⁺ was modelled as the major long-term N leachate in phase 3. Therefore, the assumption in the present study of distributions of N in leachate was based on their study [79]. Besides, as shown in Table D.4, total ammonification was estimated from biodegradation rates; 100 % of WBF protein hydrolysis was achieved within 5 years. The pattern of liberated N from landfilled cardboard over the whole modelled period (100 year) was obtained from the study by Manfredi and Christensen [69]. As for NH₄⁺ leachate treatment, the assumptions are presented in Table D.1.

Besides leachate, gas is another route of N loss. According to the equation developed by Anthonisen et al. [2] where free NH_3 is a function of $\mathrm{NH_4}^+$, pH and temperature, at general landfill pH level 8, volatilization mechanism accounts for approx 23 and 5 % of liberated N at two extreme temperature 55 and 25 °C respectively. This range was confirmed by the measured data [10] and furthermore, provided an estimation for potential NH_3 release. The temperature of landfill may

fluctuate, in older landfill with the reduced biological activity, a temperature drop could be expected [10]; in current LCA model 10 % of liberated NH_4^+ -N was assumed lost via volatilization.

In addition to NH₃, other gases can be emitted from landfill, such as N₂O, NO, N₂. Although some studies indicate landfill as a source of N₂O, especially landfills in current operation period and those covered by clay, their results showed N₂O was of minor significance in comparison with CO₂ and CH₄ [105, 89], only sharing 3 % of the GWP caused by landfill emissions [89]. Actually, before being emitted formed N₂O in the landfill could be converted into N₂ due to long residence times; furthermore, N₂O can be expected from young landfills but not older landfills as depletion of organic C does not favour heterotrophic denitrification. Instead, N2 could be the major gas produced via nitrification/denitrification. This assumption has been verified by Price et al. [84] who illustrated conversion of NO₃⁻ via definitration decreased with the depletion of organic C whereas N₂ is the dominant gas, accounting for 94-100 % of gasified NO₃⁻. NO has been suggested as a minor product from denitrification [84]. In fact, previous landfill models [79, 69] and IPCC guideline (2006) considered N₂O as insignificant. Thus, in the current LCA model, the organic C content was assumed to be sufficient for rapid denitrification in the first 30 years, after which removal of NO₃⁻ declined; the denitrification rate and induced N gas were estimated based on data reported by Price et al. [84] and are given in Table D.4.

As shown in Table D.4, 97.7 % of the leachate discharge was modelled to occur in the post-closure monitoring period (year 30–100); this estimation agrees by other landfill models summarized in Table D.3. As for NH $_3$ /N $_2$ /N $_2$ O gas, they were partially released to atmosphere, but the majority of N gases (90 %) are assumed to be collected and combusted in the biogas plant. Landfill gas treatment processes together with final N fate are presented in Sect. D.5.

D.3.3 S Flow in Landfill

The distribution of S flows depends on many factors, such as pH, O_2 etc. It was found that during the microbial decomposition (oxidation) of organic matter, S is present either in soluble ionic forms e.g. SO_4^{2-} or bound to metals (Fe, Cd, Zn, Cu, Hg). With depletion of O_2 (a major electron acceptor) the anaerobic condition developes rapidly in the landfill, SO_4^{2-} acts as an alternative electron acceptor and transformed into H_2S and S^{2-} occurs via biochemical reactions [28, 65]. A fraction of formed sulphide is bound to metallic ions and precipitated [e.g. Fe (HS)₂ and Fe(HS)₃] [77], highly depends on the landfill conditions e.g. waste composition, pH. In gas phase, besides H_2S , other S compounds including methyl mercaptan (CH₃SH), dimethyl sulfide ((CH₃)₂S), carbon disulfide (CS₂) were also detected; but H_2S is the dominant S components, accounting for 80 - 98 % (w/w) of all S gases measured [57, 58, 65, 43] in addition the knowledge about desulphurization of landfill gas has been limited [86]. Thus in the current LCA model, without

considering other S gases (except H_2S) and desulphurization, the possible fates of S are modelled including SO_4^{2-} leachate, fugitive H_2S , SO_2 generated from landfill gas combustion, and S present in insoluble form.

Via searching of empirically based study, it was found that there is lack of knowledge about the S flow in landfill sites. Few landfill models discuss S fate and their assumptions varied. Some authors e.g. Obersteiner et al. [79] or de Cortazar et al. [20] considered all the S present in the leachate form; other authors e.g. Manfredi and Christensen [69] mainly estimated the S in the gas phase but did not indicate the S in leachate; only limited landfill studies present the inventory for both, but different S element flows were concluded. According to Menard et al. [73] who included both SO_4^{2-} leachate and oxidized S gas from combustion as emissions, most S loss was estimated as gas (96.5 % of S loss if SOx was assumed as SO₂). In contrast, Eco-invent database v 2.0 estimates SO₂ only accounts for 10-15 % of S loss. None of studies above concern the insoluble S fraction and only Nielsen and Hauschild [77] give estimation of HS⁻ (50 % of total S input) but no information is available for the fate of HS⁻. In the case of WBF/cardboard disposed of in an MSW landfill site, a rapid O₂ depletion and the presence of metallic ions was assumed. The assumption for S fate was H₂S and insoluble HS⁻ accounting for 50 % of S each with negligible SO₄²⁻ present. For the H₂S destruction during combustion, a default high efficiency (99 %) as recommended in the Gassim model [43] was applied with SO₂ assumed as the combustion product.

D.4 Biogas Plant

The collected landfill gas was assumed to be transported to the on-site CHP system to generate heat and electricity where complete combustion was assumed with CO₂, N₂O and SO₂ assumed as the main products released. The landfill gas energy recovery rate is given in Table D.4. Assuming no thermal energy recovered and taking into account the CHP in-plant electrical power consumption, the net electric energy delivered to grid was estimated as 30 % of landfill gas energy content according to the range reported by Gohlke [42]. A system expansion allocation approach was applied to the electricity produced, i.e. the equivalent quantity of electrical power generated by the average electricity supply mix for the UK grid was credited to the landfill system.

D.5 Inventory for Landfill

Base on the assumptions made and data analysis above, a detailed inventory for landfill scenario was developed where the infrastructure and other inputs e.g. water were mainly derived from WRATE model [35]. As for energy balance and element fate, it is discussed below.

MJ/kg received waste	WBF	PSBF	MSBF	Cardboard
Total Electricity generated ^{a, b}	4.436E+00	4.323E+00	4.515E+00	2.169E+00
Thermal energy generated ^{a, b}	6.654E+00	6.485E+00	6.773E+00	3.254E+00
Electricity exported	3.914E+00	3.815E+00	3.984E+00	1.914E+00
Diesel consumption ^{c, d}	8.701E-02	8.701E-02	8.701E-02	8.701E-02

Table D.6 Energy balance of landfill scenarios

Notes

- ^a Density $CH_4 = 0.717 \text{ kg/m}^3$, $CO_2 = 1.977 \text{ kg/m}^3$
- b Net calorific value of landfill gas is 19 MJ/m³ [30, 21]
- ^c Diesel consumption derived from WRATE model [35]

D.5.1 Energy Balance

Energy balance is presented in Table D.6, where the electric and thermal power recovered was estimated by applying energy recovery rate assumed in Table D.4. Based on the composition of landfill gas (Table D.4) and low heating value of CH₄ [27], the net calorific value of landfill gas was estimated as 18–19 MJ/m³, which agrees with the range (19–23 MJ/m³) recommended by DTI [30, 21]. As assumed, 100 % of the heat produced from landfill gas combustion was not recovered; taking into account the in-plant electricity consumption, the net electric energy exported varied between 3.8 and 3.9 MJ per kg foams, but much less surplus electric energy was produced from landfilled cardboard due to its low biodegradability.

Besides electricity input, diesel consumption during on-site operation was also considered. According to Manfredi et al. [70], the fuel consumption depends on the degree of compaction and the amount of soil moved for daily cover at the landfill site. They reviewed literature data and found typical values to be within the range of 1–3 L diesel per tonne of waste landfilled. This range was also confirmed in the WRATE model [43]: diesel consumption for operations tends to decrease with the scaling-up of landfill site, varying from 1 to 2.4 L/tonne waste. The upper range (2.4 L/tonne) was applied as it represents the small-scale landfill site modelled here (see Sect. 5.2.3).

D.5.2 Emissions and Leachate

As presented in Sect. 5.6, three emission sources were modelled: (1) uncollected landfill gases (containing CH_4 , CO_2 , and trace amount of H_2S , NH_3 , N_2O and N_2) which diffused through the landfill cover or escaped via cracks/fissures, (2) CO_2 , N_2O , and SO_2 generated from landfill-gas complete combustion in CHP plus trace amount of un-destructed H_2S fraction, (3) the emissions from diesel combustion.

^d Diesel density = 0.85 kg/L; net calorific value = 43.4 MJ/kg [31]

C/N leachate was also taken into account—large fraction of leachate (80 % TOC and 99.5 % of $\mathrm{NH_4}^+$) was removed during the monitoring period with the remaining untreated leachte either discharged to surface water or released to ground water within 100 year. There was no S leachate assumed.

Besides emission/leachate, a proportion of elements were assumed to be stored in landill.

Landfill site was assumed as net C sink sequestrating nearly 50 % of cardboard-C and approx 11–16 % of C contained in foams. A large fraction of N/S was assumed as stored N or precipitated HS⁻. These stored chemical elements may be removed via various pathways and eventually released to environment under infinite time horizon, which should be taken into account in LCA model.

Appendix E Further Discussion on GWP 100 Profiles of WBF

In this thesis, the GWP 100 impacts of WBF were estimated in a conservative way. As discussed in Sect. 3.4.2, the temporal boundary for Soisson crop cycle was defined as the time period from Soisson cultivation to the subsequent crop cultivation. According to the defined temporal boundary, a proportion of the residual nutrients carried over from previous crops and a fraction of wheat residue left on the land and their induced emissions/leaching occurring within the Soisson crop cycle were allocated to the Soisson crop. Therefore, the CO₂ field emissions within the Soisson crop cycle were primarily derived from several sources: the decomposition of the fractions of previous crop residues and part of the wheat residue as well as the decomposition of soil organic matter. A certain fraction of C sequestered in wheat residues (both above-ground and below-ground) was taken in the model to be released in subsequent crop cycles. However, the various sources for CO₂ field emissions could not be differentiated by using the DNDC model. Moreover, it was not possible to calculate the C sequestration in the wheat crop residues on a field-by-field basis as only generic values were available. Thus, to keep transparency and clarity in the LCA model and to avoid mixing the sitespecific emission data with global generic values, only C sequestration in the wheat grain was included in the LCA model; the C sequestered in the crop aboveground and below-ground residues, which were ploughed back into the agricultural land have been included in the DNDC model but excluded from the current LCA model. Therefore, the GWP100 profiles for WBF products presented in the current study are very conservative in that all the gross CO₂ field emissions from all aspects of the wheat cultivation were allocated to the wheat grain.

To further explore the GWP100 score for WBF in the LCA model it would be possible also to investigate sharing of these gross CO₂ field emissions (DNDC-generated results) between the various wheat crop C-absorbers, i.e. wheat grain, wheat straw and below ground residues—subject to the availability of robust data for the C-balance between these components of the whole crop, ideally on a field-by-field basis to maintain the site specificity of the LCA. In effect this could be

done by developing a factor to 'allocate' to the wheat grain only those CO2 field emissions appropriate to the grain by subtracting the CO₂ equivalent of the C sequestered into the wheat crop residues from the gross CO2 field emissions released. The availability of appropriate data for the C-distribution within the whole crop and consideration of an appropriate temporal boundary for C sequestration and release (e.g. temporal boundary could be the Soisson crop cycle or, alternatively, it could be the time period over which the residues 'fully' degrade in field etc.) on which to base this allocation would be critical to the development of such an allocation factor. This aspect of the integration of DNDC with LCA models should be investigated in further research. However, for the reasons given in the first paragraph above, all the gross CO₂ field emissions were allocated to the wheat grain in the current LCA model.

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