3.2. DATA ACQUISITION AND ANALYSIS

SAMPLING OF CONTINUOUS TIME DYNAMIC MODELS

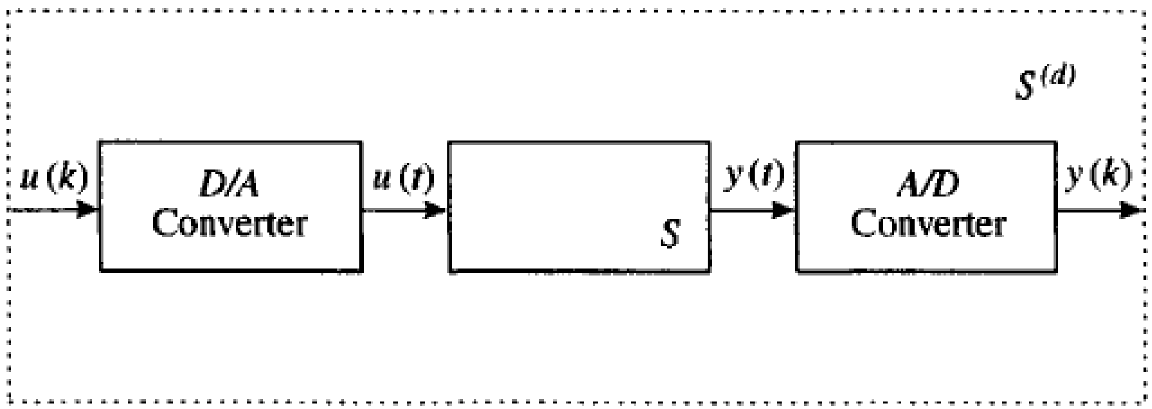
- Process models are usually constructed from **balance equations with suitable constitutive equations.**
- The balance equations can be either **ordinary or partial differential equations** depending on the assumptions on the spatial distribution of process variables.
- In order to solve balance equations, we need to **discretize** them somehow both in space (if needed) and in time.
- This section discusses discretization in time assuming that we have already lumped our PDE model as needed. In other words, **only lumped process models** are considered here.

- The lumped balance equations are **naturally continuous time differential equations** whereas almost any known method in mathematical statistics **works with discrete sets of data** and uses underlying discrete time models.

- Therefore, the need **to transform continuous time process models into their discrete time counterparts** naturally arises. This type of time discretization is called **sampling**.

- Almost any kind of **data acquisition, data logging or control system** is implemented on computers where **continuous time signals are sampled by the measurement devices**.

- Therefore, it is convenient **to generate the discrete counterpart of a process model** by simply **forming a composite system from the original continuous time process system**, the measurement devices taking the sampled output signals and from the actuators generating the continuous time manipulated input signals to the system as shown in Fig. below.



- The box labelled S is the original continuous time process system, the box D/A converter converts **continuous time signals to discrete time ones** and the box A/D converter converts **discrete time signals to continuous time ones**.

- The sampled data discrete time composite system S^d is in the dashed line box. The discrete time input and output variables (or signals) to the discrete time system S^d are

$$u : \{u(k) = u(t_k) \mid k = 0, 1, 2, \ldots\},$$
$$y : \{y(k) = y(t_k) \mid k = 0, 1, 2, \ldots\},$$

- where $T = \{t_0, t_1, t_2, \ldots\}$ is the **discrete time sequence**.

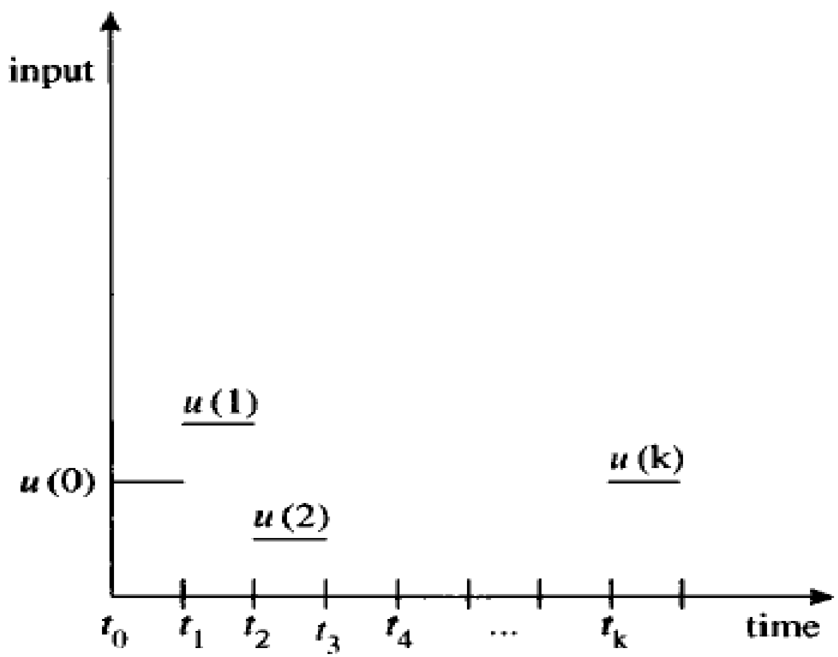
- Most often **equidistant zero-order hold** sampling is applied to the system, which means that we sample (measure) the continuous time signals and generate the manipulated discrete time signals in **regular equidistant time instances**, i.e.

$$t_{k+1} - t_k = h, \quad k = 0, 1, \ldots,$$

- where the constant h is the **sampling interval**. Moreover, a **zero-order hold** occurs in the D/A converter to generate a continuous time manipulated input signal u(t) from the discrete time one *u(k):*

$$u(\tau) = u(k), \quad \text{for all } \tau \in [t_k, t_{k+1}).$$

- Equidistant zero-order hold sampling is illustrated in Fig. below.



- In the general case, we should transform a continuous time process model describing the continuous time system S to its discrete time sampled version in the following steps:

  1. Take the **sampled discrete time signals** of the input and output signals.

  2. Make a **finite difference approximation** (FDA) of the derivatives in the model equations by using Taylor series expansion of the nonlinear operators if needed.

- Let us consider a process model in the usual LTI state space form:

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = \mathbf{A}x(t) + \mathbf{B}u(t), \qquad y(t) = \mathbf{C}x(t) + \mathbf{D}u(t)$$

with the constant matrices (A, B, C, D)

- Then, its sampled version using equidistant zero-order hold sampling with sampling time h is a discrete time LTI state space model in the form

$$x(k+1) = \mathbf{\Phi} x(k) + \mathbf{\Gamma} u(k), \qquad y(k) = \mathbf{C} x(k) + \mathbf{D} u(k),$$

- Where the constant matrices (Φ, Γ, C, D) in the discrete time model are

$$\mathbf{\Phi} = \mathrm{e}^{\mathbf{A}h} = \left(I + h\mathbf{A} + \frac{h^2}{2!}\mathbf{A}^2 + \cdots \right),$$

$$\mathbf{\Gamma} = \mathbf{A}^{-1}(\mathrm{e}^{\mathbf{A}h} - \mathbf{I})\mathbf{B} = \left(h\mathbf{I} + \frac{h^2}{2!}\mathbf{A} + \frac{h^3}{3!}\mathbf{A}^2 + \cdots \right)\mathbf{B}$$

- If numerical values of the continuous time model matrices (A, B, C, D) are given, then there are ready MATLAB functions to compute the matrices (Φ, Γ, C, D) . Most often, if h is small enough, it is sufficient to consider only the first order (containing h but not its higher powers) approximation of the Taylor series .

- EXAMPLE (Sampled linearized state space model of a CSTR). Consider the CSTR described earlier with its linearized state space model and assuming full observation of the state variables. Derive the sampled version of the model assuming zero-order hold equidistant sampling with sampling rate.

- The state space model matrices in symbolic form are as follows:

$$\mathbf{A} = \begin{bmatrix} -\frac{F}{V} - k_0 \mathrm{e}^{-E/(RT_0)} & -k_0 \left(\frac{E}{RT_0^2} \right) \mathrm{e}^{-E/(RT_0)} C_{A_0} \\ -\frac{k_0 \mathrm{e}^{-E/(RT_0)} (-\Delta H_\mathrm{R})}{\rho c_P} & -\frac{F}{V} - k_0 \left(\frac{E}{RT_0^2} \right) \mathrm{e}^{-E/(RT_0)} C_{A_0} \frac{(-\Delta H_\mathrm{R})}{\rho c_P} - \frac{UA}{V \rho c_P} \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} \frac{(C_{A_\mathrm{i}} - C_{A_0})}{V} & 0 \\ \frac{(T_\mathrm{C} - T)}{V} & \frac{F}{V} + \frac{UA}{V \rho c_P} \end{bmatrix},$$

$$\mathbf{C} = \mathbf{I}, \quad \mathbf{D} = 0.$$

- Applying zero-order hold equidistant sampling to the model matrices above with the first-order approximation in the above Eqs. we obtain :

$$\Phi = \begin{bmatrix} 1 - \left(\frac{F}{V} - k_0 e^{-E/(RT_0)} \right) h & -hk_0 \left(\frac{E}{RT_0^2} \right) e^{-E/(RT_0)} C_{A_0} \\ -h \frac{k_0 e^{-E/(RT_0)} (-\Delta H_R)}{\rho c_P} & 1 - h \left(\frac{F}{V} - k_0 \left(\frac{E}{RT_0^2} \right) e^{-E/(RT_0)} C_{A_0} \frac{(-\Delta H_R)}{\rho c_P} - \frac{UA}{V \rho c_P} \right) \end{bmatrix},$$

$$\Gamma = \begin{bmatrix} \frac{(C_{A_i} - C_{A_0})}{V} h & 0 \\ \frac{(T_C - T)}{V} h & \left(\frac{F}{V} + \frac{UA}{V \rho c_P} \right) h \end{bmatrix}.$$

DATA SCREENING

- If we have collected any real data either steady-state or dynamic, we have to assess **the quality and reliability of the data** before using it for model calibration or validation.

- Data screening methods are used for this purpose assuming that we have a set of measured data.

$$D[1, k] = \{d(1), d(2), \ldots, d(k)\}$$

- with vector-valued data items $d(i) \in R^V$, *i = 1,...K: arranged in a sequence* according to the time of the collection (experiment).

- Data screening is **a passive process** in nature, i.e. if poor quality data are detected then it is usually **better not to use them and preferably repeat the experiment** than to try to "repair" them by some kind of filtering.

Data Visualization

- The most simple and effective way of data screening is **visual inspection**. This is done by plotting the collected set of measured data against

  - time or sequence number (time domain),
  - frequency (frequency domain),
  - one another

- When we plot data on a single signal, that is on a time dependent variable against time or sequence number, then we get visual information on

  - **trends and seasonal changes** due to some equipment changes,
  - **outliers, gross errors or jumps** detected just from the pattern.

- It is important to visualize the data using different scales on both the **time and the magnitude axis**.

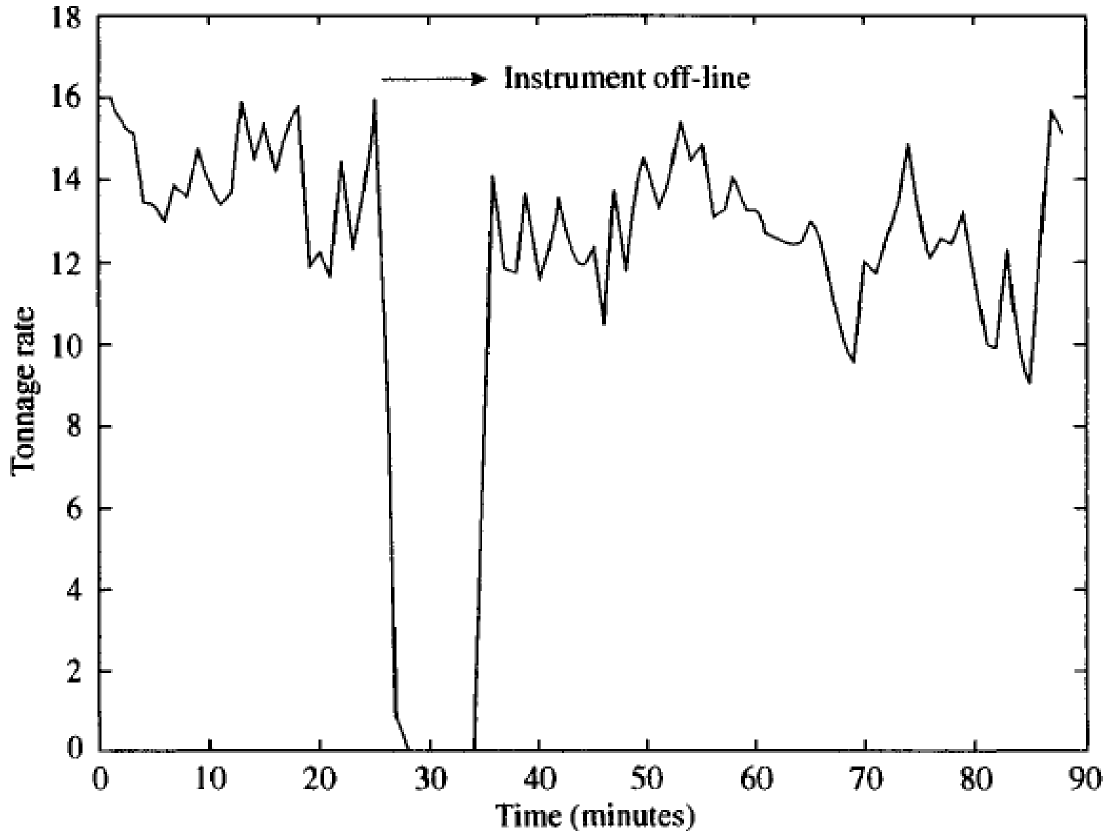
- This plot carries diagnostic information about **the nature of the disturbances affecting the quality of the data**.

- If we plot **one signal against another one, then we may discover**
  - cross-correlation, and/or
  - linear dependence between them.

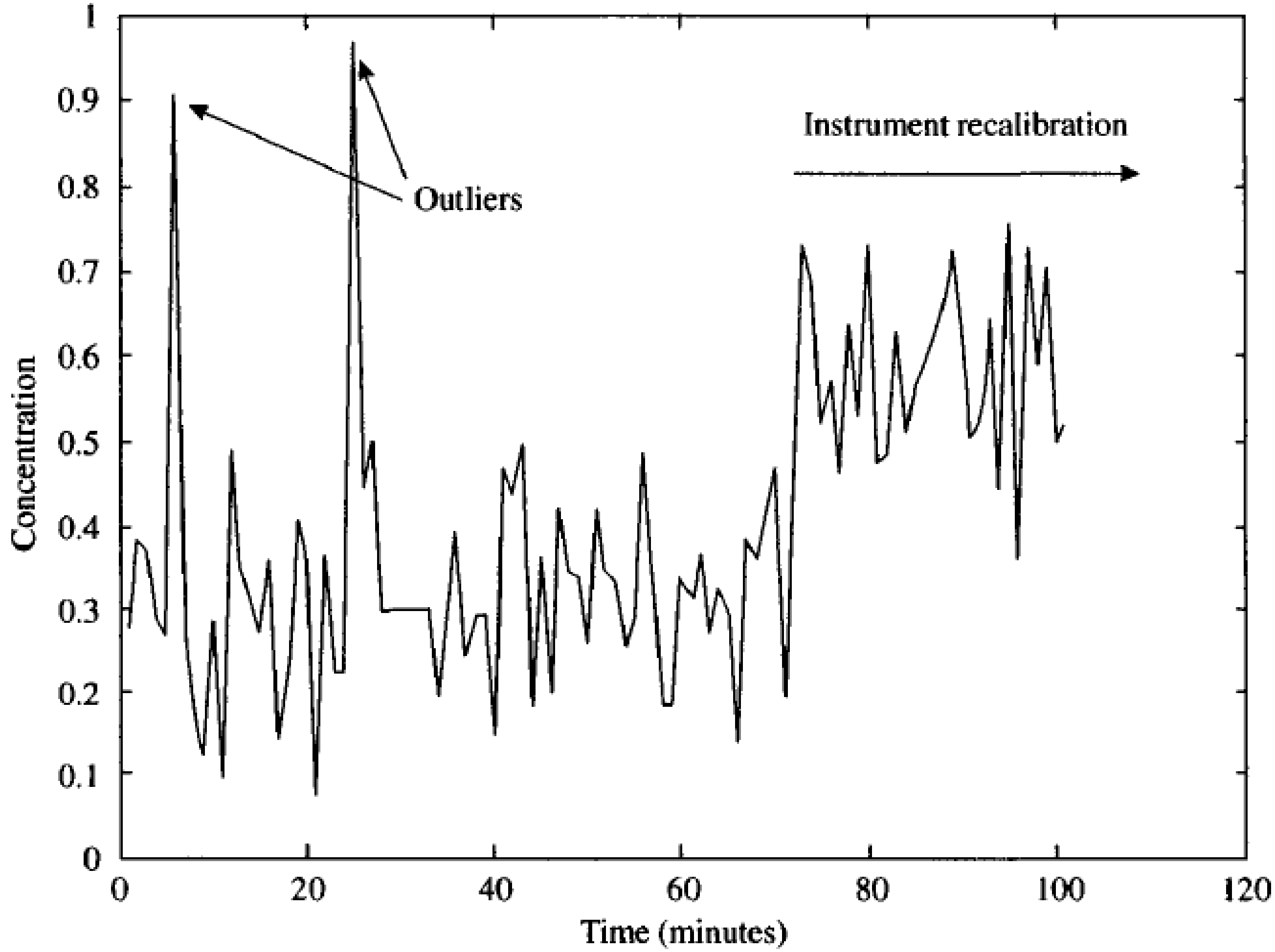
- Visualization helps in identifying quickly **abnormal data** which does not conform to the usual patterns.

- As a supplement to data visualization plots simple statistics, such as
  - signal mean value,
  - auto-correlation coefficients,
  - signal value distribution

- Example time-plots of data records of real valued data signals are shown below



- **Two jumps forming a gross error** are seen in the Figure. The reason for the gross error was a measurement device failure: the corresponding automated sensor went off-line when the first jump was observed and then went back online causing the second jump.



- The first part (in time) of the shows **two big outliers and a slow trend**. These anomalies initiated a recalibration of the corresponding instrument which is seen in the form of a positive jump on the plot

Outlier Tests

- The outlier test methods are based on two different principles: either they are looking for deviations from
  - the "usual" distribution of the data (**statistical methods**)
  - or they detect outlier data by **limit checking**.

- In both cases, we may apply the fixed or the adaptive version of the methods depending on whether the normal (non-outlier) data statistics are given a priori or they should be first estimated from test data.

Trends, Steady-State Tests

- If we want to perform **a parameter** and/or **structure estimation** of static models, then we need to have **steady-state data**.

- Steady state or stationarity includes **the absence of trends**. There can be other circumstances when we want to have data with no trends.

- Trend detection is therefore **an important data screening procedure** and can be an efficient and simple process system diagnosis tool.

- The trend detection or steady-state test methods can be divided into two groups: methods based on **parameter estimation and methods based on other statistics**.

1. Methods based on parameter estimation

- The simplest way to detect trends is to fit a straight line through the measured data and check **whether its slope is zero**.

- If the measurement errors are independent of each other and are normally distributed, then standard statistical hypothesis tests can be applied to check their constant mean.

2. Methods based on other statistics

- The most well known and commonly used method is the so-called **Cumulative SUMmation (CUSUM) method**.

- CUSUM is a recursive method which is based on **a recursive computation of the sample mean** with growing sample sizes.

- This cumulative sum based mean is then plotted against time and inspected either by limit checking or by parameter estimation **whether it has any slope different from zero**.

Gross Error Detection

- Gross errors are caused by equipment failures or malfunctions.

- They can be detected by different methods depending on the nature of the malfunctioning and on the presence of other "healthy" nearby signals.

- The available methods for gross error detection can be grouped as follows:

  1. Bias or slow trend detection

  Gross errors can be visible bias or slow trend in the recorded signal of the sensor or sensors related to the equipment in question. **Trend detection methods** can then be applied to detect them.

  2. Jump detection

  In case of sudden failure, a **jump arises in the corresponding signal**(s) which can be detected via bias or jump detection in time series by standard methods

  3. Balance violation detection

  The group of related **signals of the equipment subject to failure** or malfunction can also be used for detecting gross error causing the violation of the causal deterministic relationship between them.

EXPERIMENT DESIGN FOR PARAMETER ESTIMATION OF STATIC MODELS

- The parameter estimation for static models requires steady-state data because of the model. Therefore, the first step in designing experiments is to ensure and test that the system is in steady state.

- This is done by *steady-state tests.* Thereafter, we decide **the number of measurements**, the **spacing of the test points** and the **sequencing of the test points**.

Number of Measurements

- The number of measurements depends on the **number of test points** *and on the* number of **repeated measurements** in the test points.

- If we repeat measurements at the test points, then we may have **a good estimate on the variances** of the measurement errors which is very useful to assess the fit of the estimate.

- The number of test points depends critically on **the number of state variables of the process system** and on **the number of estimated parameters**.

- In general, we need to make sufficient measurements to estimate unknown parameters and possibly unknown states, i.e. the number of measurements **should be significantly greater than** the number of unknown parameters and states.

Test Point Spacing

- It is important that we have a set of measurements **which "span" the state space of the process system** the model is valid for.
- This means that we have to space experimental measurement points **roughly uniformly over the validity region of the process model** we are going to calibrate or validate.
- It is equally important that we stay **within the validity region** of our process model.
- For linear or linearized models, this validity region can be quite narrow **around the nominal operating point of the model**.

Test Point Sequencing

- For static models and process systems in steady-state, the sequence of measurements **should not affect the result of parameter estimation**.

- That is, because measurement errors of the individual measurements are usually **independent and equally distributed with zero mean**.

- For some kinds of process systems, however, we can achieve the above properties of independence and zero mean only by **randomization of the measurements**.

- This artificially transforms **systematic errors** into **random measurement errors**.

EXPERIMENT DESIGN FOR PARAMETER ESTIMATION OF DYNAMIC MODELS

- The experimental design for parameter and structure estimation of dynamic models involves a number of **additional issues compared with static models**.

- The reason for this is that we can **only design the input variable as** part of the independent variables in the model and then the output variables are **determined by the dynamic response of the process system itself**.

Sampling Time Selection

- **Proper sampling of continuous time signals** and process models is essential.
- The selection of the sampling time is **closely connected with the selection of the number of measurements**.
- We want to have sufficiently **rapid sampling for a sufficient length of time**.
- Moreover, we want to have **information about all time response characteristics** of our dynamic process model.
- For this reason, we have to select the sampling time to be **roughly one third or one quarter of the fastest time response of the process system**, which is usually in the order of seconds for process systems.

3.3 STATISTICAL MODEL CALIBRATION AND VALIDATION

- **Model validation** is one of the most difficult steps in the modelling process.

- It needs a **deep understanding of modelling**, **data acquisition** as well as basic notions and **procedures of mathematical statistics**.

GREY-BOX MODELS AND MODEL CALIBRATION

- In practical cases, we most often have **an incomplete model if we build a model from first principles** according to Steps 1 -4 of the SEVEN STEP MODELLING PROCEDURE.

- The reason for this is that we **rarely have a complete model together with all the parameter values for all of the controlling mechanisms** involved.

- An example of this is a case when we have **complicated reaction kinetics**, where we rarely have all the reaction kinetic parameters given in the literature or measured independently and often the form of the reaction **kinetic expression is only partially known.**

Grey-box Models

- **Grey-box Models** is used in contrast to the so-called empirical or black-box models where the model is **built largely from measured data using model parameter and/or structure estimation techniques**.

- The opposite case is the case of white-box models **where the model is constructed only from first engineering principles** with all its ingredients known as a well-defined set of equations which is mathematically solvable.

- In practice, of course, **no model is completely "white" or "black"** but all of them are "grey", since practical models are somewhere in between.

- Process models developed using first engineering principles but with part of their model parameters and/or structure unknown is termed as **grey-box models**.

Model Calibration

- We **often do not have available values** of the model parameters and part of the model structure.

- Therefore, we want to obtain these **model parameters and structural elements using experimental data from the real process**.

- Because measured data contains measurement errors, we can only estimate the missing model parameters and structural elements. This estimation step is called **Statistical Model Calibration**.

- The **model calibration** is performed using
  - the developed grey-box model by the steps 1-4 of the SEVEN STEP MODELLING PROCEDURE,
  - measured data from the real process system which we call **calibration data**,
  - a predefined measure of fit, which measures the quality of the process model **with its missing parameters and estimated structural elements**.

Conceptual Steps of Model Calibration

- In realistic model calibration, there are other important steps which one should carry out besides just a simple model parameter and structure estimation.

- These steps are needed to check and to transform the grey-box model and the measured data **to a form suitable for the statistical estimation and then to check the quality of the obtained model**.

- These conceptual steps to be carried out when doing model calibration are as follows:

1. Analysis of model specification

- Here, we have to **consider all of the ingredients of our grey-box process model** to determine which parameters and/or structural elements need to be estimated **to make the process model equations solvable for generating their solution** for dynamic models.

- This step may involve a DOF analysis and the analysis of the non-measurement data available for the model building.

2. Sampling of continuous time dynamic models

- Statistical procedures use a discrete set of measured data and a model. To get an estimate, we need **to discretize our grey-box process models** to be able to estimate its parameters and/or structural elements

3. Data analysis and preprocessing

- Measurement data from a real process system are usually of varying quality. We may have data with outliers or large measurement errors **due to some malfunctions in the measurement devices** or **unexpectedly large disturbances**.

- From the viewpoint of good quality estimates **it is vital to detect and remove data of unacceptable quality.**

4. Model parameter and structure estimation

5. Evaluation of the quality of the estimate

- The evaluation is done by using either empirical, usually graphical methods or by exact hypothesis testing if the mathematical statistical properties of the estimates are available.

- Model calibration is usually followed by model validation where we decide on **the quality of the model obtained by modelling and model calibration**.

- Model validation is in some sense similar to model calibration because here we **also use measured data, but another, independently measured data set** *(**validation data**) and also statistical* methods.

MODEL PARAMETER AND STRUCTURE ESTIMATION

- During model calibration we use the developed grey-box model and measured experimental data to obtain **a well-defined or solvable process model.**

- In the model validation step, we again use measured experimental data (**the validation data**) distinct from what has been applied for model calibration.

- We do this in two different ways:
  - to compare the **predicted outputs of the model** to the **measured data**, or
  - to compare the **estimated parameters of the model based on validation data to the "true'' or previously estimated parameters**.

STATISTICAL MODEL VALIDATION VIA PARAMETER ESTIMATION

- The principle of statistical model validation is to compare by the methods of mathematical statistics either
  - the (measured) **system output with the model output**, or
  - **the estimated system parameters with the model parameters**.

- In other words "validation" means "comparison" of

$$(y \text{ and } y_M) \quad \text{or} \quad (p \text{ and } p_M).$$

- Statistical methods are needed because the measured output y is corrupted by measurement (observation) errors

$$y = y^{(M)} + \varepsilon.$$

- The items of a model validation problem are as follows:
  - a developed and **calibrated process model**,
  - **measured data from the real process system** which we call validation data,
  - a predefined measure of fit, or **loss function which measures the quality of the process model**.

- The conceptual steps to be carried out when performing model validation are also similar to that of model calibration and include:

1. Analysis of the process model

This step may involve the analysis of the uncertainties in the calibrated process model and its **sensitivity analysis**. The results can be applied for designing experiments for the model validation.

2. Sampling of continuous time dynamic models

3. Data analysis and preprocessing

4. Model parameter and structure estimation

5. Evaluation of the quality

3.4. ANALYSIS OF DYNAMIC PROCESS MODELS

- **BASIC DYNAMICAL PROPERTIES: OBSERVABILITY CONTROLLABILITY, AND STABILITY**

State Observability

- The state variables of a system are not often directly observable.
- Therefore, we need to determine **the value of the state variables at any given time from the measured inputs and outputs** in such a way that we only use functions of inputs and outputs and their derivatives together with the known system model and its parameters.
- A system is called (state) observable, **if from a given finite measurement record of the input and output variables, the state variable can be reconstructed at any given time**.

State Controllability

- For process control purposes over a wide operation range, we need to drive a process system from its given initial state to **a specified final state**.

- A system is called (state) controllable **if we can always find an appropriate manipulable input function which moves the system from its given initial state to a specified final state in finite time**.

- This applies **for every given initial state to final state**.

Stability

- There are two related but different kinds of stability :
  - **BIBO stabilit**y which is also known as **external stability**,
  - **asymptotic stability**, known as **internal stability**

BIBO Stability

- The system is BIBO or externally stable **if it responds to any bounded-input signal with a bounded-output signal**.

Asymptotic or Internal Stability

- A solution to the state equation of a system is asymptotically stable **if a "neighbouring“ solution described by a different initial condition has the same limit as t $\rightarrow\infty$**.

MODEL SIMPLIFICATION AND REDUCTION

- The term "**model simplicity**" may have different meanings depending on the context and on the set of models we consider.
- A process model may be more simple than another one in terms of

  - **model structure**

    We can say, for example, that a **linear model** is simpler than a **nonlinear one**.

  - **model size**

- For process models of the same type of structure (for example both linear) the model size can be measured in **the number and dimension of model variables and parameters.**
- Most often the number of the input and output variables **are fixed by the problem statement**, therefore, the number of state variables and that of parameters play a role.

Simplification of Linear Process Models

- The model simplification can be carried out in a graphical way using two basic simplification operations:

  - **variable removal** by assuming steady state,
  - **variable coalescence** by assuming similar dynamics.

- With these two elementary transformations, we can simplify a process model structure by applying them consecutively in any required order.

Elementary Simplification Transformations

- The elementary transformations of model structure simplification are as follows.

  1. **Variable lumping: lump(xj, *xl)***

  Applicability conditions: We can lump two state variables X_j and x_l together to form a lumped state variable if they have "similar dynamics", that is,

$$x_j(t) = Kx_\ell(t), \quad K > 0.$$

2. **Variable removal: remove(xj)**

- Applicability conditions:

  We can remove a state variable Xj from the structure graph if it **is either changing much faster or much slower than the other variables**.

  Note that a "perfect" controller forces the variable under control to follow the setpoint infinitely fast, therefore **a controlled variable can almost always be removed from the structure graph**.

  In both cases the time derivative of the variable to be removed is negligible, that is,

$$\frac{\mathrm{d}x_j(t)}{\mathrm{d}t} = 0 \quad \Rightarrow \quad x_j(t) = \text{constant}.$$

- **EXAMPLE((Variable lumping and variable removal of the three jacketted CSTR in series model.**

- Simplify the structure graph of the system by:

  1. lumping of all the cooling water temperatures together,
  2. removing all the cooling water temperatures.

Variable lumping

- We may assume that the temperature state variables belonging to the cooling water subsystem, i.e.

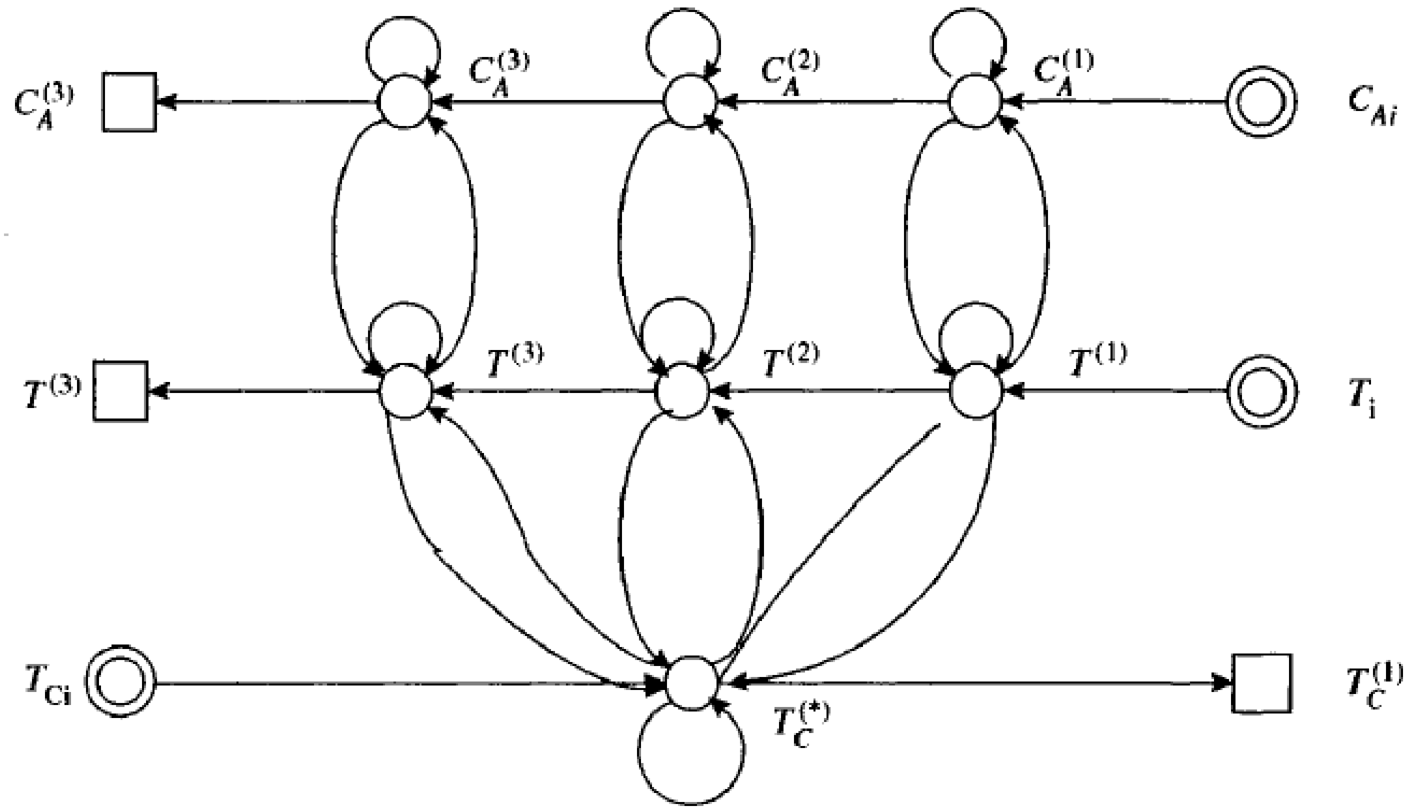
$$T_{\mathrm{C}}^{(1)},\ T_{\mathrm{C}}^{(2)},\ T_{\mathrm{C}}^{(3)}$$

  have similar dynamical behaviour with respect to changes in the manipulated input and disturbance variables.

- Therefore, we can form a lumped cooling water temperature T_C^* from them by applying the variable lumping transformation twice:

$$T_{\mathrm{C}}^{(*)} = \mathrm{lump}\left(T_{C}^{(1)}, \mathrm{lump}(T_{C}^{(2)}, T_{C}^{(3)})\right)$$

- The resultant structure graph is shown in Fig below.



- **Simplified structure graph of three jacketted CSTRs by variable removal.**

Variable removal

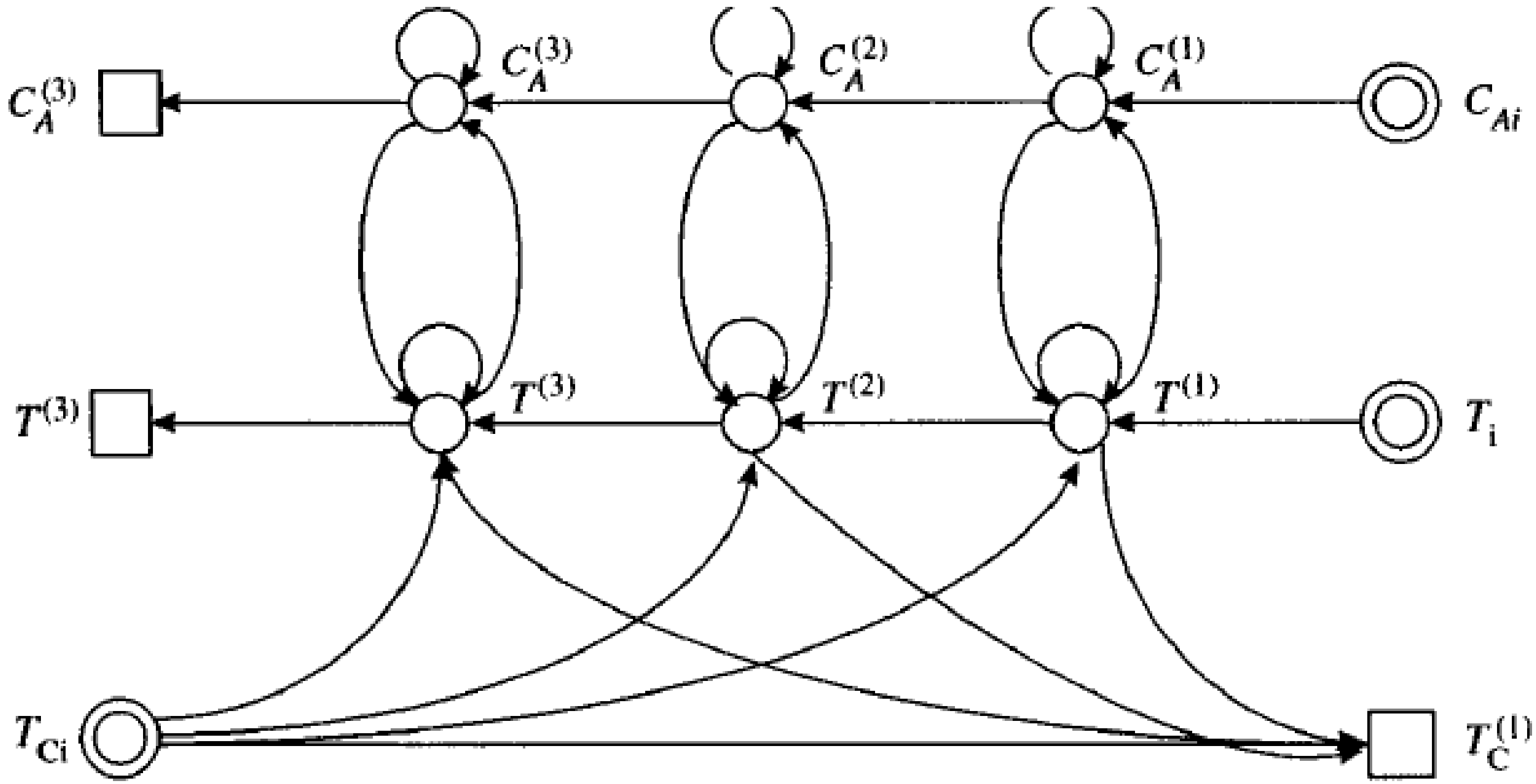
- For a cooling system with **large overall heat capacity**, we can assume that the temperature state variables belonging to the cooling water subsystem

$$T_C^{(1)},\ T_C^{(2)},\ T_C^{(3)}$$

are in quasi-steady state and are **regarded as constants**. Therefore, we can remove them from the structure graph by applying the variable removal transformation three times:

$$\text{remove}\left(T_C^{(1)}\right) \circ \text{remove}\left(T_C^{(2)}\right) \circ \text{remove}\left(T_C^{(3)}\right).$$

- The resultant structure graph is shown in the next Fig.



Simplified structure graph of three jacketted CSTRs by variable removal