Process Dynamics and Control

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Chapter Two

Theoretical Models of Chemical Processes

- Mathematical Modeling is a mathematical abstraction of a real process.
- It is at best approximation of real process.
- To analyze the behavior of a process, a mathematical representation of the physical and chemical phenomenon taking place in it..
- The activities leading to the construction of the model is called modeling.

The main uses of mathematical modeling are:

- To improve understanding of the process
- To train plant operating personal
- To design control strategy for new plant
- To select controller settings
- To design the controller law
- To optimize process operating conditions

Six-step modeling procedure

- Define goals
- Prepare information
- Formulate the model
- Determine the solution
- Analyze results
- Validate the model

We apply this procedure

- to many physical systems
- overall material balance
- component material balance
- energy balances

Examples of variable selection

- liquid level $\rightarrow$ total mass in liquid
- pressure $\rightarrow$ total moles in vapor
- temperature $\rightarrow$ energy balance
- concentration $\rightarrow$ component mass

- **Overall Material Balance**:
- Accumulation of mass= Mass in - Mass out
- **Component Material Balance**:
- Accumulation of component mass= Component mass in - Component mass out + Generation of component mass
- **State variables** is a set of fundamental quantities whose value describe the natural state of a given system.
- **State equations** is a set of equations in the variables which describe how the natural state of the given system change with time.

- Modeling objectives is to describe process dynamics based on the laws of conservation of mass, energy and momentum.
  - Mass Balance (Stirred tank)
  - Energy Balance (Stirred tank heater)
  - Momentum Balance (Car speed)
- Degree of Freedom: $Nf = Nv - Ne$; where
  - NV is the total number of process variables, and
  - NE is the number of independent equations.

Mathematical Modeling of Common Chemical Processes

General balances taken in mathematical modeling

- Total Mass Balance

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} = \sum_i \rho_i F_i - \sum_j \rho_j F_j$$

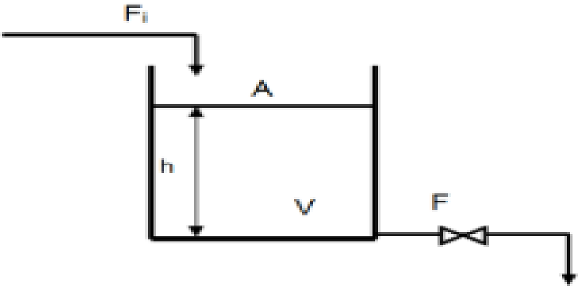
- Component Balance on A

$$\frac{dn_A}{dt} = \frac{d(C_A V)}{dt} = \sum_i C_{Ai} F_i - \sum_j C_{Aj} F_j \pm r_A V$$

- Total Energy Balance

$$\frac{dE}{dt} = \frac{d(U + K + P)}{dt} = \sum_i \rho_i F_i h_i - \sum_j \rho_j F_j h_j \pm Q$$

1) Mathematical Model: Surge tank (Liquid)



- Modeling objective: Control of tank level
- Assumptions: Incompressible flow

✓ Total mass balance:

$$\frac{dm}{dt} = \sum m_i - \sum m_0$$

$$\Rightarrow \frac{d(\rho V)}{dt} = \rho_i q_i - \rho_0 q \quad \text{but} \quad \rho_i = \rho_0 = \rho$$

$$\Rightarrow \rho \frac{dV}{dt} = \rho(q_i - q)$$

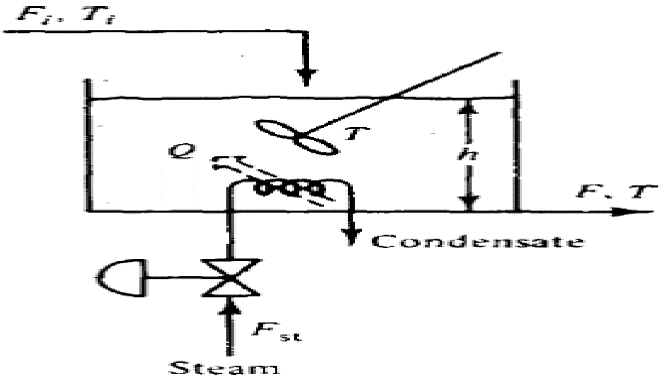
$$\Rightarrow \frac{dV}{dt} = q_i - q$$

✓ This is the dynamic model of surge tank in liquid.

✓ To calculate degree of freedom

- NV = 5(A, h, q, q_i, ρ)
- Parameter: 2(A, ρ)
- Inputs: 2(q, q_i)
- Equation: 1
- $DF = NV - NE = 4 - (1 + 2 + 2) = 0$
- It has unique solution.

2) Mathematical Model: A Stirred Tank Heater



- Modeling objective: Control of tank level and temperature
- Assumptions: Incompressible flow, $T_{ref} = 0$

Modeling objective:

- Control of tank level and temperature

Assumptions:

- Incompressible flow,
- $T_{ref} = 0$

Total mass balance:

$$\frac{dm}{dt} = \sum \dot{m}_i - \sum \dot{m}_o$$

$$\Rightarrow \frac{d(\rho V)}{dt} = \rho_i F_i - \rho_o F \quad \text{but} \quad \rho_i = \rho_o$$

$$\Rightarrow \rho \frac{dV}{dt} = \rho(F_i - F)$$

$$\Rightarrow A \frac{dh}{dt} = F_i - F \text{ ------------------(1)}$$

Total energy balance:

$$\frac{dE}{dt} = \sum \dot{E}_i - \sum \dot{E}_0 + Q$$

$$\Rightarrow \frac{dE}{dt} = \sum m_i h_i - \sum m_o h_o + Q$$

$$\Rightarrow \frac{d(mC_p(T-Tr))}{dt} = \sum(m_i C_p T_i) - \sum m_o C_p T) + Q$$

$$\Rightarrow \frac{d(\rho V C_p T)}{dt} = \rho F_i C_p T_i - \rho F C_p T + Q$$

$$\Rightarrow \rho C_p \frac{d(VT)}{dt} = \rho C_p [F_i T_i - FT] + Q$$

$$\Rightarrow \frac{VdT}{dt} + \frac{TdV}{dt} = F_i T_i - FT + \frac{Q}{\rho C_p}$$

By substituting equation (1) in eq. (2)

$$\Rightarrow \frac{VdT}{dt} + T(F_i - F) = F_iT_i - FT + \frac{Q}{\rho C_p}$$

$$\Rightarrow \frac{VdT}{dt} = F_i(T_i - T) + \frac{Q}{\rho C_p}$$

$$\Rightarrow \frac{dT}{dt} = \frac{F_i}{V}(T_i - T) + \frac{Q}{\rho V C_p} \text{ ----------- } (3)$$

- The two state equations are:

$$\frac{dV}{dt} = F_i - F$$

$$\frac{dT}{dt} = \frac{F_i}{V}(T_i - T) + \frac{Q}{\rho V C_p}$$

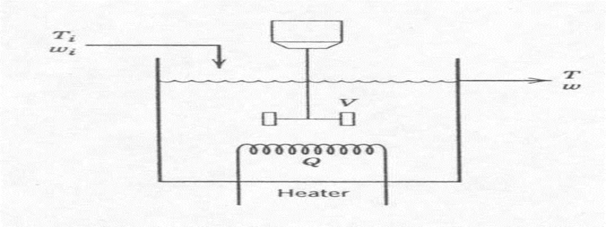
- State variables are: h, T
- Parameters are: A, C_p, ρ

- Model Consistency:
- Variables = 9 (A, C_p, ρ, F_i,Ti, Q, F, h, T)
- Equations = 2
- Constants = 3(A, C_p, ρ)
- Inputs = 4 (F_i,Ti, Q, F)
- Unknowns = 2 (h, T)
- Degree of freedom = NV − NE

$$= 9 - (2 + 3 + 4) = 0$$

➢It has unique solution.

3) Mathematical Model: A Stirred Tank Heater



- Modeling objective: Control of tank level and temperature
- Assumptions: Incompressible flow, $T_{ref} = 0$
- Perfect mixing; thus, the exit temperature T is also the temperature of the tank contents.
- The inlet and outlet flow rates are equal; thus, the liquid holdup V is constant.
- The density ρ and heat capacity C of the liquid are assumed to be

Modeling objective:

- Control of tank temperature

Assumptions:

- Incompressible flow,
- $T_{ref} = 0$

Total mass balance:

$$\frac{dm}{dt} = \sum m_i - \sum m_0$$

$$\Longrightarrow \frac{d(\rho V)}{dt} = \rho_i w_i - \rho_0 w \quad \text{but} \quad \rho_i = \rho_0$$

$$\Longrightarrow \rho \frac{dV}{dt} = \rho(w_i - w)$$

$$\Longrightarrow A \frac{dh}{dt} = w_i - w$$

$$\Longrightarrow 0 = w_i - w$$

$$\Longrightarrow w_i = w \text{ ------------------(1)}$$

Total energy balance:

$$\frac{dE}{dt} = \sum E_i - \sum E_0 + Q$$

$$\Rightarrow \frac{dE}{dt} = \sum m_i h_i - \sum m_o h_o + Q$$

$$\Rightarrow \frac{d(mC_p(T-Tr))}{dt} = \sum(m_i C_p Ti) - \sum mC_p T) + Q$$

$$\Rightarrow \frac{d(\rho V C_p T)}{dt} = \rho w_i C_p T_i - \rho w C_p T + Q$$

$$\Rightarrow \rho C_p \frac{d(VT)}{dt} = \rho C_p [w_i T_i - wT] + Q$$

$$\Rightarrow \frac{VdT}{dt} + \frac{TdV}{dt} = w_i T_i - wT + \frac{Q}{\rho C_p}$$

By substituting eq. (1) in eq. (2)

$$\Rightarrow \frac{VdT}{dt} + 0 = w_i T_i - wT + \frac{Q}{\rho C_p}$$

$$\Rightarrow \frac{dT}{dt} = \frac{w}{V}(T_i - T) + \frac{Q}{\rho V C_p} \text{------} (3)$$

- The two state equation is:

$$\frac{dT}{dt} = \frac{w}{V}(T_i - T) + \frac{Q}{\rho V C_p}$$

- State variables is: T
- Parameters are: A, C_p, ρ

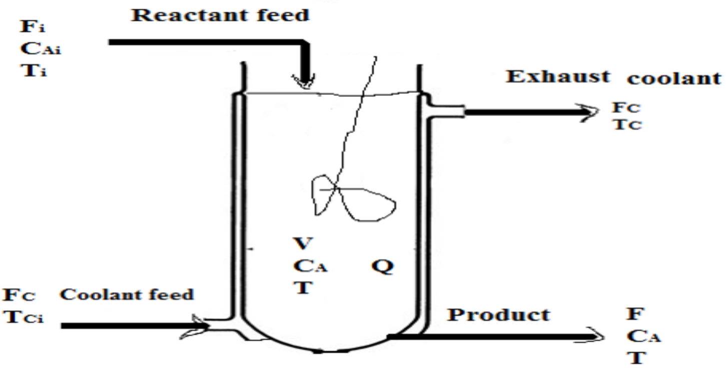
- Model Consistency:
- Variables = 9 (A, C_p, ρ, w_i, w, Ti, Q, h, T)
- Equations = 1
- Constants = 4(A, C_p, ρ, h)
- Inputs = 4 (w_i,Ti, Q, w)
- Unknowns = 1 (T)
- Degree of freedom = NV − NE

$$= 9 - (1 + 4 + 4) = 0$$

- It has unique solution.

- The effluent flow rate F can be considered either as input or output.
- If there is a control valve on the effluent stream so that its flow rate can be manipulated by a controller, the variable
- F is an input, since the opening of the valve is adjusted externally, otherwise F is an output variable.

4) Mathematical Model: A Stirred Tank Heater in jacketed Consider a simple liquid phase, non-isothermal, irreversible, exothermic reaction: $A \rightarrow B$ where $r_A = kC_A^{\alpha}$, $\triangle H_r = -\lambda$ kJ/kmol and the state variables are V, C_A, T, T_c.



The balance performed are

- Total mass balance
- Component balance on A
- Energy balance inside the reactor
- Energy balance around the reactor

The assumption taken are

- First degree
- reference temperature is zero
- constant density
- constant specific heat capacity
- exothermic reaction

❖ The dynamics behavior of the process

A) From total mass balance, V

$$\Rightarrow \frac{dm}{dt} = \dot{m}_i - \dot{m} = \sum \rho_i F_i - \sum \rho_j F$$

$$\Rightarrow \frac{d(\rho V)}{dt} = \rho(F_i - F)$$

$$\Rightarrow \frac{dV}{dt} = F_i - F \text{ ---------------------------(1)}$$

B) From component balance, C_A

$$\frac{dn_A}{dt} = \sum \dot{n}_{Ai} - \sum \dot{n}_A - V(-r_A)$$

$$\Rightarrow \frac{d(VC_A)}{dt} = F_i C_{Ai} - FC_A - VkC_A$$

$$\Rightarrow \frac{VdC_A}{dt} + \frac{C_A dV}{dt} = F_i C_{Ai} - FC_A - VkC_A$$

By substituting equation (1)

$$\Rightarrow \frac{VdC_A}{dt} + C_A(F_i - F) = F_i C_{Ai} - FC_A - VkC_A$$

$$\Rightarrow \frac{VdC_A}{dt} + F_i C_A = F_i C_{Ai} - VkC_A$$

$$\Rightarrow \frac{dC_A}{dt} = \frac{Fi}{V}(C_{Ai} - C_A) - kC_A \text{ ------------------(2)}$$

C) Energy balance inside the reactor, T

$$\frac{dE}{dt} = \sum m_i h_i - \sum m_j h_j + \lambda V(-r_A) - Q$$

$$\Rightarrow \frac{d(mC_p(T-Tr))}{dt} = \sum(m_i C_p Ti) - \sum(m_j C_p T) + \lambda V k C_A - Q$$

$$\Rightarrow \frac{d(\rho V C_p T)}{dt} = \rho F_i C_p T_i - \rho F C_p T + \lambda V k C_A - Q$$

$$\Rightarrow \frac{d(\rho V C_p T)}{dt} = \rho F_i C_p T_i - \rho F C_p T + \lambda V k C_A - Q$$

$$\Rightarrow \frac{VdT}{dt} + \frac{TdV}{dt} = F_i T_i - FT + \lambda VkCA - \frac{Q}{\rho C_p}$$

$$\Rightarrow \frac{VdT}{dt} + T(F_i - F) = F_i T_i - FT + \frac{\lambda VkCA}{\rho C_p} - \frac{Q}{\rho C_p}$$

$$\Rightarrow \frac{dT}{dt} = \frac{F_i}{V}(T_i - T) + \frac{\lambda kCA}{\rho C_p} - \frac{Q}{\rho V C_p} \text{-----------------------} (3)$$

D) Energy balance around the reactor, T_c

$$\frac{dE}{dt} = \sum m_{ic}h_{ic} - \sum m_{jc}h_{jc} + Q$$

$$\Rightarrow \frac{d(m_c C_{pc}(T_c - Tr))}{dt} = \sum(m_{ic}C_{pc}(T_{ci} - Tr)) - \sum(m_{jc}C_{pc}(T_c - Tr)) + Q$$

$$\Rightarrow \rho_c C_{pc}\frac{d(V_c T_c)}{dt} = \rho_c C_{pc}(F_{ic}Tci - F_c T_c) + Q$$

$$\Rightarrow \rho_c C_{pc}(\frac{dT_c}{dt} + \frac{d(V_c)}{dt}) = \rho_c C_{pc}(F_{ic}Tci - F_c T_c) + Q$$

$$\Rightarrow \rho_c C_{pc}\frac{dT_c}{dt} = \rho_c C_{pc}(F_{ic}Tci - F_c T_c) + Q$$

$$\Rightarrow \frac{dT_c}{dt} = F_{ic}Tci - F_c T_c + \frac{Q}{\rho_c C_{pc}} \text{-----------------------------------} (4)$$

➢The state equations are:

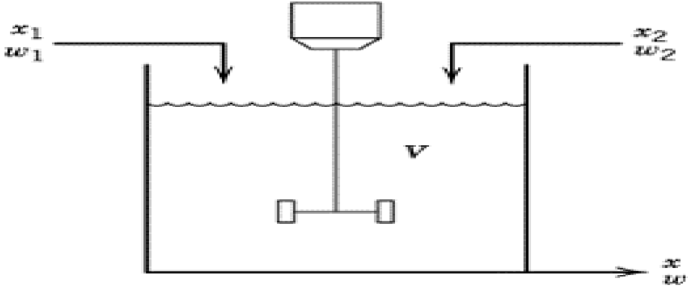
- $\frac{dV}{dt} = F_i - F$
- $\frac{dC_A}{dt} = \frac{Fi}{V}(C_{Ai} - C_A) - kC_A$
- $\frac{dT}{dt} = \frac{F_i}{V}(Ti - T) + \frac{\lambda k C_A}{\rho C_p} - \frac{Q}{\rho V C_p}$
- $\frac{dT_c}{dt} = \frac{F_c}{Vc}(T_{ci} - T_c) + \frac{Q}{V_c \rho_c C_{pc}}$

➢State variables are: V, C_A, T and T_C

➢Degree of freedom

- Variables = 19 (V, Fi, F, C_A, C_{Ai}, k, T, Ti, λ, C_p, ρ, ρ_c, C_{pc}, Q, Tc, Tci, Fci, Fc, Vc)
- Equations = 4
- Constants = 8(F_c, V_c, C_p, ρ, ρ_c, C_{pc}, λ, k)
- Inputs = 7 (F_i, Ti, Tci, C_{Ai}, Fci, Q, F)
- DF = 19 − (4 + 8 + 7) = 0
- It has unique solution.

5) Mathematical Model: A Blending Process stirred-tank system



Develop the dynamics behavior of the process

The dynamics behavior of the process

A) From total mass balance, V

$$\Rightarrow \frac{dm}{dt} = \sum w_i \ - \sum w$$

$$\Rightarrow \frac{d(\rho V)}{dt} = (w_1 + w_2 - w)$$

$$\Rightarrow \frac{dV}{dt} = \frac{1}{\rho}(w_1 + w_2 - w) \text{ ------------------------------(1)}$$

B) From component balance, C_A

$$\frac{d(\rho V x)}{dt} = w_1 x_1 + w_2 x_2 - wx$$

$$\Rightarrow \rho\left(\frac{xdV}{dt} + \frac{Vdx}{dt}\right) = w_1 x_1 + w_2 x_2 - wx$$

$$\Rightarrow \rho\left(x\left(\frac{1}{\rho}(w_1 + w_2 - w)\right) + \frac{Vdx}{dt}\right) = w_1 x_1 + w_2 x_2 - wx$$

$$\Rightarrow \rho V\frac{dx}{dt} + x(w_1 + w_2 - w) = w_1 x_1 + w_2 x_2 - wx$$

$$\Rightarrow \rho V\frac{dx}{dt} = w_1(x_1 - x) + w_2(x_2 - x)$$

$$\Rightarrow \frac{dx}{dt} = \frac{w_1}{\rho V}(x_1 - x) + \frac{w_2}{\rho V}(x_2 - x) \text{ --------------------------(2)}$$

Example 1: A stirred-tank blending process shown in figure below with a constant liquid holdup is used to blend two streams whose densities (which does not change during mixing) are both approximately $250 kg/m^3$. Assume that the process has been operating for a long period of time with flow rates of $\omega_1 = 300$ kg/min and $\omega_2 = 200$ kg/min.

a) Develop the model that describes the dynamics behavior of the process.

b) What is the steady-state value of output flow rate w?

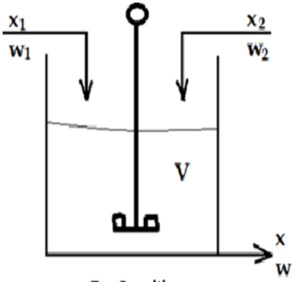
c) If the output flow rate is 400kg/min, then what is the volume of the tank at a period of 20 min?

d) If feed compositions (mass fractions) are $x_1 = 0.35$ and $x_2 = 0.55$, then what is the steady-state value of composition, x?

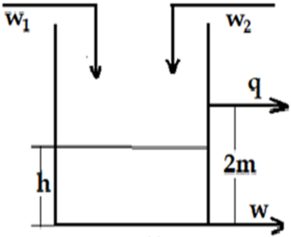
Example 2: The liquid storage tank shown in figure below has two inlet streams with mass flow rates ω_1 and ω_2 and an exit stream with flow rate w. The cylindrical tank is 6.5m tall and 2m in diameter. The liquid has a density of $800 kg/m^3$. Normal operating procedure is to fill the tank until the liquid level reaches a maximum value of the tank using constant flow rates: $\omega_1 = 250$kg/min, $\omega_2 = 150$kg/min and $\omega = 300$kg/min. Particular day, corrosion of the tank has opened up a hole in the wall at a height of 2m, producing a leak whose volumetric flow rate $q(m^3/min)$ can be approximated by: $q = 0.0625\sqrt{h-2}$ where h is height in meters.

a) If the tank was initially empty, then determine the time to reach leak point.

b) If mass flow rates ω_1, ω_2 and w are kept constant indefinitely, then determine the maximum value of liquid level when no overflow occurs



For Quesition 4



For Quesition 5

Modeling Difficulties:

- Poorly understood processes
- Imprecisely known parameters
- Size and complexity of a model