Modelling & Simulation of Chemical Engineering Systems

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LECTURE # 3
Examples of Lumped Parameter Systems

Last Lecture

- Conservation Laws; mass, momentum ,energy
- Assumptions
- Macroscopic & microscopic balances
- Transport rates
- Thermodynamic relations
- Phase Equilibrium
- Chemical kinetics
- Degree of Freedom
- Examples of Mathematical Models for Chemical Processes

Conservation Laws:
General Form

Conservation laws describe the variation of the amount of a "conserved quantity" within the system over time:

$$\begin{pmatrix} \text{rate of} \\ \text{accumulation} \\ \text{of conserved} \\ \text{quantity} \\ \text{within system} \end{pmatrix} = \begin{pmatrix} \text{rate of} \\ \text{flow of} \\ \text{conserved} \\ \text{quantity} \\ \text{into system} \end{pmatrix} - \begin{pmatrix} \text{rate of} \\ \text{flow of} \\ \text{conserved} \\ \text{quantity} \\ \text{from system} \end{pmatrix} + \begin{pmatrix} \text{rate of} \\ \text{generation of} \\ \text{conserved} \\ \text{quantity} \\ \text{within system} \end{pmatrix} \tag{1.1}$$

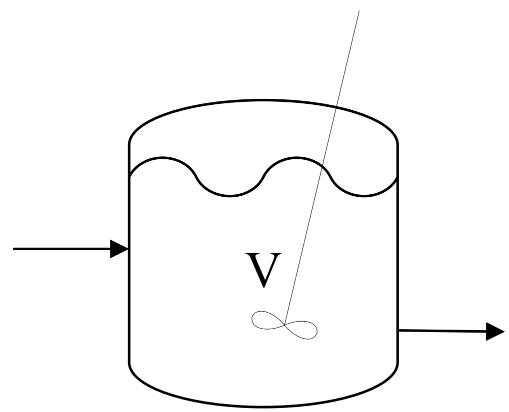
Conserved Quantities

Typical conserved quantities:

- Total mass (kg)
- Mass of an individual species (kg)
- Number of molecules/atoms (mol)
- Energy (J)
- Momentum (kg.m/s)

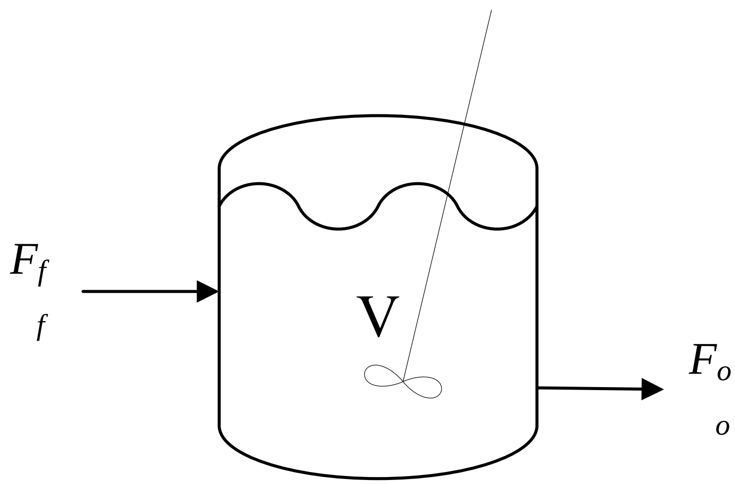
Examples of Mathematical Models for Chemical Processes
Lumped Parameter Systems

- Example 1. Liquid Storage Tank
- Our objective is to develop a model for the variations of the tank holdup, i.e. volume of the tank



Example 1. Liquid Storage Tank Assumptions

- Perfectly mixed (Lumped) → density of the effluent is the same as that of tank content.
- Isothermal



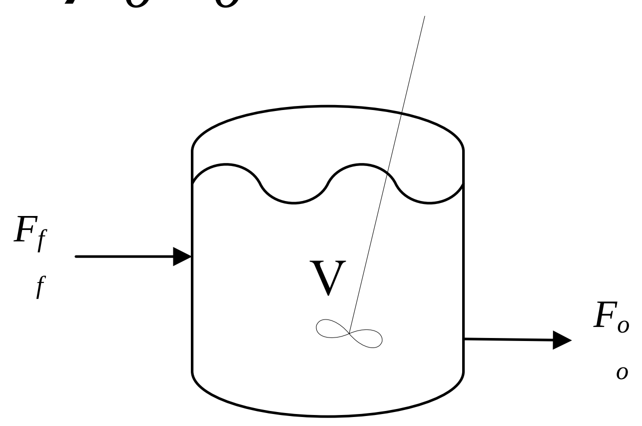
Example 1. Liquid Storage Tank Model

Rate of mass accumulation = Rate of mass in - rate of mass out

$$m\big|_{t+\Delta t} - m\big|_{t} = \rho_f F_f \Delta t - \rho_o F_o \Delta t$$

$$\lim \frac{m\big|_{t+\Delta t} - m\big|_{t}}{\Delta t} = \rho_f F_f - \rho_o F_o$$

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} = \rho_f F_f - \rho_o F_o$$



Example 1. Liquid Storage Tank Model

- Under isothermal conditions we assume that the density of the liquid is constant.

$$\frac{dV}{dt} = F_f - F_o$$

$$A\frac{dL}{dt} = F_f - F_o$$

Example 1. Liquid Storage Tank Model Degree of Freedom

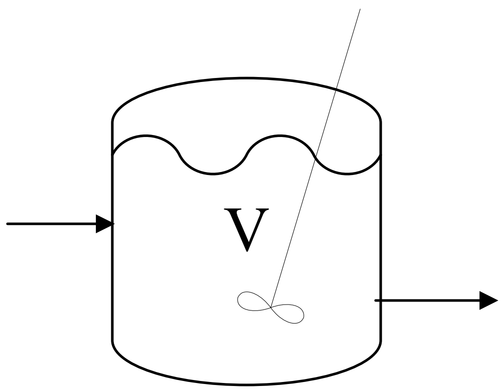
- Parameter of constant values: *A*
- Variables which values can be externally fixed (Forced variable): *Ff*
- Remaining variables: *L* and F_o
- Number of equations: 1
- Number of remaining variables – Number of equations = 2 – 1 = 1

$$F_o = \alpha\sqrt{L}$$

Example 2. Isothermal CSTR

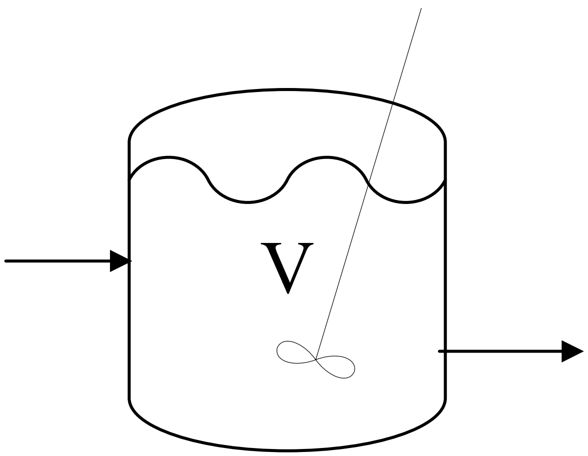
- Our objective is to develop a model for the variation of the volume of the reactor and the concentration of species *A* and *B*.
- a liquid phase chemical reactions taking place:

$$A \xrightarrow{k} B$$



Example 2. Isothermal CSTR：Assumptions

- Perfectly mixed
- Isothermal
- The reaction is assumed to be irreversible and of first order.



Example 2. Isothermal CSTR : Model

- Component balance
  - Flow of moles of *A* in:

$$F_f C_{Af}$$

  - Flow of moles of *A* out:

$$F_o C_{Ao}$$

  - Rate of accumulation:

$$\frac{dn}{dt} = \frac{d(VC_A)}{dt}$$

  - Rate of generation: $-rV$

where r ($moles/m^3 s$) is the rate of reaction.

Example 2. Isothermal CSTR : Model

$$\frac{d(VC_A)}{dt} = F_f\, C_{Af} - F_o\, C_A - rV$$

$$\frac{d(VC_A)}{dt} = V\frac{d(C_A)}{dt} + C_A\frac{d(V)}{dt} = F_f\, C_{Af} - F_o\, C_A - rV$$

$$V\frac{d(C_A)}{dt} = F_f(C_{Af} - C_A) - kC_AV$$

Example 2. Isothermal CSTR：Degree of Freedom

- Parameter of constant values: A
- (Forced variable): F_f and C_{Af}
- Remaining variables: V, Fo, and C_A
- Number of equations: 2
- The degree of freedom is

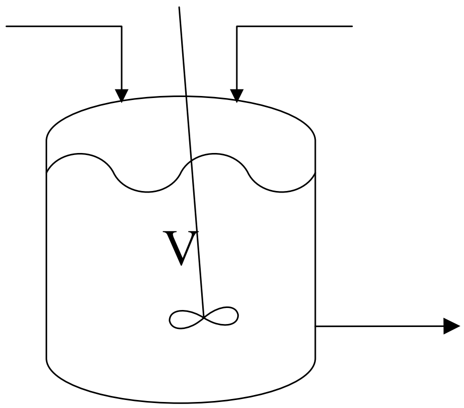
$$f = 3 - 2 = 1$$

The extra relation is obtained by the relation between the effluent flow Fo and the level in open loop

Example 3. CSTR Example

- $A + B \rightarrow P$
- Two streams are feeding the reactor. One concentrated feed with flow rate $F1$ ($m3/s$) and concentration $CB1$ ($mole/m3$) and another dilute stream with flow rate $F2$ ($m3/s$) and concentration $CB2$ ($mole/m3$). The effluent has flow rate Fo ($m3/s$) and concentration CB ($mole/m3$). The reactant A is assumed to be in excess.
- The reaction rate:

$$r = \frac{k_1 C_B}{(1 + k_2 C_B)^2} \qquad (mole/m^3.s)$$



Example 3. CSTR Example

- Assumptions: Isothermal, Constant density
- Total mass balance:

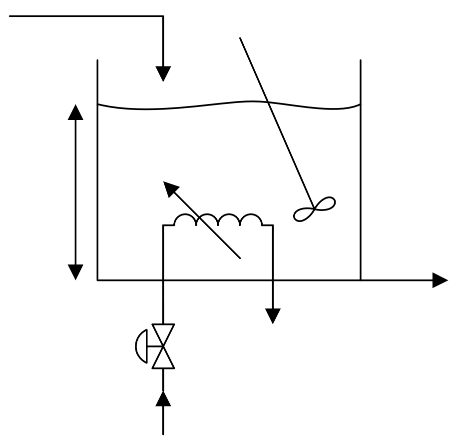
$$A\frac{dL}{dt} = F_1 + F_2 - F_o$$

- Component *B* balance:

$$V\frac{d(C_B)}{dt} = F_1(C_{B1} - C_B) + F_2(C_{B2} - C_B) - \frac{k_1 C_B}{(1 + k_2 C_B)^2}V$$

Example 4. Stirred Tank Heater

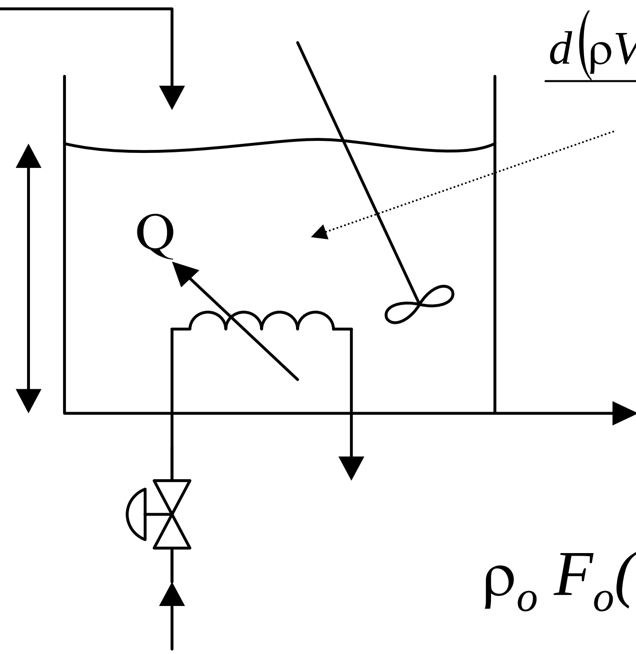
- The liquid enters the tank with a flow rate F_f (m^3/s), density ρ_f (kg/m^3) and temperature T_f (K). It is heated with an external heat supply of temperature T_{st} (K), assumed constant. The effluent stream is of flow rate F_o ($m3/s$), density ρ_o (kg/m^3) and temperature T(K). Our objective is to model both the variation of liquid level and its temperature



Example 4. Stirred Tank Heater

$\rho_f F_f(\tilde{U}_f + \tilde{K}_f + \tilde{\phi}_f)$

Flow work: $F_f P_f$



$$\frac{d\left(\rho V(\tilde{U} + \tilde{K} + \tilde{\phi})\right)}{dt}$$

F_f, T_f, ρ

$\rho_o F_o(\tilde{U}_o + \tilde{K}_o + \tilde{\phi}_o)$

Flow work: $F_o P_o$

the rate of energy generation is

$$Q_e + Q_r - (W_o + F_o P_o - F_f P_f)$$

L

Example 4. Stirred Tank Heater

$$\frac{d\left(\rho V(\tilde{U} + \tilde{K} + \tilde{\phi})\right)}{dt} = \rho_f F_f\left(\tilde{U}_f + \tilde{K}_f + \tilde{\phi}_f\right) - \rho_o F_o\left(\tilde{U}_o + \tilde{K}_o + \tilde{\phi}_o\right) + Q_e + Q_r - (W_o + F_o P_o - F_f P_f)$$

$$\frac{d\left(\rho V(\tilde{U} + \tilde{K} + \tilde{\phi})\right)}{dt} = \rho_f F_f\left(\tilde{U}_f + \tilde{K}_f + \tilde{\phi}_f\right) - \rho_o F_o\left(\tilde{U}_o + \tilde{K}_o + \tilde{\phi}_o\right) + Q_e + Q_r - W_o - F_o \rho_o \frac{P_o}{\rho_o} + F_f \rho_f \frac{P_f}{\rho_f}$$

$$\frac{d\left(\rho V(\tilde{U} + \tilde{K} + \tilde{\phi})\right)}{dt} = \rho_f F_f\left(\tilde{U}_f + P_f \tilde{V}_f + \tilde{K}_f + \tilde{\phi}_f\right) - \rho_o F_o\left(\tilde{U}_o + P_o \tilde{V}_o + \tilde{K}_o + \tilde{\phi}_o\right) + Q_e + Q_r - W_o$$

$$\frac{d\left(\rho V(\tilde{U} + \tilde{K} + \tilde{\phi})\right)}{dt} = \rho_f F_f\left(\tilde{h}_f + \tilde{K}_f + \tilde{\phi}_f\right) - \rho_o F_o\left(\tilde{h}_o + \tilde{K}_o + \tilde{\phi}_o\right) + Q_e + Q_r - W_o$$

Example 4. Stirred Tank Heater

- We can neglect kinetic energy unless the flow velocities are high.
- We can neglect the potential energy unless the flow difference between the inlet and outlet elevation is large.
- All the work other than flow work is neglected, i.e. $W_o = 0$.
- There is no reaction involved, i.e. $Q_r = 0$.

$$\frac{d\left(\rho V\widetilde{U}\right)}{dt} = \rho_f F_f \widetilde{h}_f - \rho_o F_o \widetilde{h}_o + Q_e$$

Example 4. Stirred Tank Heater

$$\tilde{h} = \tilde{C}p(T - T_{ref})$$

$$\rho\tilde{C}_p \frac{d\left(V(T - T_{ref})\right)}{dt} = \rho F_f \tilde{C}_p (T_f - T_{ref}) - \rho F_o \tilde{C}_p (T - T_{ref}) + Q_e$$

$$\rho\tilde{C}_p A \frac{d\left(LT\right)}{dt} = \rho F_f \tilde{C}_p T_f - \rho F_o \tilde{C}_p T + Q_e$$

$$A\frac{d\left(LT\right)}{dt} = AT\frac{d\left(L\right)}{dt} + AL\frac{d\left(T\right)}{dt}$$

$$AL\frac{dT}{dt} + T(F_f - F_o) = F_f T_f - F_o T + \frac{Q_e}{\rho\tilde{C}_p}$$

$$AL\frac{dT}{dt} = F_f (T_f - T) + \frac{Q_e}{\rho\tilde{C}_p}$$

Example 4. Stirred Tank Heater

- The stirred tank heater is modeled, then by the following coupled ODE's:

$$A\frac{dL}{dt} = F_f - F_o$$

$$AL\frac{dT}{dt} = F_f(T_f - T) + \frac{Q_e}{\rho\tilde{C}_p}$$

$$L(ti) = Li \qquad \text{and } T(ti) = Ti$$

Example 4. Stirred Tank Heater
Degree of Freedom

- Parameter of constant values: *A*, ρ *and Cp*
- (Forced variable): *Ff* and *Tf*
- Remaining variables: *L*, *Fo*, *T*, *Qe*
- Number of equations: 2
- The degree of freedom is therefore,

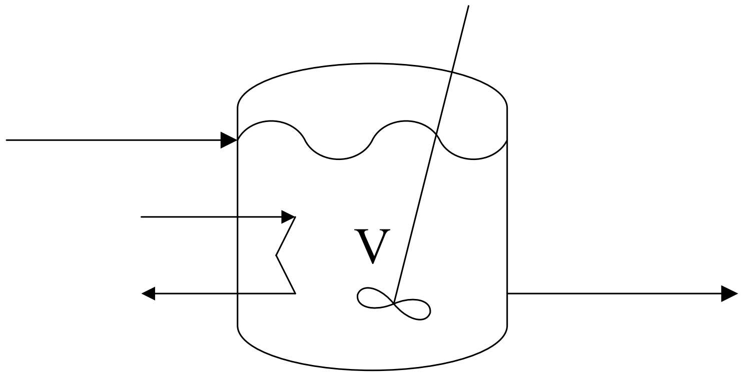
$$4 - 2 = 2$$

$$Qe = UA_H(Tst - T), \qquad F_o = \alpha\sqrt{L}$$

Example 5. Non-Isothermal CSTR

- The reaction A → B is exothermic and the heat generated in the reactor is removed via a cooling system as shown in figure 2.7. The effluent temperature is different from the inlet temperature due to heat generation by the exothermic reaction.
- The dependence of the rate constant on the temperature:

$$r = kC_A = k_o e^{-E/RT} C_A$$



Example 5. Non-Isothermal CSTR

- The general energy balance for macroscopic systems applied to the CSTR yields, assuming constant density and average heat capacity
- The rate of heat exchanged *Qr* due to reaction is given by:

$$Q_r = -(\Delta H_r)\ V\ r$$

$$\rho \tilde{C}_p \frac{d\left(V(T - T_{ref})\right)}{dt} = \rho F_f \tilde{C}_p (T_f - T_{ref}) - \rho F_o \tilde{C}_p (T - T_{ref}) + Q_r - Q_e$$

$$\rho \tilde{C}_p V \frac{dT}{dt} = \rho F_f \tilde{C}_p (T_f - T) + Q_r - Q_e$$

Example 5. Non-Isothermal CSTR

- The non-isothermal CSTR is modeled by three ODE's:

$$\frac{dV}{dt} = F_f - F_o$$

$$V \frac{d(C_A)}{dt} = F_f (C_{Af} - C_A) - rV$$

$$\rho \widetilde{C}_p V \frac{dT}{dt} = \rho F_f \widetilde{C}_p (T_f - T) + (-\Delta H_r) Vr - Q_e$$

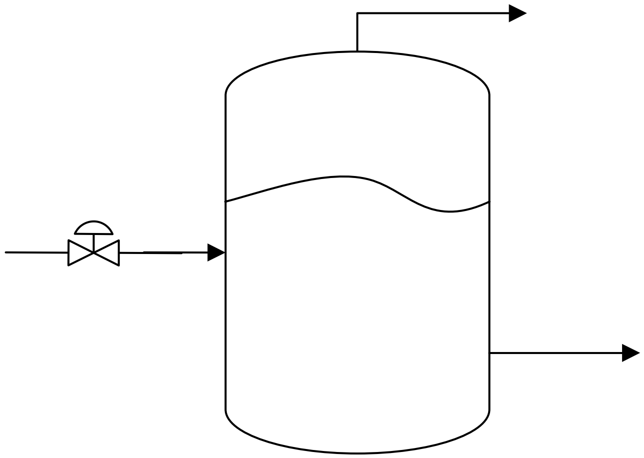
$$r = k_o e^{-E/RT} C_A$$

$$V(ti) = Vi \qquad T(ti) = Ti \qquad \text{and} \qquad CA(ti) = CAi$$

Example 6. Single Stage Heterogeneous Systems:

Multi-component flash drum

- A multi-component liquid-vapor separator. The feed consists of *Nc* components with the molar fraction z_i (i=1,2... *Nc*). The feed at high temperature and pressure passes through a throttling valve where its pressure is reduced substantially. As a result, part of the liquid feed vaporizes. The two phases are assumed to be in phase equilibrium.



Example 6. Single Stage Heterogeneous Systems: Multi-component flash drum

- Assumption: Since the vapor volume is generally small neglect the dynamics of the vapor phase and concentrate only on the liquid phase
- *For liquid phase:* Total mass balance:

$$\frac{d(\rho_L V_L)}{dt} = \rho_f F_f - \rho_L F_L - \rho_v F_v$$

- Component balance (*i=1,2,....,Nc*-1) :

$$\frac{d(\rho_L V_L x_i)}{dt} = \rho_f F_f z_i - \rho_L F_L x_i - \rho_v F_v y_i$$

- Energy balance:

$$\frac{d(\rho_L V_L \tilde{h})}{dt} = \rho_f F_f \tilde{h}_f - \rho_L F_L \tilde{h} - \rho_v F_v \tilde{H}$$

Example 6. Single Stage Heterogeneous Systems: Multi-component flash drum

- Liquid-vapor Equilibrium (*i=1,2,....,Nc*)
-

$$y_i = \frac{x_i P_i^s}{P}$$

$$\sum_{i=1}^{Nc} y_i = 1 \qquad \sum_{i=1}^{Nc} x_i = 1$$

- Physical Properties

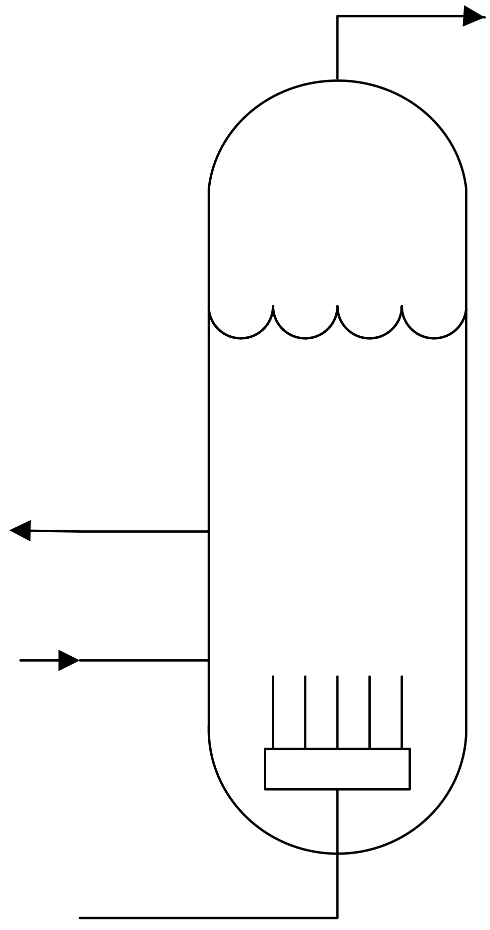
$\rho_L = f(xi, T, P)$ $\qquad \rho_V = f(yi, T, P)$

$h = f(xi, T)$ $\qquad H = f(yi, T)$

Example 7. Reaction with Mass Transfer

- The reactant *A* enters the reactor as a gas and the reactant *B* enters as a liquid. The gas dissolves in the liquid where it chemically reacts to produce a liquid *C*. The product is drawn off the reactor with the effluent *FL*. The un-reacted gas vents of the top of the vessel. The reaction mechanism is given as follows:

$$A + B \rightarrow C$$



Example 7. Reaction with Mass Transfer

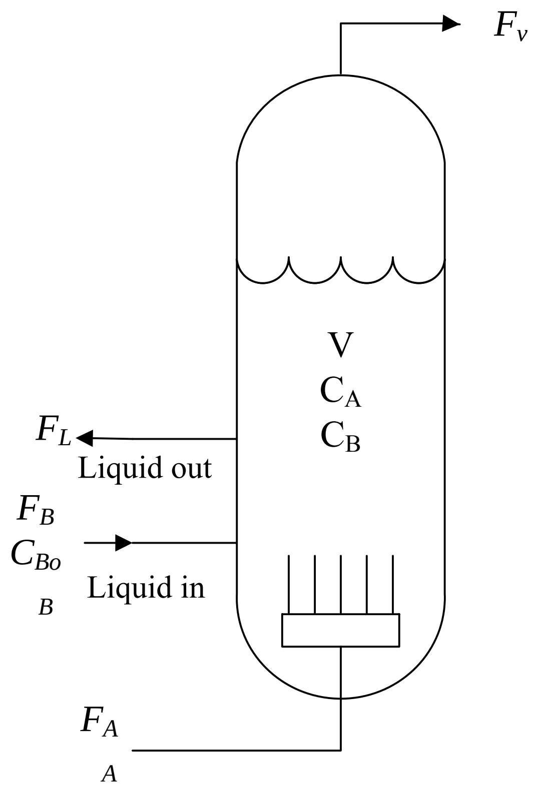
Assumptions:

- Perfectly mixed reactor
- Isothermal operation
- Constant pressure, density, and holdup.
- Negligible vapor holdup.
- mass transfer of component *A* from the bulk gas to the bulk liquid is approximated by the following molar flux:

$$N_A = K_L \left(C^*_A - C_A \right)$$

where K_L is mass transfer coefficient C_A^* is gas concentration at gas-liquid interface

C_A is gas concentration in bulk liquid



Example 7. Reaction with Mass Transfer

- ***Liquid phase:***

$$\frac{d\rho V}{dt} = \rho_B F_B + M_A A_m N_A - \rho F_L$$

$$V\frac{dC_A}{dt} = A_m N_A - F_L C_A - rV$$

$$V\frac{dC_B}{dt} = F_B C_{Bo} - F_L C_B - rV$$

Vapor phase:

$$Fv = F_A - M_A\, Am\, N_A/\rho_A$$