Lecture 3: Modelling Lumped Parameter Systems

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(Plus material from Ian Cameron)

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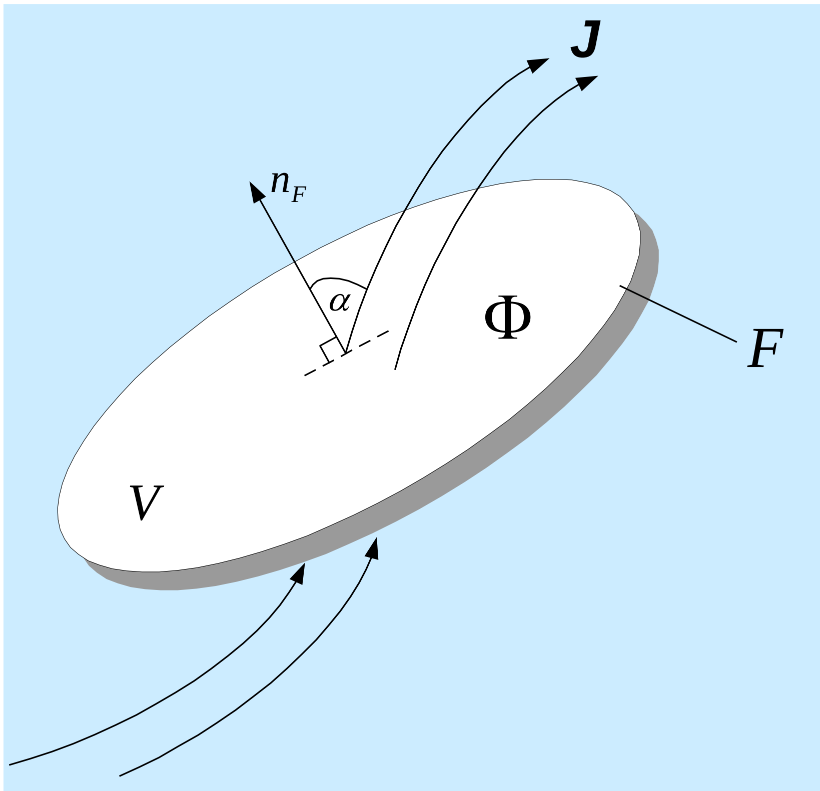
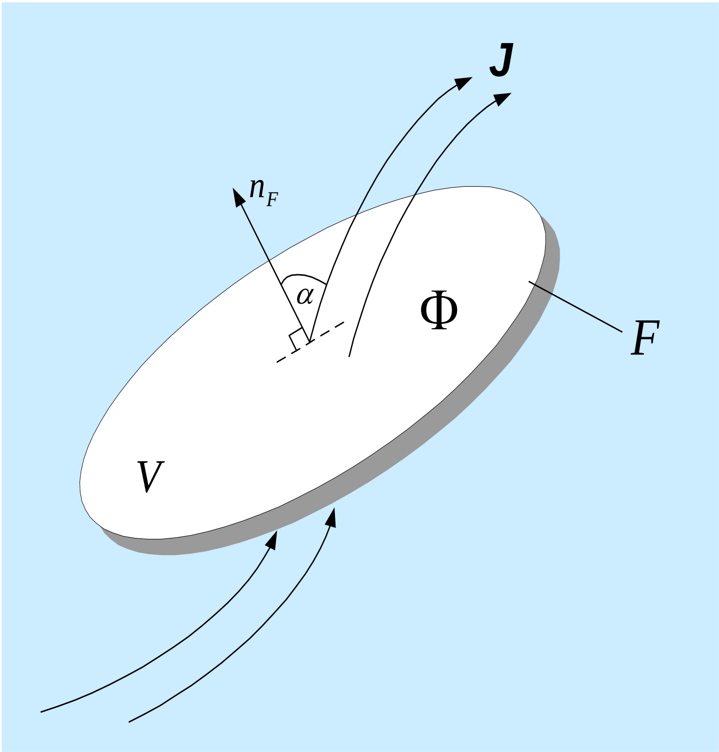
General 3D conservation space



Governing equation

$$\frac{\partial \Phi}{\partial t} = -\nabla \bullet J + q$$

General 3D conservation space



Governing equation

General differential form
where Φ can vary in space and time

$$\frac{\partial \hat{\Phi}}{\partial t} = -\nabla \bullet J + \hat{q}$$

Governing equation

Lumped form where Φ does *not* vary in space but varies in time

$$\frac{d\Phi}{dt} = \Delta J_C + q$$

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The lumped conservation balance

General conservation balance

$$\frac{d}{dt}\left\{\int_v \hat{\Phi}(r,t)dv\right\} = -\oint_F J(r,t)\bullet n_F(r)df + \int_V \hat{q}(r,t)dv$$

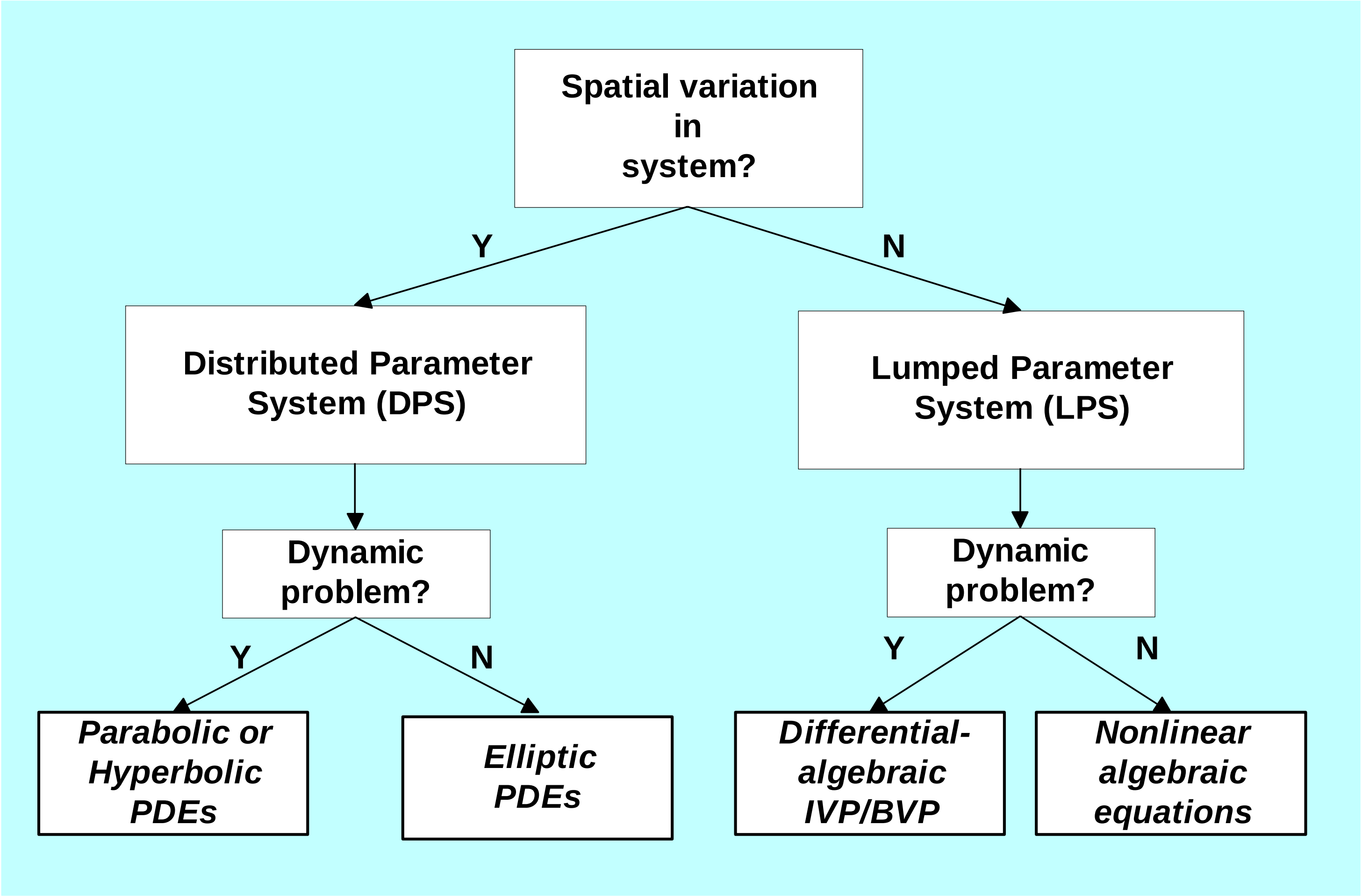
Assuming homogeneity in the conserved quantity

$$\frac{d}{dt}\left\{\hat{\Phi}\int_v dv\right\} = \Delta J + \hat{q}\int_V dv \longrightarrow \frac{d}{dt}\left\{\hat{\Phi}V\right\} = \Delta J + \hat{q}V$$

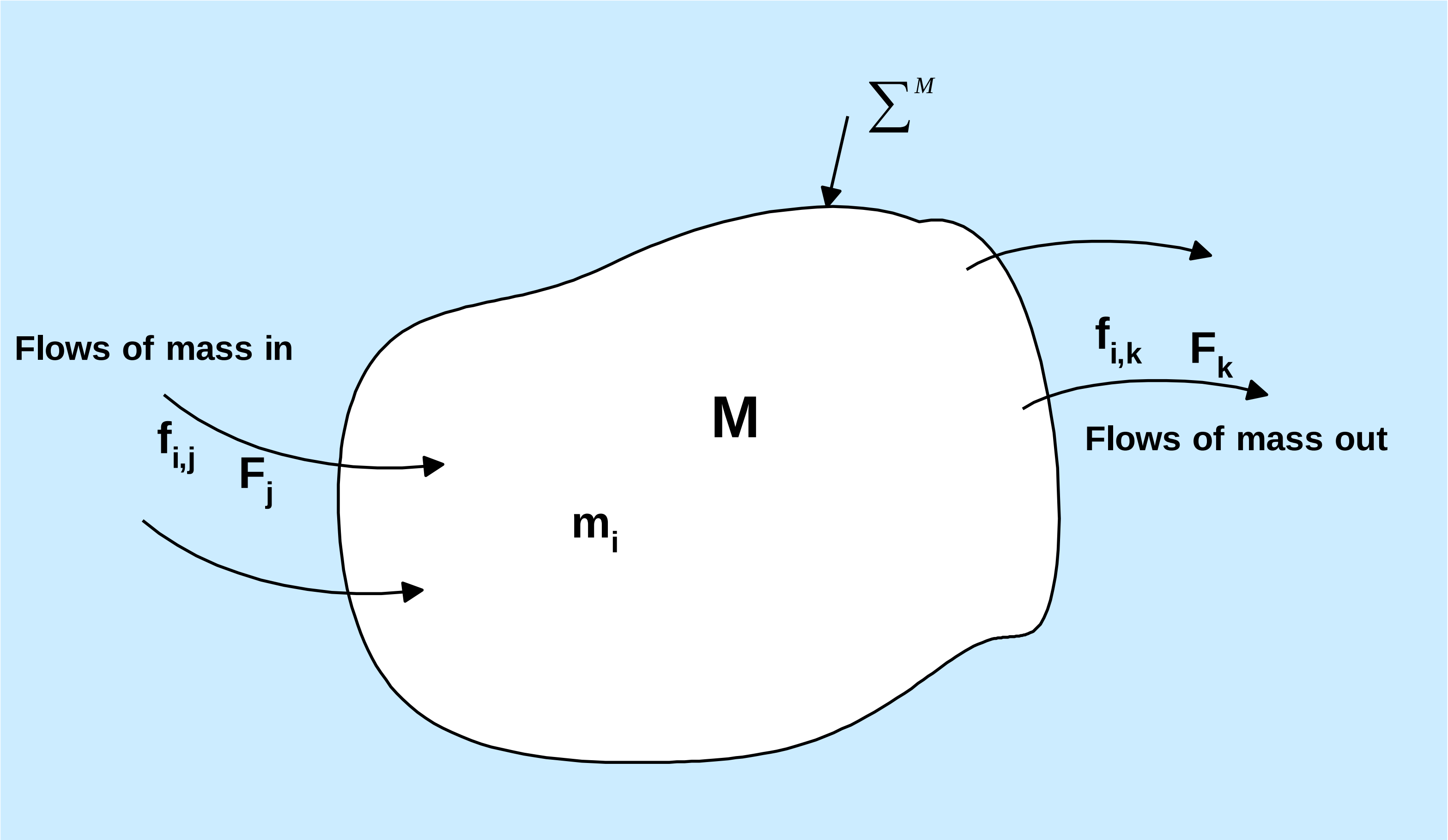
Lumped conservation balance

$$\frac{d}{dt}\Phi = \Delta J + q$$

Model Characteristics

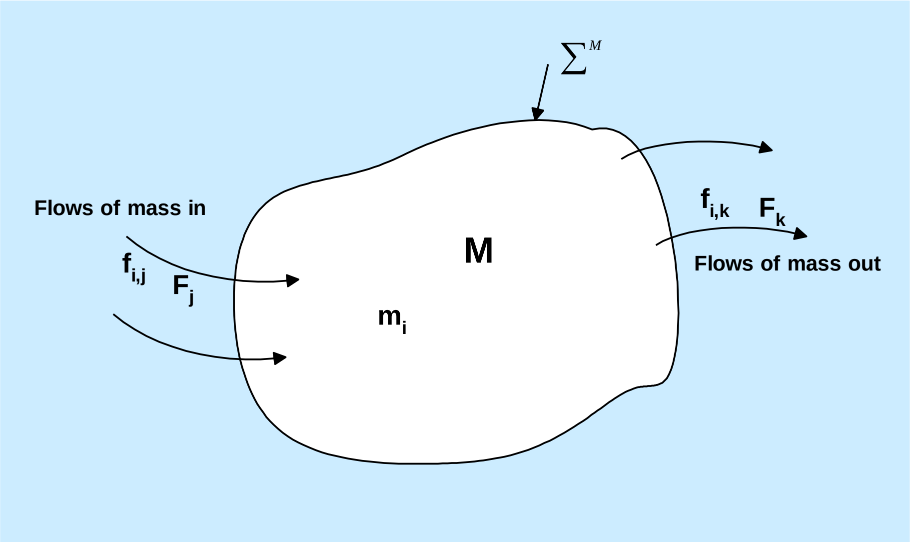


The mass balance volume



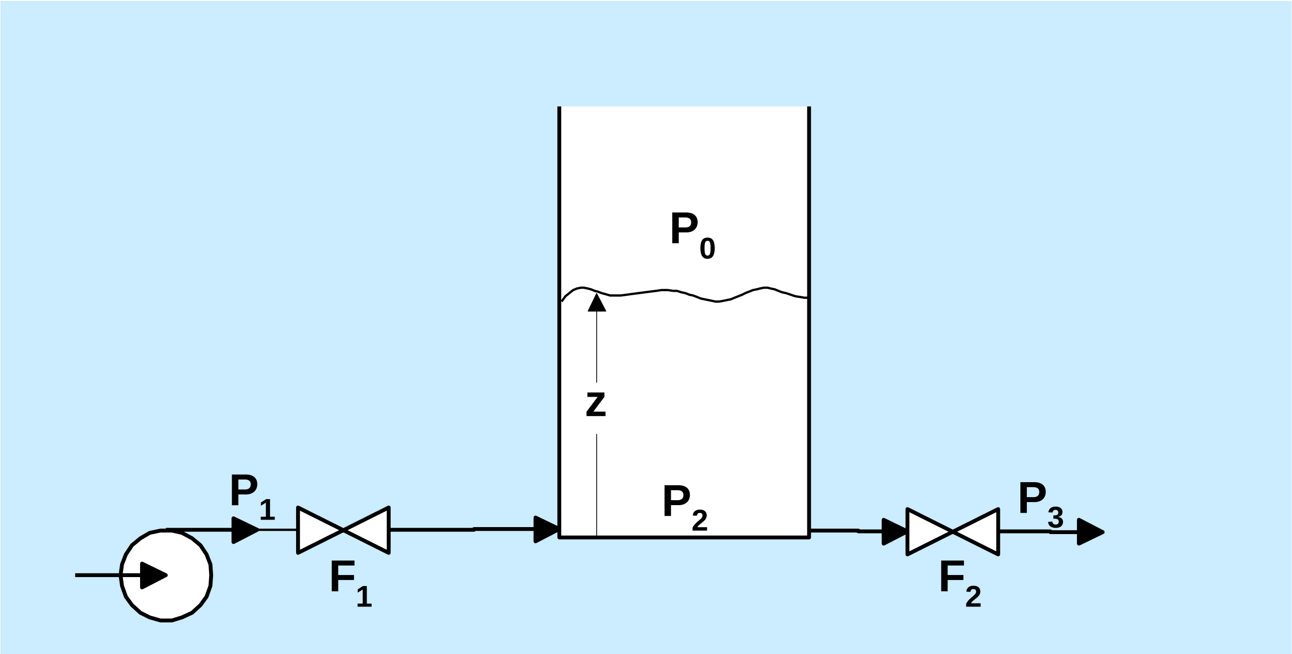
Overall mass balance

$$\left\{\begin{matrix}\text{rate of change}\\ \text{of total mass}\end{matrix}\right\} = \left\{\begin{matrix}\text{flow of mass}\\ \text{into the system}\end{matrix}\right\} - \left\{\begin{matrix}\text{flow of mass}\\ \text{out of the system}\end{matrix}\right\}$$

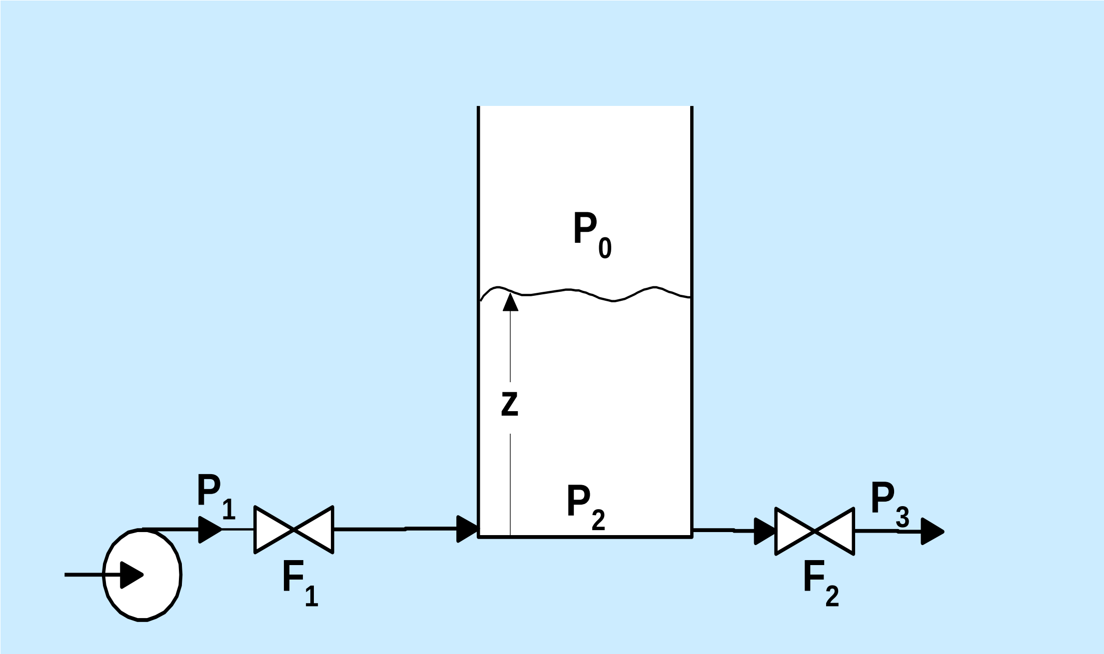


$$\frac{dM}{dt} = \sum_{j=1}^{p} F_j - \sum_{k=1}^{q} F_k$$

A Process Example



A Process Example



$$\frac{dz}{dt} = \frac{(F_1 - F_2)}{A}$$

$$F_1 - C_V \sqrt{P_1 - P_2} = 0$$

$$F_2 - C_V \sqrt{P_2 - P_3} = 0$$

$$P_2 - P_0 - \rho g z = 0$$

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Component mass balances

$$\begin{Bmatrix}\text{rate of change of} \\ \text{mass of species}\ i\end{Bmatrix} = \begin{Bmatrix}\text{mass flow of species}\ i \\ \text{into the system}\end{Bmatrix} - \begin{Bmatrix}\text{mass flow of species}\ i \\ \text{out of the system}\end{Bmatrix} + \begin{Bmatrix}\text{generation or consumption} \\ \text{of species}\ i\ \text{in volume}\end{Bmatrix}$$

$$\frac{dm_i}{dt} = \sum_{j=1}^{p} f_{i,j} - \sum_{k=1}^{q} f_{i,k} + g_i \qquad i = 1, \ldots n$$

Molar Balance

Mass balances that involve reactions are most conveniently expressed as molar balances, i.e.,

$$\frac{dn_i}{dt} = \sum_{j=1}^{p} \tilde{f}_{i,j} - \sum_{k=1}^{q} \tilde{f}_{i,k} + \tilde{g}_i \qquad i = 1, \ldots\ldots, n$$

where $\tilde{g}_i$ is the rate of generation or consumption of species *i* through reaction, i.e.,

$$\tilde{g}_i = r_i \left[\frac{moles}{m^3 .\text{sec}} \right] V \left[m^3 \right]$$

where

$r_i = rate\ of\ \ generation\ of\ \ species\ i$

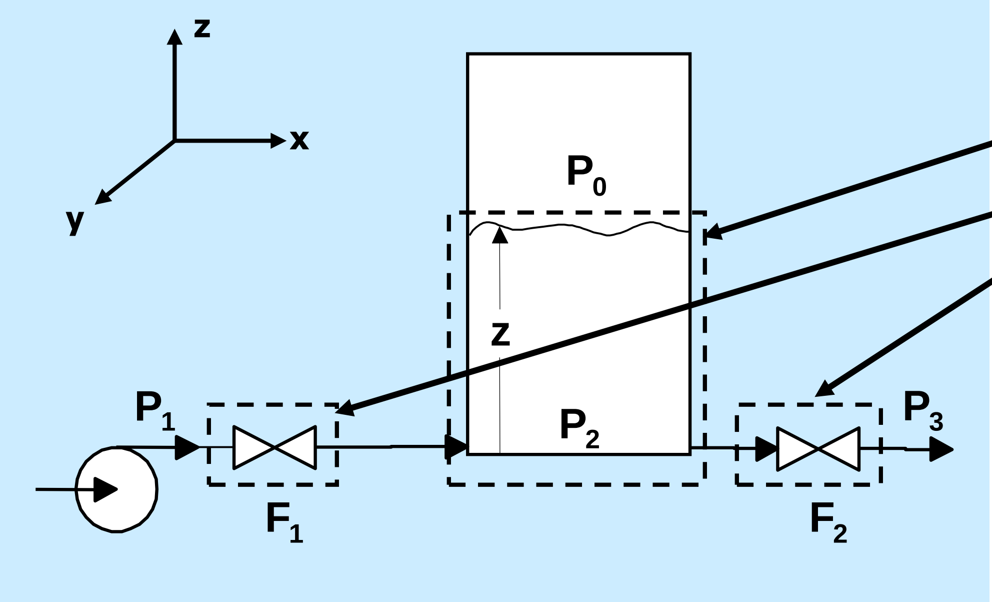
$\quad = \nu_i\, r$

where

$\nu_i = stochiometric\ coefficient$

$r = overall\ reaction\ rate$

Tank mass balance



Balance volumes

- **tank holdup**
- **valves**

Conservation

$$\frac{dM}{dt} = F_1 - F_2$$

Constitutive

$$F_1 = C_V \sqrt{P_1 - P_2}$$

$$F_2 = C_V \sqrt{P_2 - P_3}$$

$$P_2 = P_0 + \rho g z$$

$$z = M / A\rho$$

Assumptions

A1: Well mixed in x,y,z directions

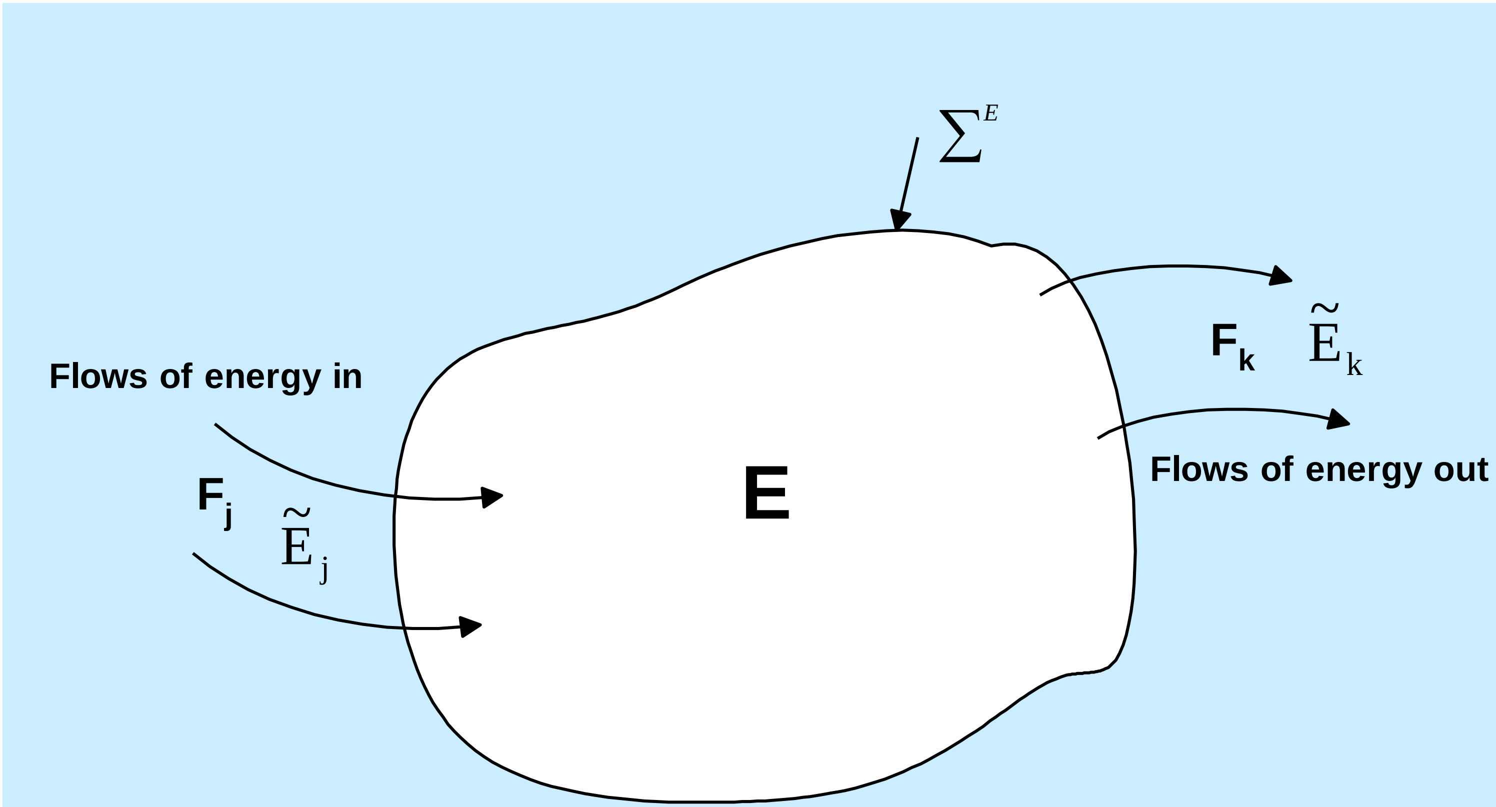
A2: no mass holdup in valves

A3: no physical losses from system

A4: no mass losses from evaporation

A5: Isothermal operation

The energy balance volume



Energy balance

$$\left\{\begin{array}{l}\text{rate of change}\\ \text{of total energy}\end{array}\right\} = \left\{\begin{array}{l}\text{flow of energy}\\ \text{into the system}\end{array}\right\} - \left\{\begin{array}{l}\text{flow of energy}\\ \text{out of the system}\end{array}\right\}$$

Components of the balance

- Convective energy flows
- Conductive/radiative flows
- Work terms

Energy Balance Terms

- Convective flows → $\sum_{j=1}^{p} F_j(\hat{U} + \hat{K}_E + \hat{P}_E)_j$

  $\sum_{k=1}^{q} F_j(\hat{U} + \hat{K}_E + \hat{P}_E)_k$

- Heat flows → $Q = Q_C + Q_R$

- Work terms
  - shaft work → W_S
  - expansion work → $W_E = -\iiint_V P(r,t)dV = -P\frac{dV}{dt}$
  - flow work → $W_F = \sum_{j=1}^{p} F_j(P\hat{V})_j - \sum_{k=1}^{q} F_k(P\hat{V})_k$

Total energy balance

$$\frac{dE}{dt} = \sum_{j=1}^{p} F_j \hat{E}_j - \sum_{k=1}^{q} F_j \hat{E}_k + Q + W$$

$$\frac{dE}{dt} = \sum_{j=1}^{p} F_j (\hat{U} + \hat{K}_E + \hat{P}_E)_j - \sum_{k=1}^{q} F_k (\hat{U} + \hat{K}_E + \hat{P}_E)_k + Q + \left\{ \sum_{j=1}^{p} F_j (P\hat{V})_j - \sum_{k=1}^{q} F_k (P\hat{V})_k + W_E + W_S \right\}$$

$$\frac{dE}{dt} = \sum_{j=1}^{p} F_j (\hat{H} + \hat{K}_E + \hat{P}_E)_j - \sum_{k=1}^{q} F_k (\hat{H} + \hat{K}_E + \hat{P}_E)_k + Q + \hat{W}$$

Reduced energy balances

❖ Neglect P_E, K_E

$$\frac{dU}{dt} = \sum_{j=1}^{p} F_j \hat{H}_j - \sum_{k=1}^{q} F_k \hat{H}_k + Q + \hat{W}$$

❖ PV constant or small

$$\frac{dU}{dt} = \frac{d(H - PV)}{dt} = \sum_{j=1}^{p} F_j \hat{H}_j - \sum_{k=1}^{q} F_k \hat{H}_k + Q + \hat{W}$$

$$\frac{dH}{dt} = \sum_{j=1}^{p} F_j \hat{H}_j - \sum_{k=1}^{q} F_k \hat{H}_k + Q + \hat{W}$$

❖ Output specific enthalpies equivalent to bulk phase

$$\frac{dH}{dt} = \sum_{j=1}^{p} F_j \hat{H}_j - \sum_{k=1}^{q} F_k \hat{H} + Q + \hat{W}$$

Reduced energy balances (cont.)

- **all enthalpies evaluated at system temperature**

$$\hat{H}_j(T_j) = \hat{H}_j(T) + c_{P_j}(T_j - T)$$

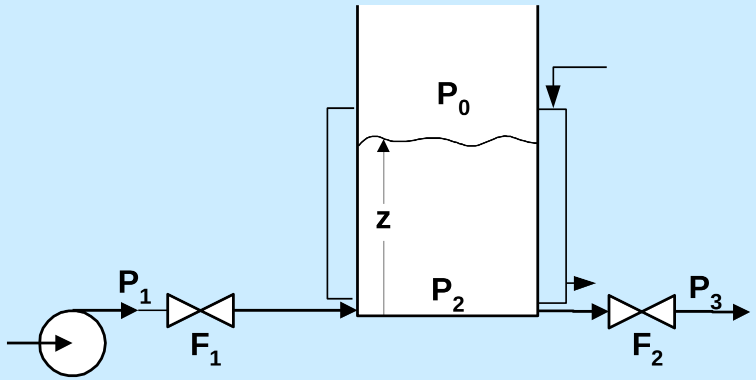
$$\frac{dH}{dt} = \sum_{j=1}^{p} F_j\left[\hat{H}_j(T) + c_{P_j}(T_j - T)\right] - \sum_{k=1}^{q} F_k \hat{H}(T) + Q + \hat{W}$$

- **explicit appearance of reaction terms and temperature**

$$V\rho c_P \frac{dT}{dt} = \sum_{j=1}^{p} F_j c_{P_j}(T_j - T) + rV(-\Delta H_R) + Q + \hat{W}$$

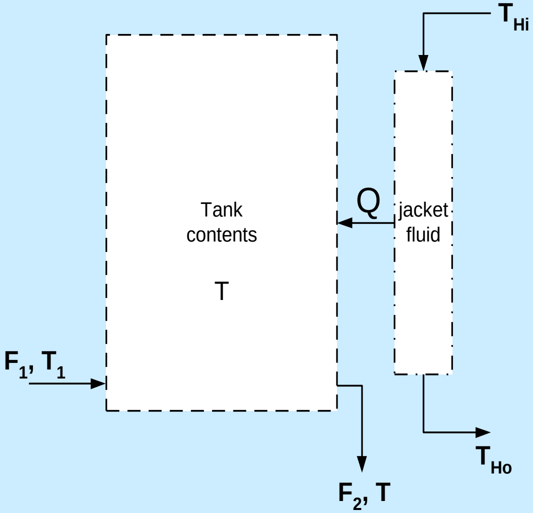
Note: $H = M\, c_p\, T$

Tank energy balance



Balance volumes

- **tank holdup**
- **jacket holdup**



Assumptions

A5: Fixed mass holdup in jacket

A6: well mixed jacket contents

A7: negligible KE terms

A8: negligible PE terms

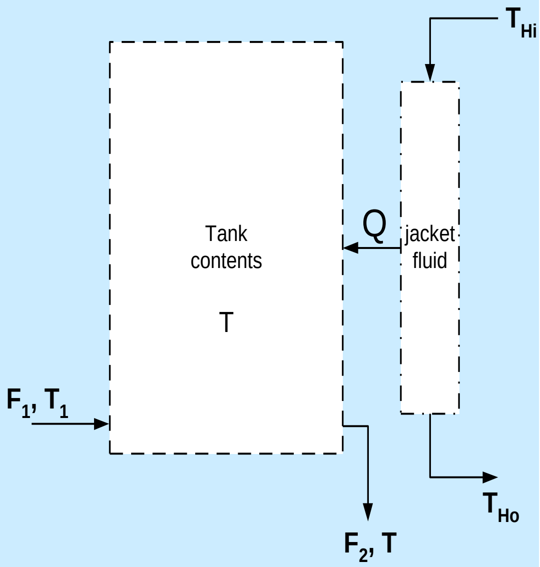
A9: negligible PV terms

A10: jacket temperature is averaged

A11: fixed heat capacities

Tank energy balances

System



Tank

Conservation

$$\frac{dH}{dt} = Q + F_1\hat{h}_1 - F_2\hat{h}_2$$

Constitutive

$$Q = UA(T_H - T)$$

$$\hat{h}_1 = f(T_1, P)$$

$$\hat{h}_2 = f(T_2, P)$$

$$H = Mc_P T$$

$$A = \pi D z$$

Jacket

Conservation

$$\frac{dH_J}{dt} = F_H\hat{h}_{Hi} - F_H\hat{h}_{Ho} - Q$$

Constitutive

$$Q = F_H c_{PH}(T_{Hi} - T_{Ho})$$

$$\hat{h}_{Hi} = f(T_{Hi}, P)$$

$$\hat{h}_{Ho} = f(T_{Ho}, P)$$

$$H_J = M_{HJ} c_{PH} T_H$$

$$T_H = (T_{Hi} + T_{Ho})/2$$

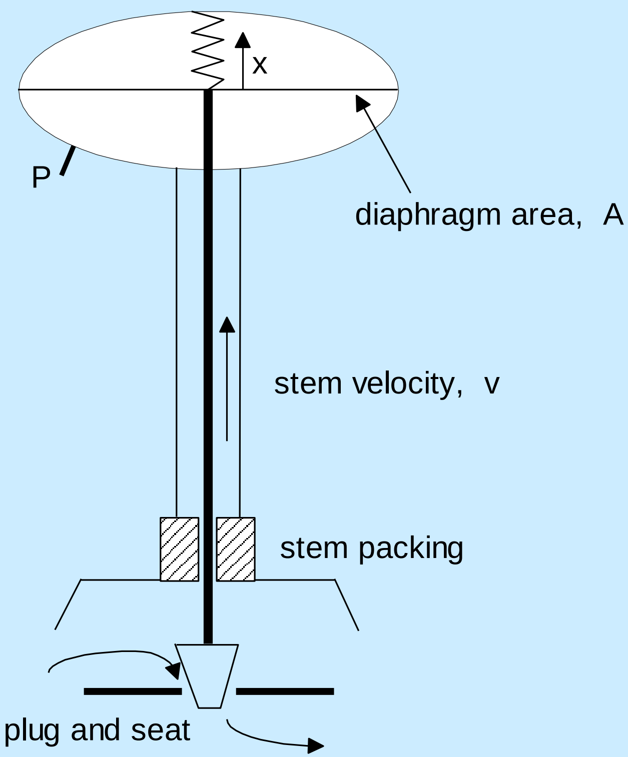
Momentum balance

$$\left\{\begin{array}{l}\text{rate of change}\\ \text{of momentum}\end{array}\right\} = \left\{\begin{array}{l}\text{rate of momentum}\\ \text{into the system}\end{array}\right\} - \left\{\begin{array}{l}\text{rate of momentum}\\ \text{out of the system}\end{array}\right\}$$

$$\left\{\begin{array}{l}\text{sum of all forces}\\ \text{on the system}\end{array}\right\}$$

$$\frac{dM}{dt} = M^{(i)} - M^{(o)} + \sum_{i=1}^{s} F_i$$

Example momentum balance



$$\frac{d\mathrm{M}}{dt} = \frac{d(Mv)}{dt} = F_D - F_S - F_P$$

$$M\frac{dv}{dt} = PA - kx - cv$$

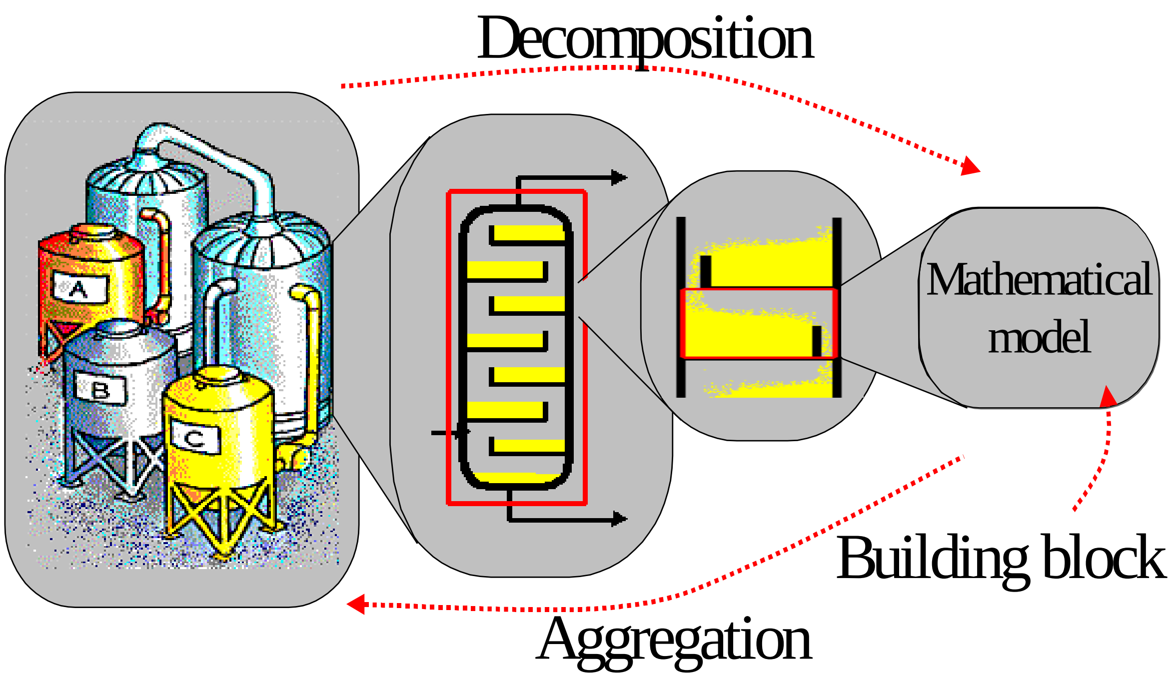
$$\left(\frac{M}{k}\right)\frac{d^2x}{dt^2} + \left(\frac{c}{k}\right)\frac{dx}{dt} + x = \left(\frac{PA}{k}\right)$$

$$\tau^2\frac{d^2x}{dt^2} + 2\xi\tau\frac{dx}{dt} + x = K$$

Incremental modelling practice

- Model mass balances first → test model
- Add energy balance as needed → test model
- Add control loops one at a time → tune & test
- Test overall integrated model
- Fully document model
  - Goal and assumptions
  - Balance volume diagrams
  - Parameter values and data references
  - Equation development
  - Test data and model performance
- Use model for intended application area

Model Construction - Generation



Three Classes of Equations

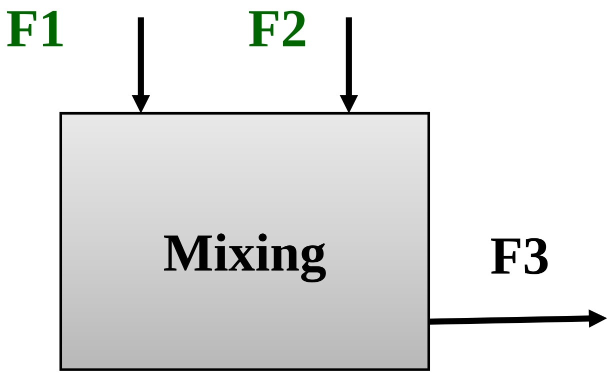
*** Balance Equations**

***Constraint Equations**

***Constitutive Equations**

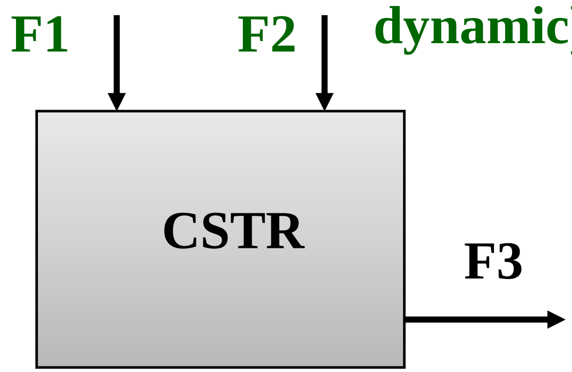
Incremental modelling: Develop a reference (generic) model & then use it multiple times or aggregate them

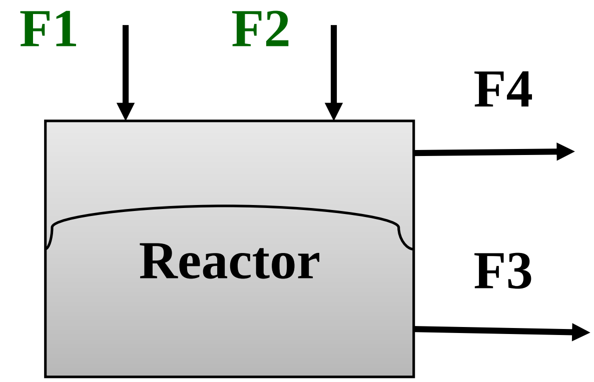
Modelling exercise -3: Incremental modelling



3a-1: Model the operation of a single phase mixer (first steady state & then dynamic)

3a-2: Add reaction A + B → C + D to the models of 4a (first steady state & then dynamic)





3a-3: Add option for one or two-phases (vapour-liquid) in equilibrium with or without reaction (first steady state & then dynamic)