Lecture 2: Model Building Framework

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(Plus material from Ian Cameron)

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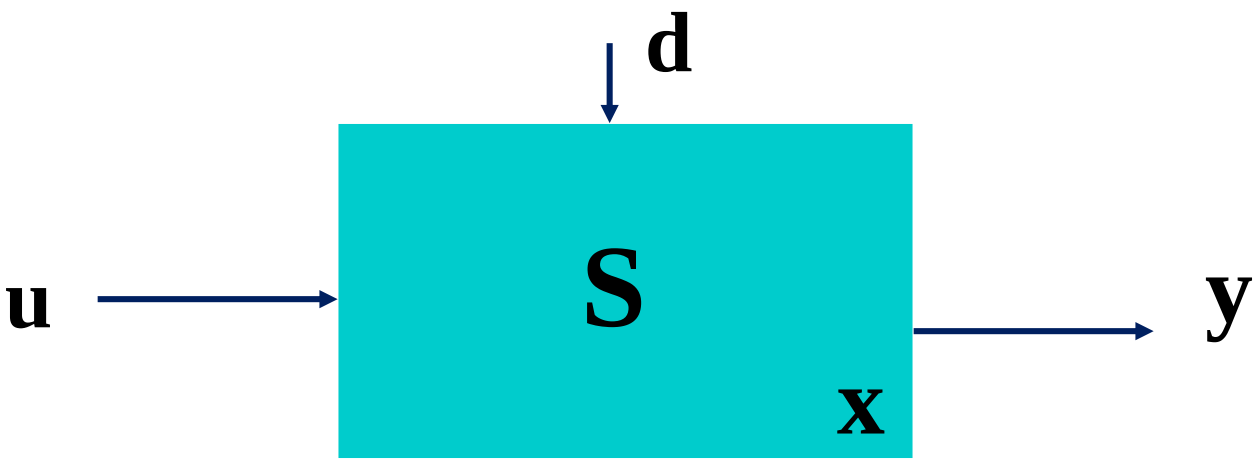
This lecture consists of 3 parts

- Modelling framework (lecture 2)
- Conservation principles (lecture 2a)
- Constitutive & conditional models (lecture 2b)

Overview: Lecture 2

- The process system (SISO, MISO,MIMO)
- The modelling goal
- A systematic approach
- The necessary ingredients

The Process System



- Inputs, **u**
- Outputs, **y**
- States, **x**
- Disturbances, **d**

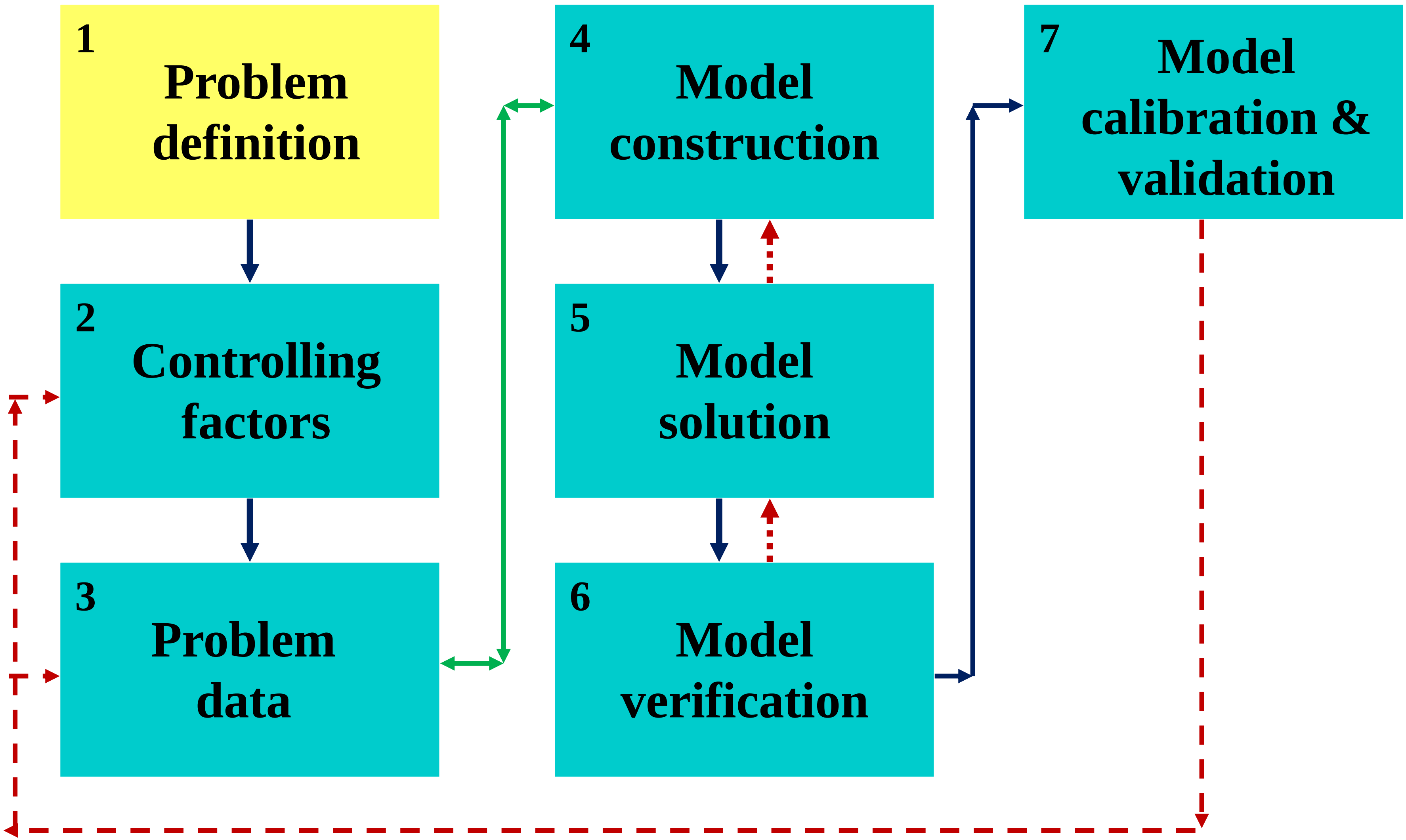
y = **S[u,d]**

(SISO, MIMO
SS or dynamic)

The Modelling Goal

- **Application areas**
  - Flowsheeting
    - simulation (rating)
    - design
    - optimization
  - Process control/analysis
    - prediction
    - regulation
    - identification
    - diagnosis
- **Performance specifications**
  - real, integer or Boolean indices

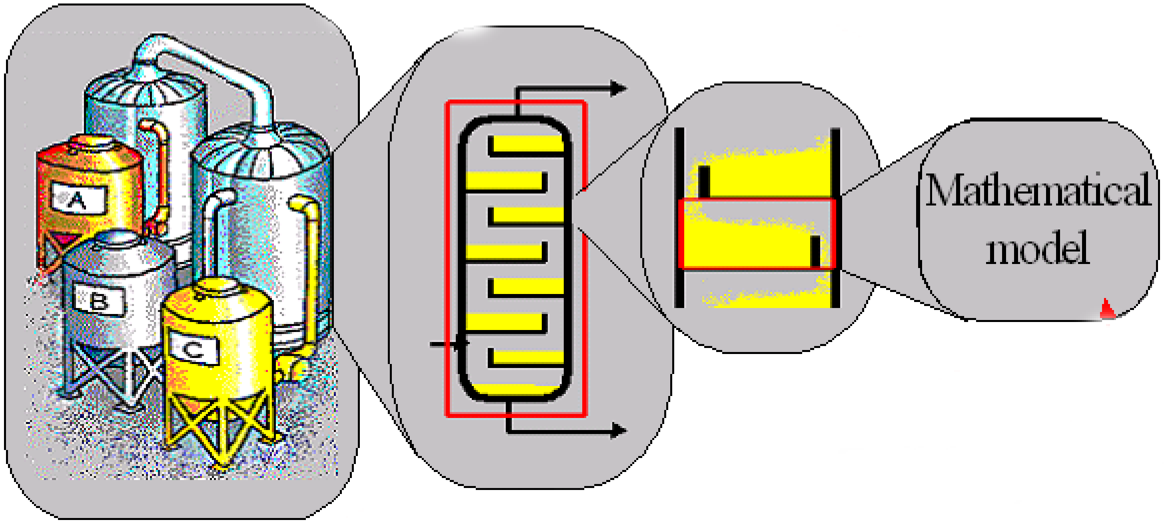
A Systematic Modelling Procedure

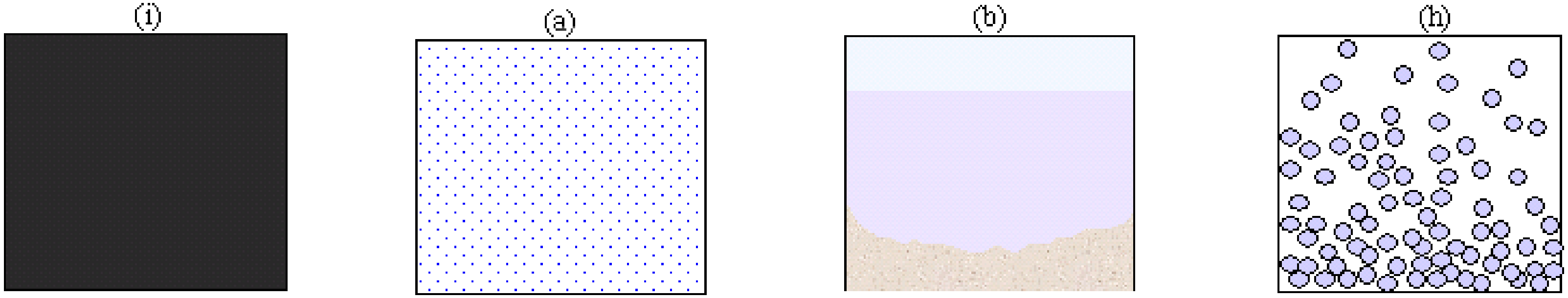


1. Problem Definition

- Clear description of system
  - establish underlying assumptions
- Statement of modelling intention
  - intended goal or use
  - acceptable error
  - anticipated inputs/disturbances

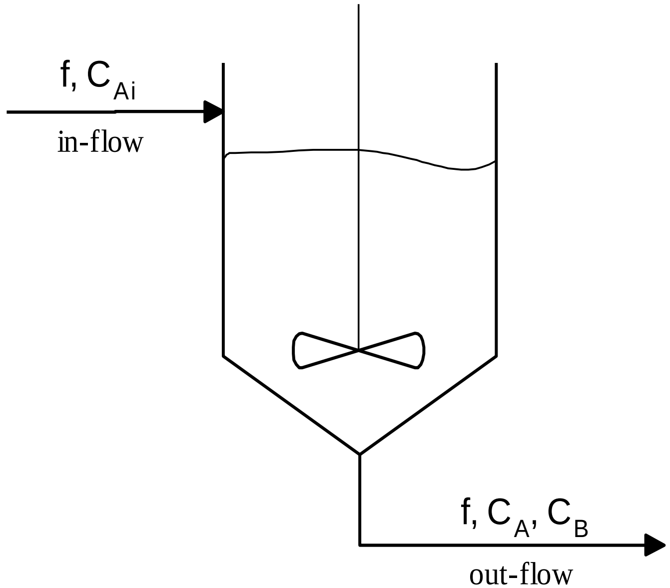
1. Problem Definition





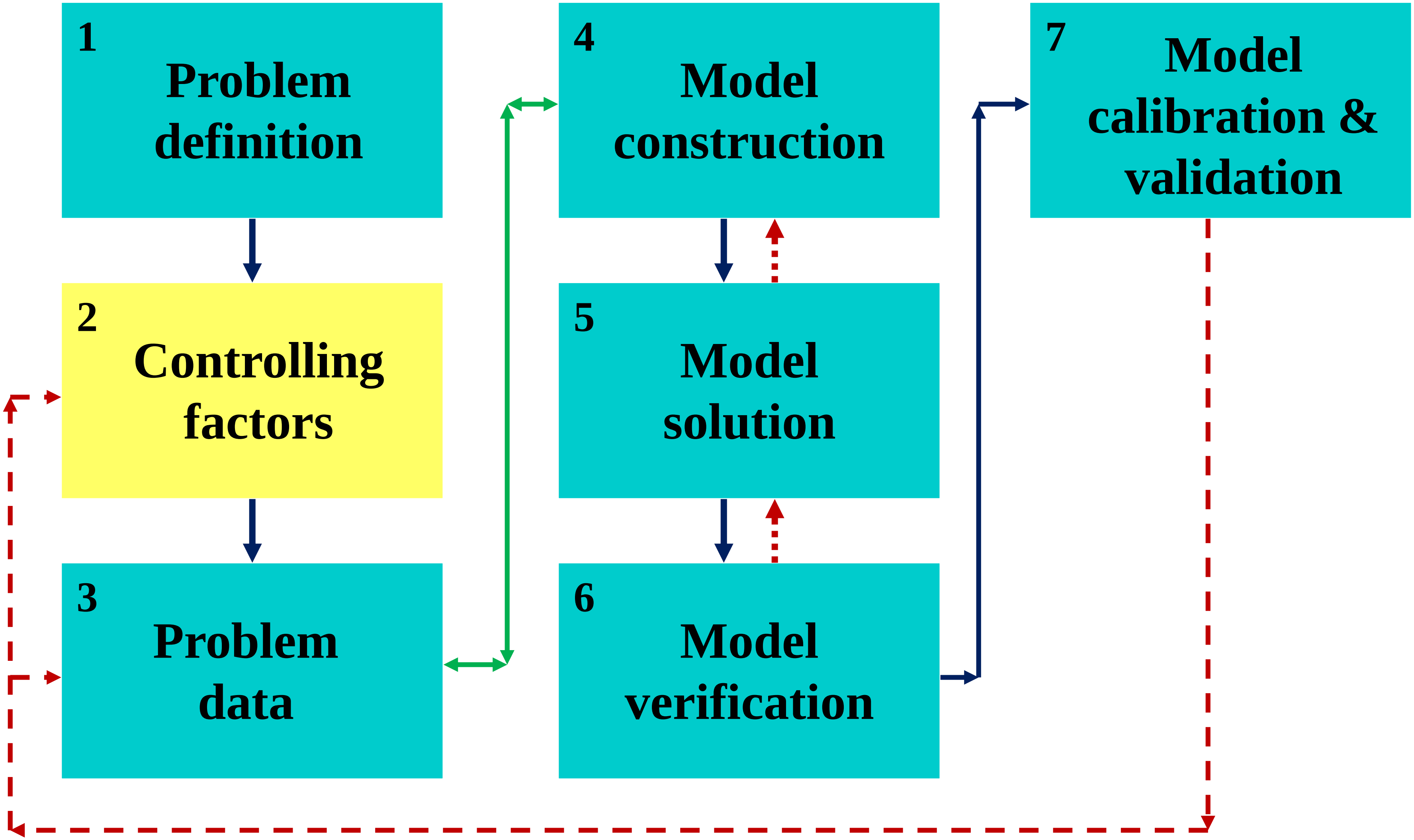
Black box | Perfectly mixed system | Equilibrium phase system | Particulated system with uniform gradient in one direction

Definition Example (Step 1)



- Goal (intent)
  - effect of inlet change
  - study dynamic behavior (control design)
  - +/-10% accuracy
- CSTR description
  - process/system details
  - lumped ? - yes
  - dynamic? - yes

A Systematic Modelling Procedure

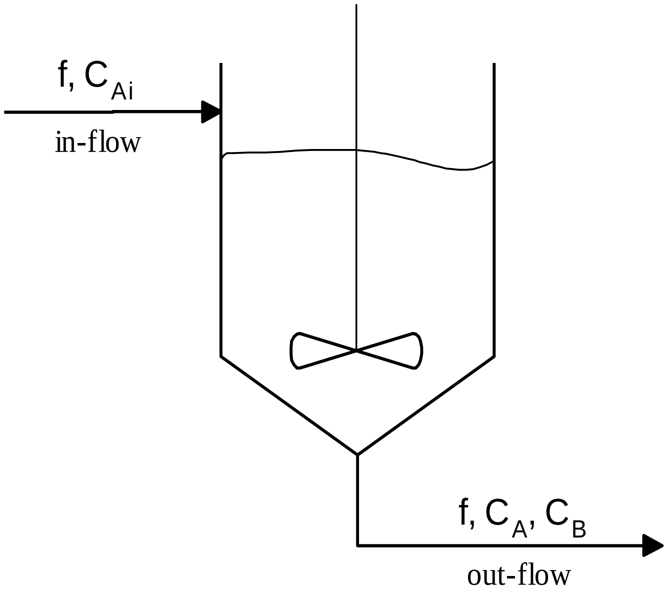


2. Controlling Factors / Mechanisms

- Chemical reaction
- Mass transfer
  - convective, evaporative, …
- Heat transfer
  - radiative, conductive, …
- Momentum transfer

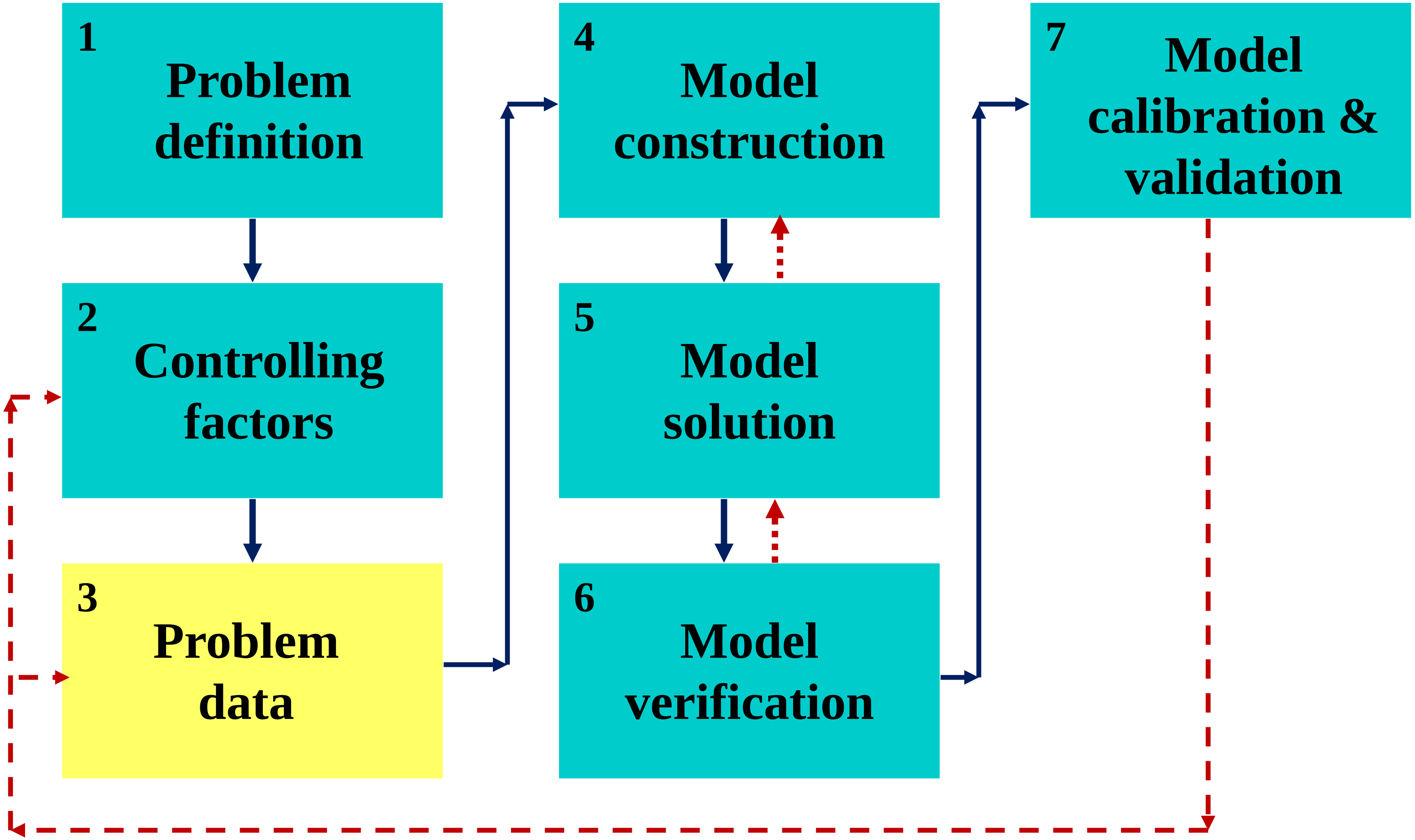
→ ASSUMPTIONS

Mechanisms - CSTR (step 2)

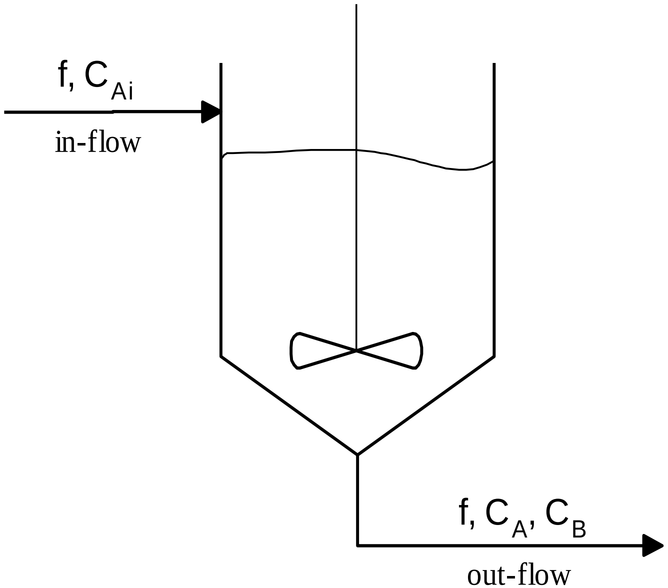


- Chemical reaction
  A → B
- Perfect mixing
- No heat loss or supplied (adiabatic)

A Systematic Modelling Procedure

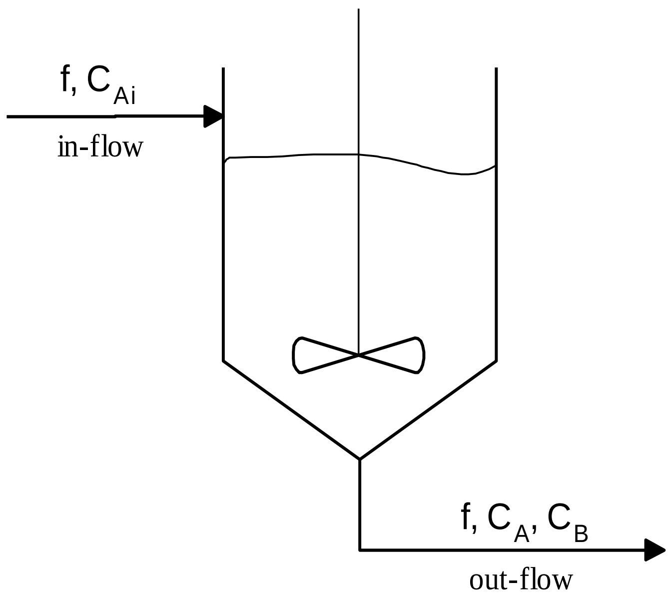


3. Data for the problem



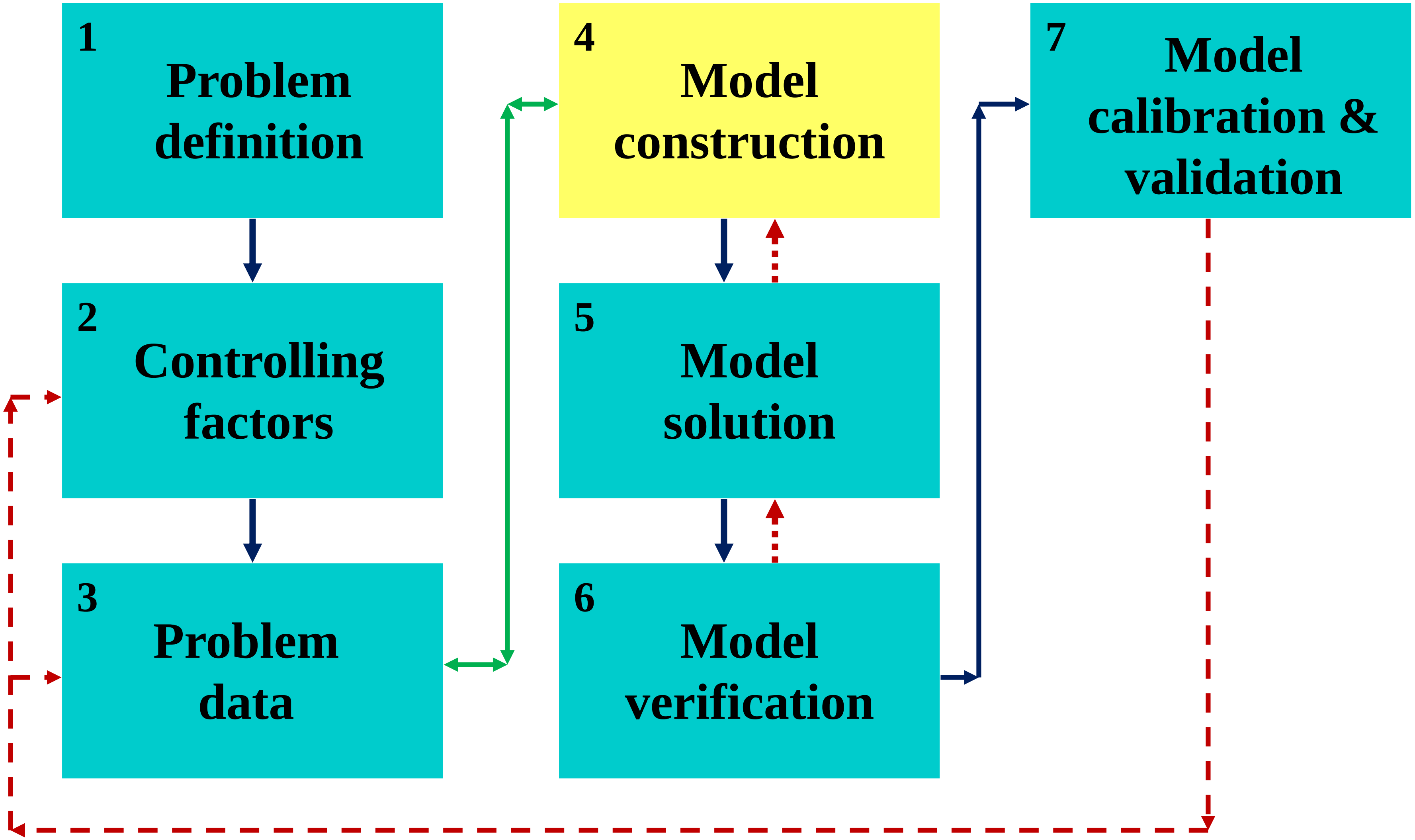
- Physico-chemical data
- Reaction kinetics
- Equipment parameters
- Plant (process) data

Data needs: Example - CSTR (step 3)

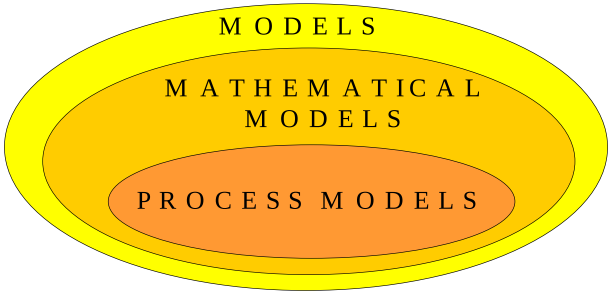


- Reaction kinetics data: k_0 , E, ΔH_R
- Physico-chemical properties
  - specific heats, enthalpies, …
- Equipment parameters: V

A Systematic Modelling Procedure



Model Construction Steps



- Derive the model equations
- Analyze model equations
- Translate the model equations to a solvable form; create library for use with a simulator or for on-line solution

A computer aided system assists the user in performing the above tasks

4. Model construction

- **Assumptions**
- **Boundaries and balance volumes**
- **Conservation equations**
  - mass
  - energy
  - momentum
- **Constitutive equations**
  - reaction rates
  - transfer rates
  - property relations
  - balance volume relations
  - control relations & equipment constraints
- **Conditions**
  - **Equilibrium; control; defined relations; initial conditions; boundary conditions**

Classification of Variables

Known (Defined by system (parameters); Defined by problem; Independent)

Unknown (state, dependent)

CSTR Model (step 4)

- Assumptions
  - A1: perfect mixing
  - A2: first order reaction
  - A3: adiabatic operation
  - A4: equal inflow, outflow
  - A5: constant properties

Equations analysis:
8 equations: 2 ODEs; 6 AEs

- Equations
  - conservation

$$\frac{dm_A}{dt} = f_{A_i} - f_A - rV$$ mass

$$\frac{dH}{dt} = f\hat{H}_i - f\hat{H}$$ energy

  - constitutive

$$r = k_0 e^{-\frac{E}{RT}} C_A$$ Reaction rate

$$m_A = C_A V$$

$$\hat{H}_i = c_P T_i$$

$$\hat{H} = c_P T$$

$$f_{Ai} = f C_{A_i}$$

$$f_A = f C_A$$

Defined relations for mass, enthalpy and flow

CSTR Model (step 4)

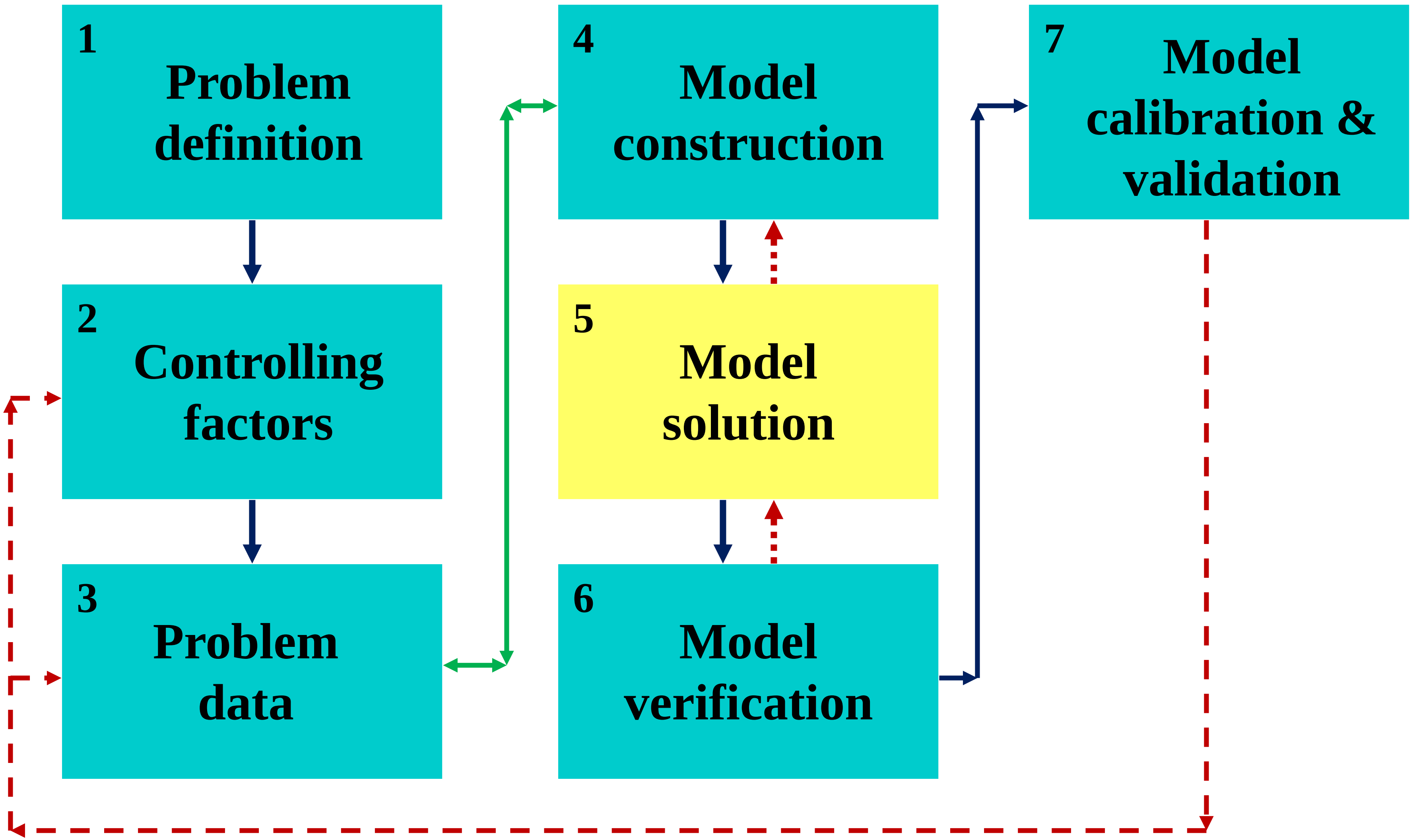
- Classification of variables (plus degree of freedom analysis: **D_F=18 variables – 8 equations = 10**)
  - Known (parameters) $R, k_0, E, \Delta H_R, c_p$ **5**
  - Known (defined) V, f, C_{Ai}, T_i **4**
  - Known (independent) t **1**
  - Unknown $M_A, H, r, C_A, T, \hat{H}_i, f_{Ai}, f_A$ **2+6**

- Boundary Conditions

$$C_A(0) = C_{A_i}$$
$$T(0) = T_i$$

Two differential equations need **initial conditions** for two dependent variables

A Systematic Modelling Procedure



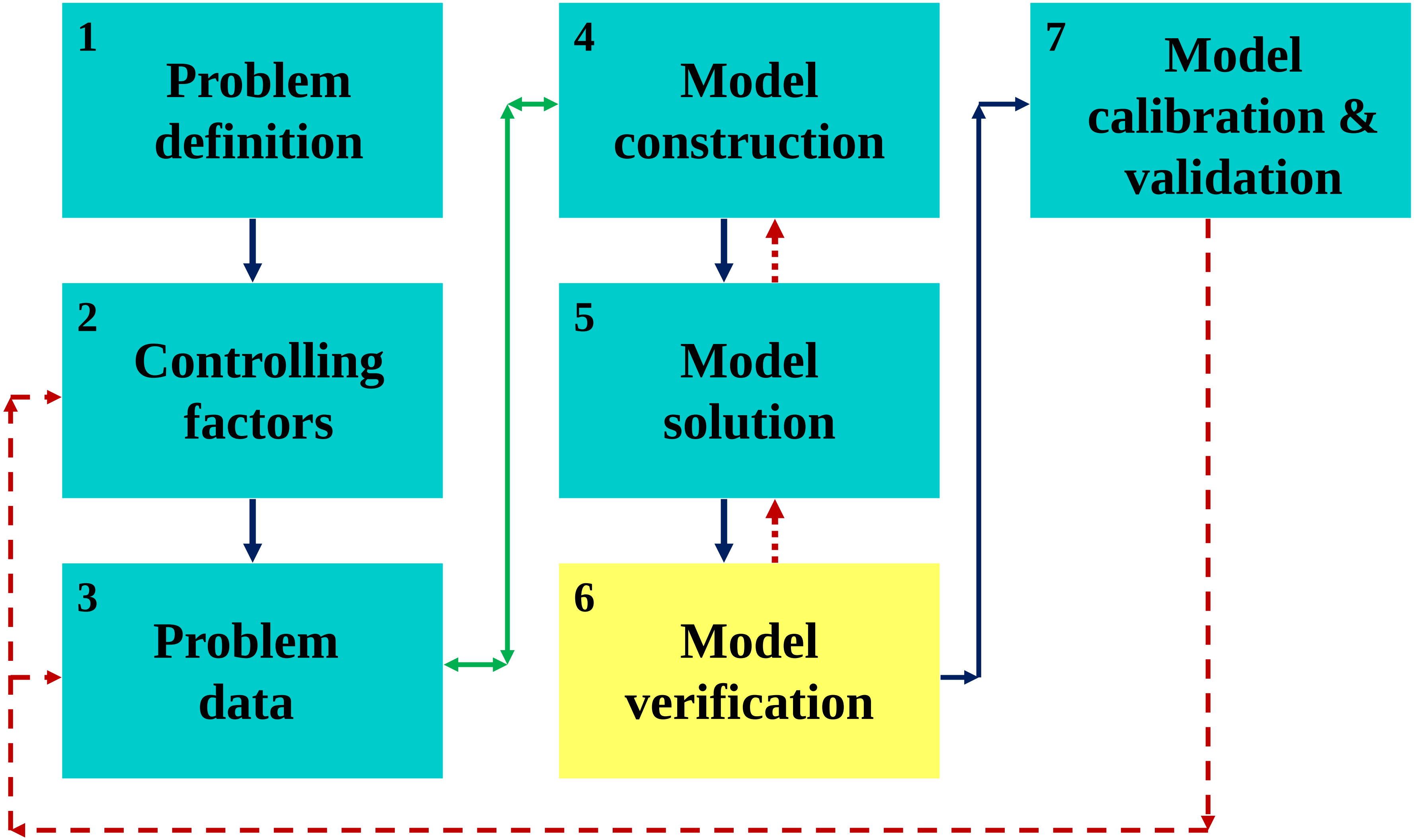
5. Model solution

- Algebraic systems
- Ordinary differential equations
- Differential-algebraic equations
- Partial differential equations
- Integro-partial differential equations

CSTR - Numerical Solution (step 5)

- Solution of differential-algebraic equations
  - using structuring techniques
  - using direct DAE solution

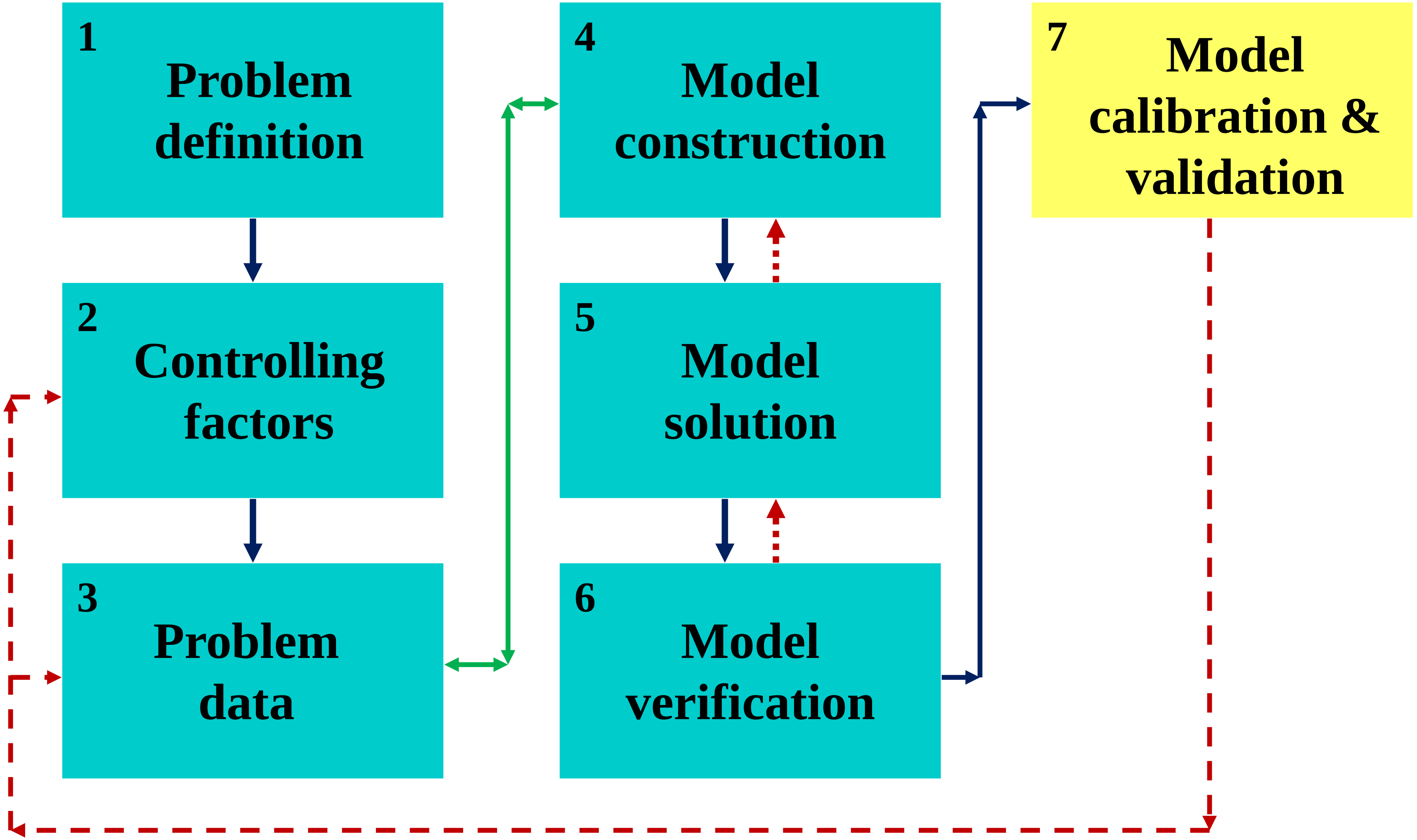
A Systematic Modelling Procedure



6. Model verification

- Structured programming approach
- Modular code
- Testing of separate modules
- Exercise all code logic
  - conditions
  - Constraints
- Quality documentation

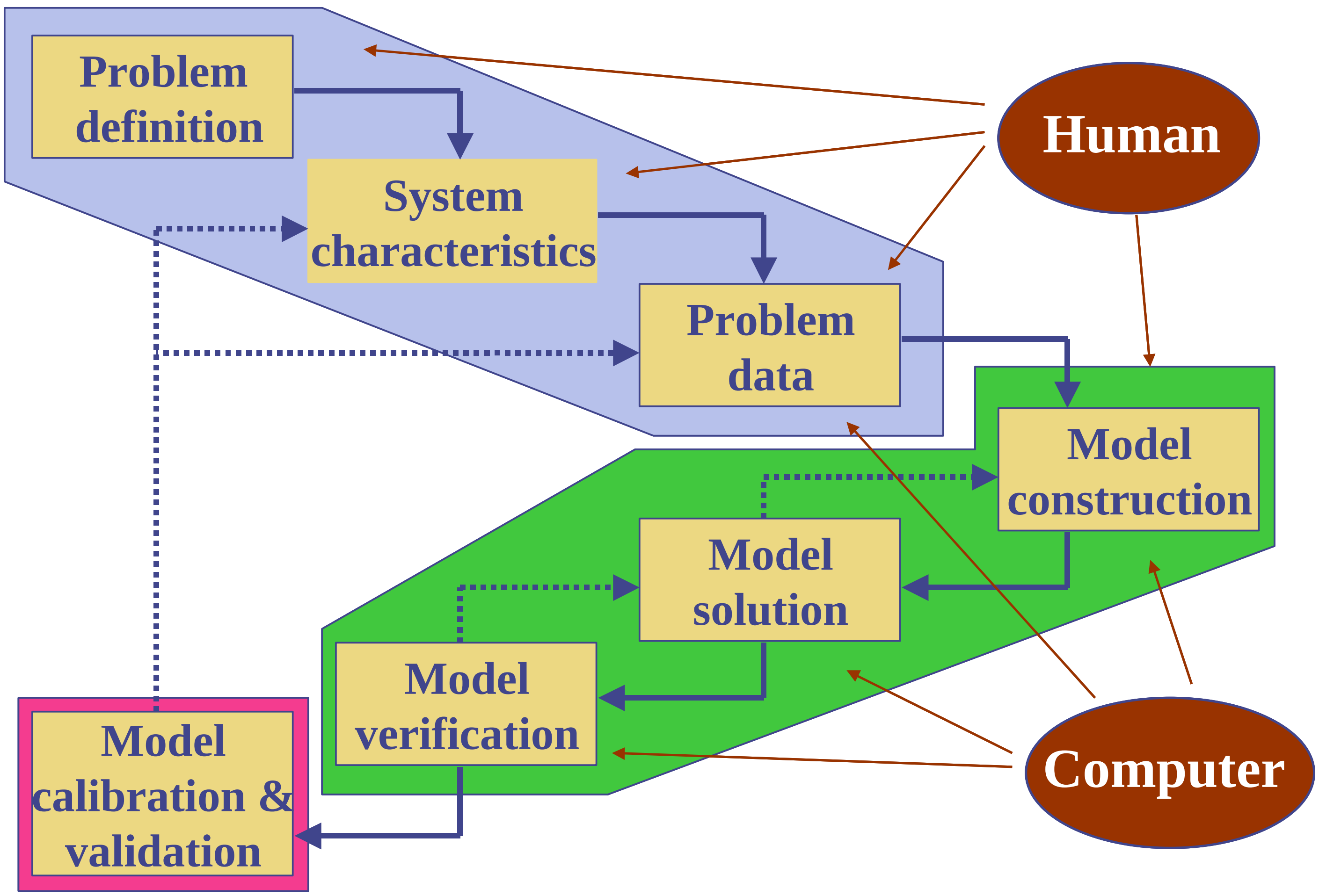
A Systematic Modelling Procedure



7. Model calibration/validation

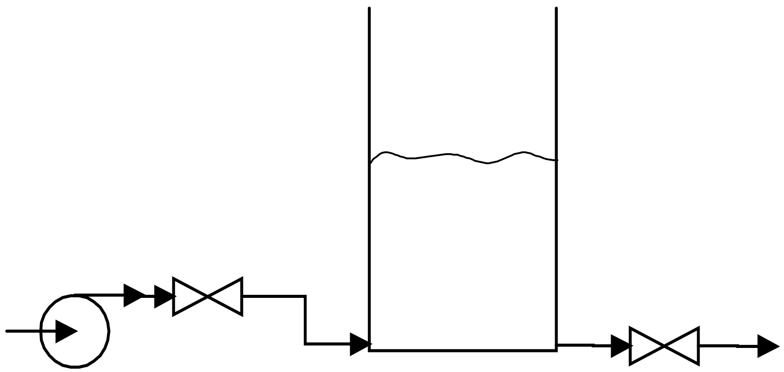
- Generate plant data
- Analyze plant data for quality
- Parameter or structure estimation
- Independent hypothesis testing for validation
- Revise the model until suitable for purpose

Systematic Computer Aided Modelling System

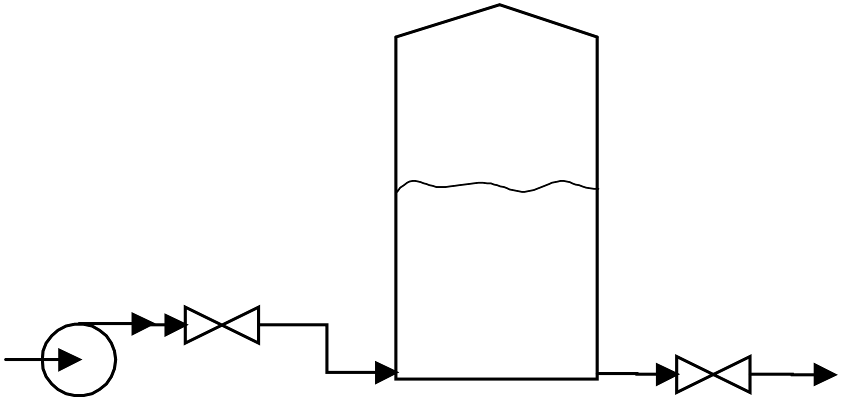


Modelling exercise - 1

For the open & closed tank systems shown below, develop the appropriate models

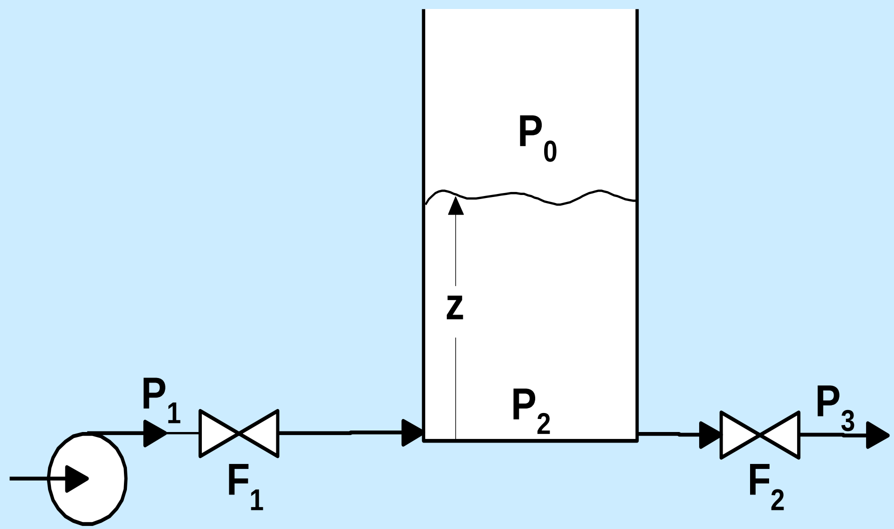


Open system



Closed system

A Process Example



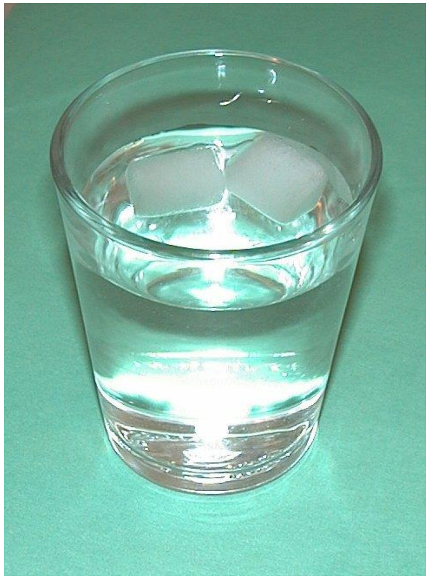
$$\frac{dz}{dt} = \frac{(F_1 - F_2)}{A}$$

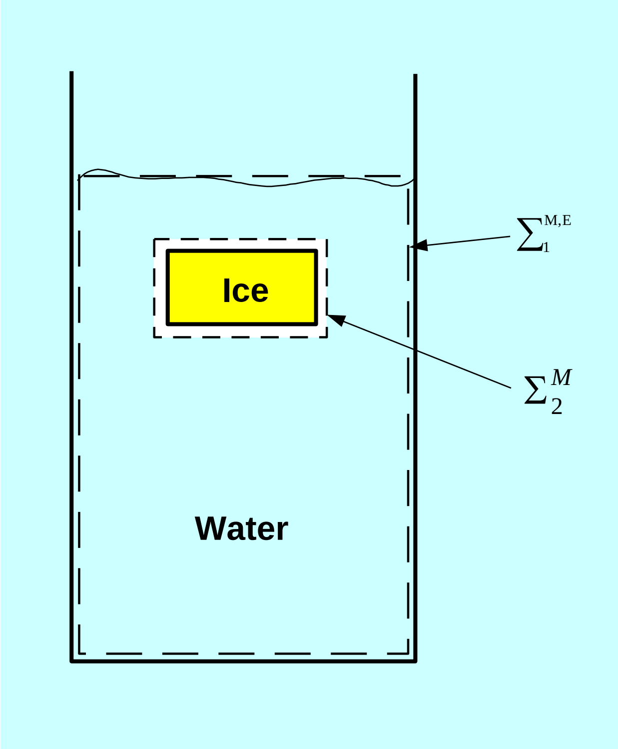
$$F_1 - C_V\sqrt{P_1 - P_2} = 0$$

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

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

Modelling exercise – 2a: Melting of ice cube






```
#Conservation equation
#*********************
#Mass balance
dMice = -m
dMwater = m

#Energy balnce
dTw = -q/(Mwater*cpwater)


Constitutive equations
#*********************
m = q/L

q = h*A*(Tw-Tice)

A = 6*(Mice/roice)^(2/3)


L = heat of vaporization (energy/mass)
h = heat transfer coefficient
[energy/(temperature*area)]
A = area of ice cube
```

Lecture 2a: Conservation Principles

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Overview of lecture 2a

- Thermodynamic system principles
- Balance volumes in process systems
- Extensive and intensive variables
- Principle of conservation
- Conservation equations
- Induced algebraic equations

Principle of Conservation

❖ Word form

$$\begin{Bmatrix}\text{net change}\\ \text{of quantity}\end{Bmatrix}=\begin{Bmatrix}\text{flow into}\\ \text{system}\end{Bmatrix}-\begin{Bmatrix}\text{flow out}\\ \text{of system}\end{Bmatrix}+\{\text{generation}\}-\{\text{consumption}\}$$

❖ Integral equation form

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

❖ Differential form (rectangular coordinates)

$$\frac{\partial\hat{\Phi}}{\partial t} = D\left(\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{\partial y^2}+\frac{\partial^2\varphi}{\partial z^2}\right)-\left(\frac{\partial\hat{\Phi}}{\partial x}v_x+\frac{\partial\hat{\Phi}}{\partial y}v_y\frac{\partial\hat{\Phi}}{\partial z}v_z\right)+\hat{q}$$

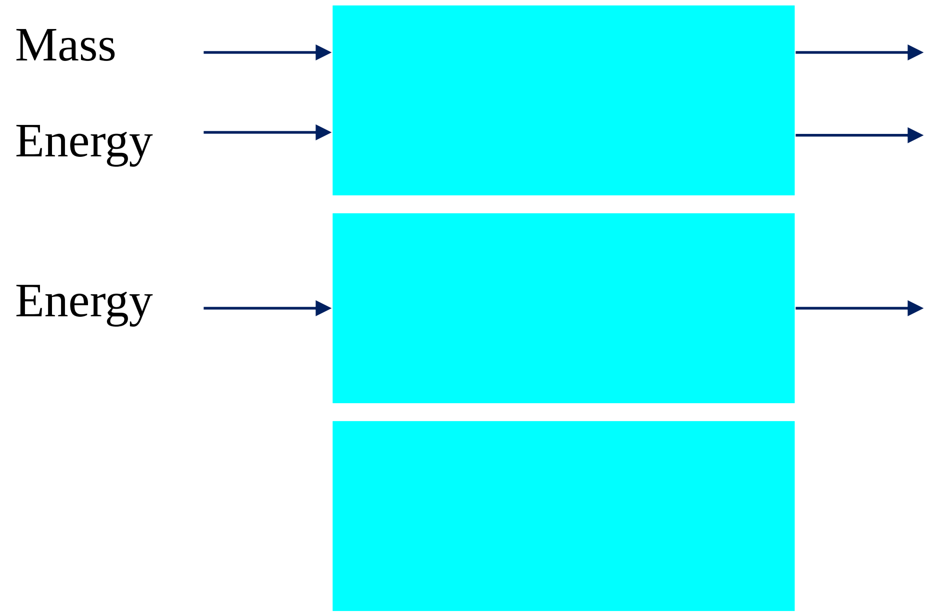
Thermodynamic system principles

Spaces and their characteristics

open systems

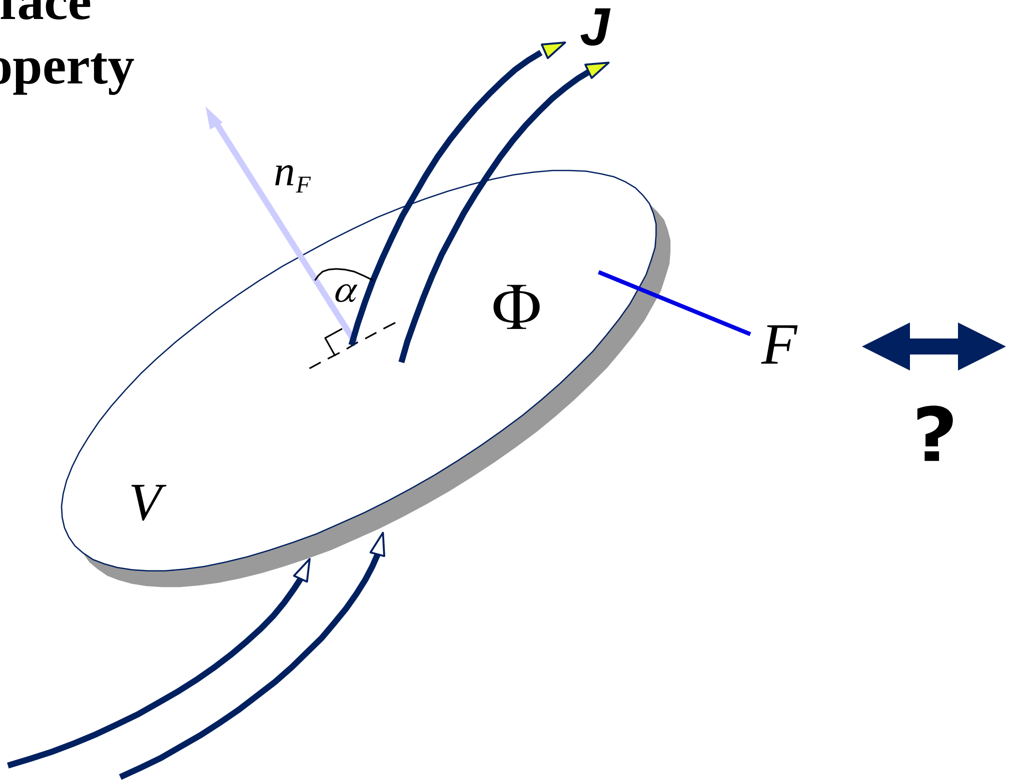
closed systems

isolated systems



Balance or "Control" Volumes

V: volume
F: surface
ϕ : property



General principle

Copper converter

Gas compressor

Particular application

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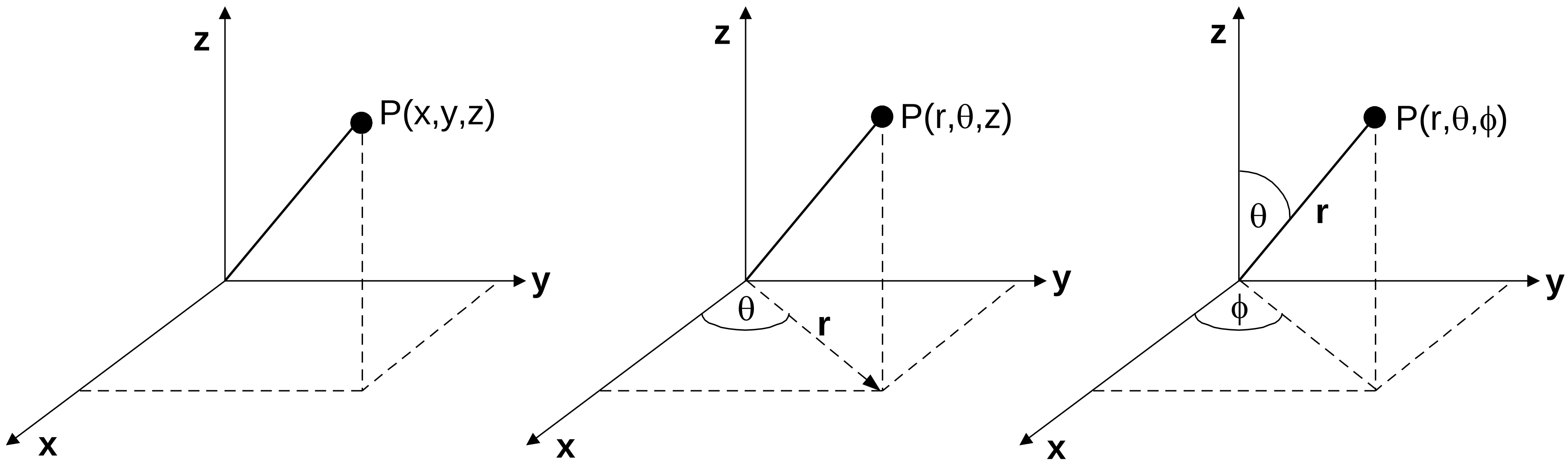
Balance Volumes

- Defined by physical equipment
- Defined by distinct phases
- Dictated by the modelling goal
- Need for a co-ordinate system
  - rectangular
  - cylindrical
  - spherical

Principal Co-ordinate Systems



Rectangular Cylindrical Spherical

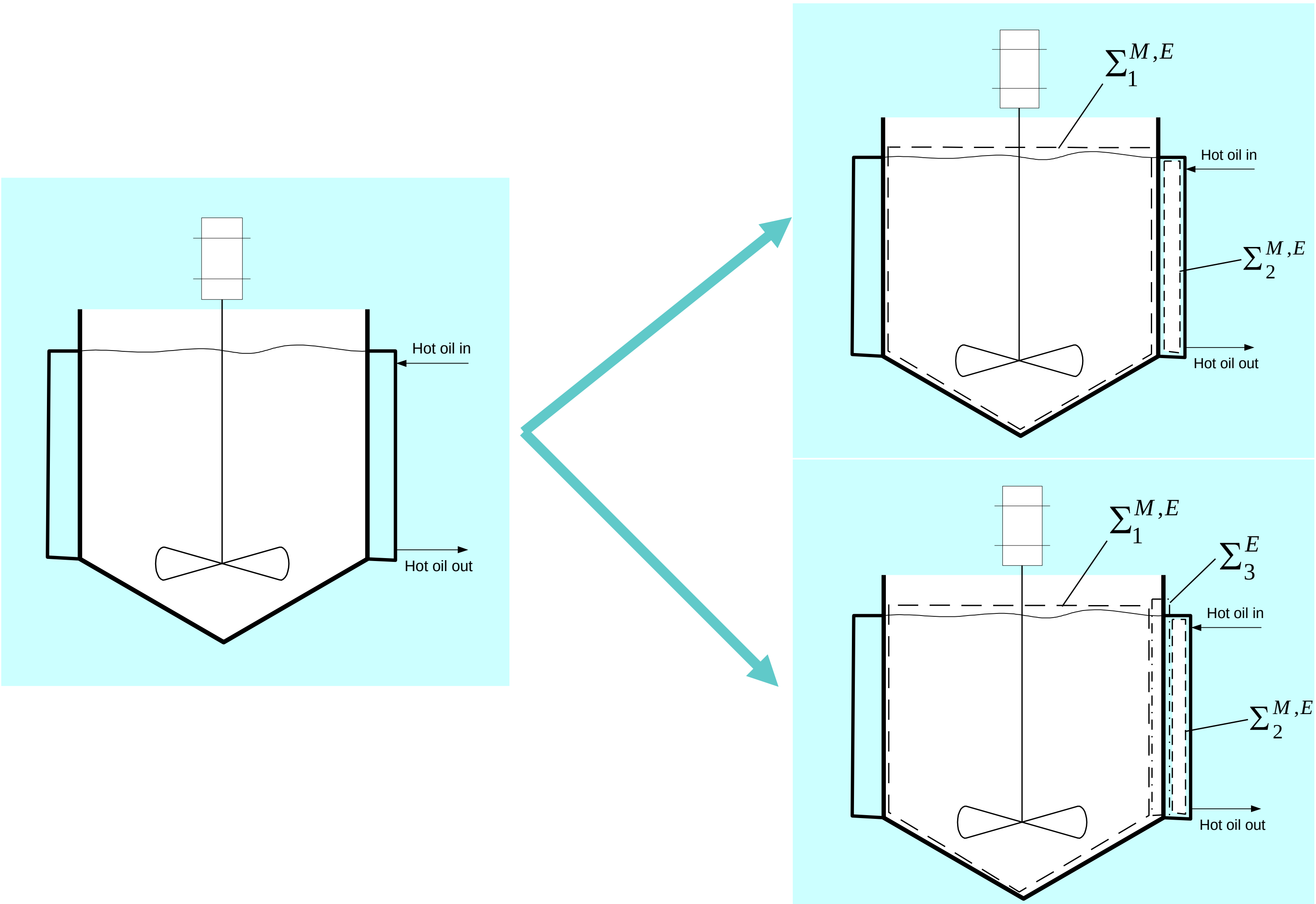
Relation Between Balance Volumes

- Mass balance volume set: *primary set*

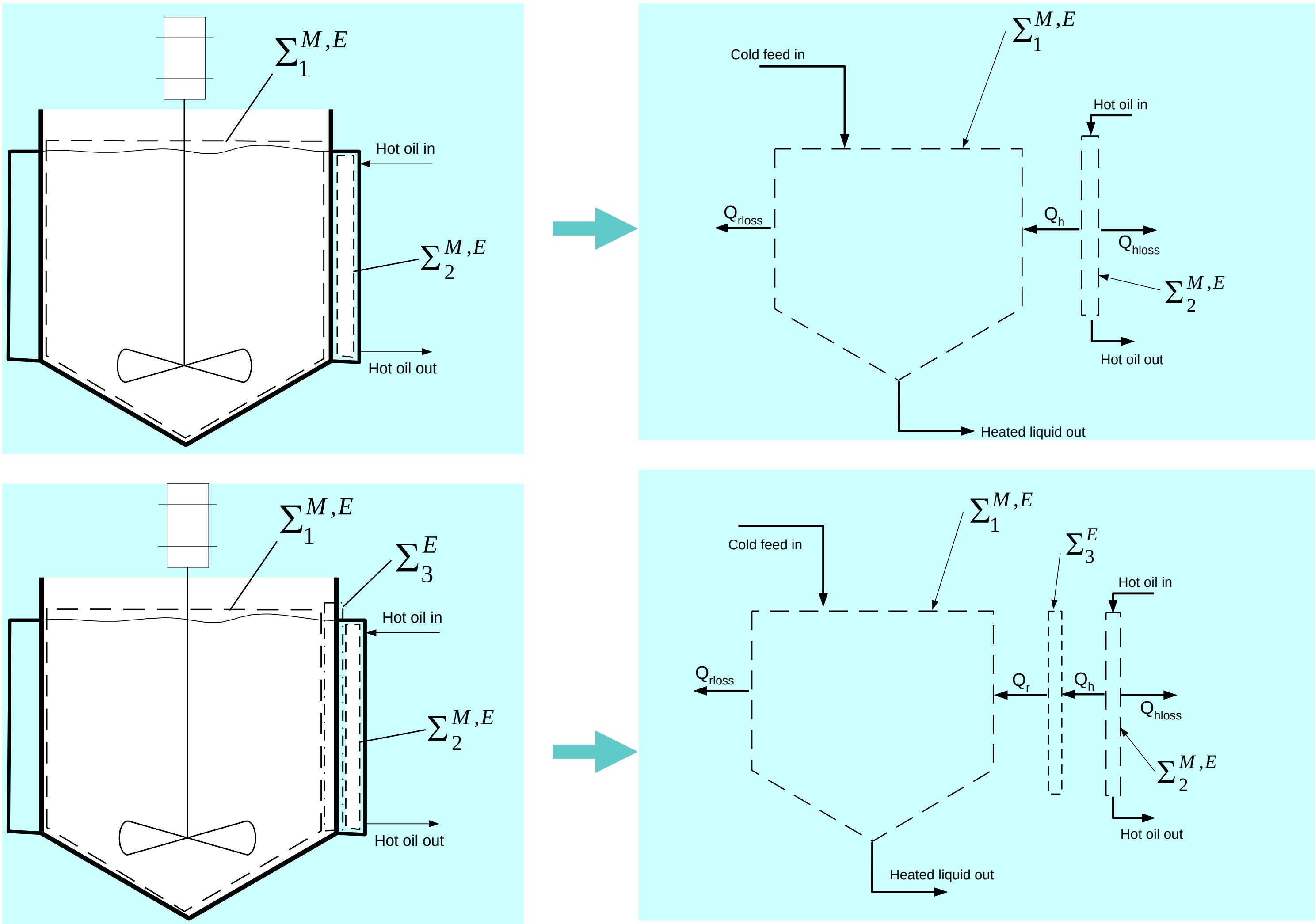
- Energy balance volume set can span or encapsulate mass balance sets

- Balance volume manipulations
  - coalescence
  - division

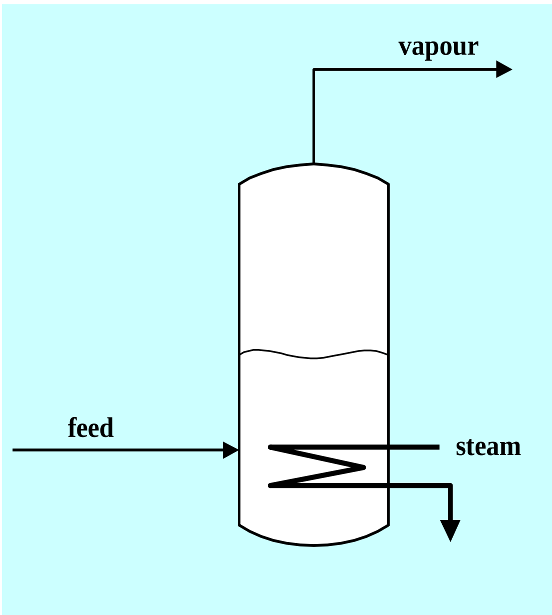
Balance Volumes for a Heated CSTR

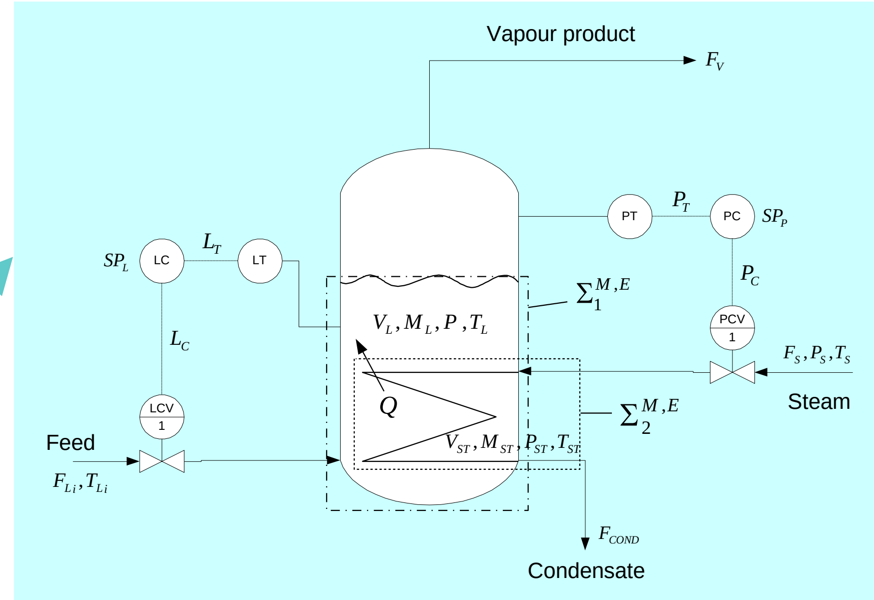


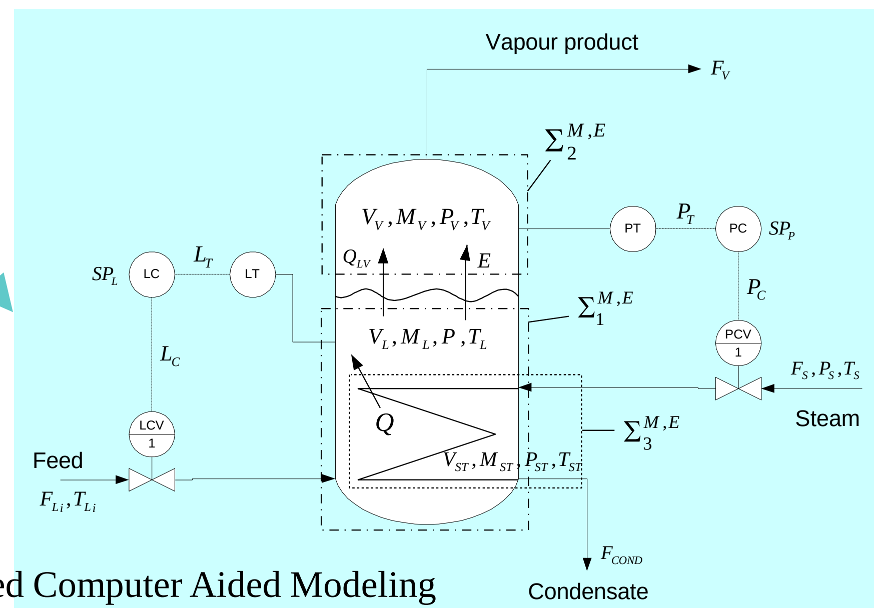
Relationship Between Balance Volumes



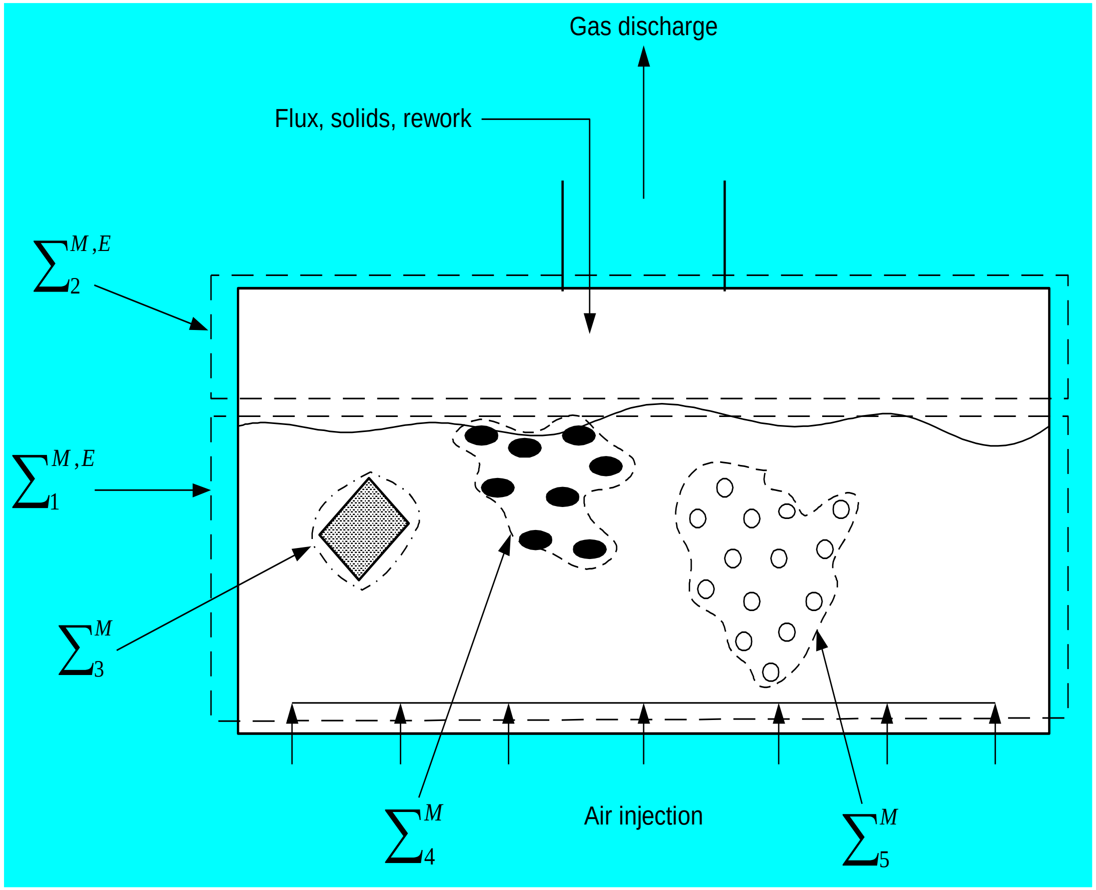
Balance Volumes for a Vaporizer







Balance Volumes for Copper Converter



Extensive and Intensive Properties

- Extensive Properties
  - depend on the extent of the system (overall mass; component masses; energy; enthalpy; …)

$$E_i^S = E_i^{S_1} + E_i^{S_2}$$

- Intensive Properties
  - do not depend on extent

$$I_k = f(I_i, I_j)$$

- Extensive properties are conserved

$$E = M\, f(I_j, I_i)$$

Intensive Properties

Intensive

- P, T, compositions
- mass specific properties

$$I_k = \frac{E_k}{M}$$

- key variables for constitutive relations

Potentials

- driving forces for diffusive flow of their extensive counterpart

Lecture 2b: Constitutive Relations

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What are constitutive relations?

- Relate conserved extensive quantities to intensive variables
- Help define physico-chemical quantities (e.g. enthalpies, densities, viscosities ,…)
- Define transfer rates (mass, energy, …)
- Other relations to "constitute" the model

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How do constitutive relations arise ?

- Related to the terms in the conservation equations for mass, energy and momentum

• Convective flow terms (process streams)

• Molecular flow streams (fluxes)

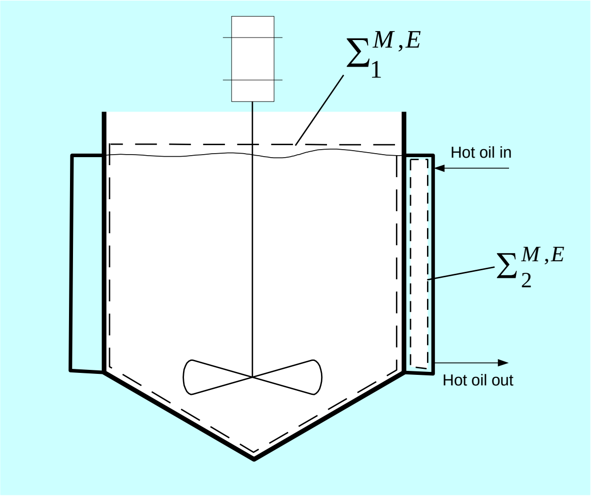
• Internal processes

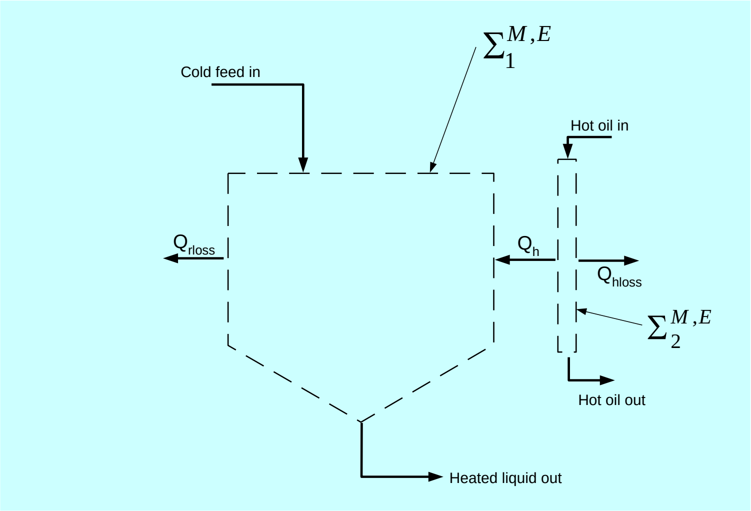
$$\frac{\partial \Phi}{\partial t} = -\nabla \bullet J + q$$

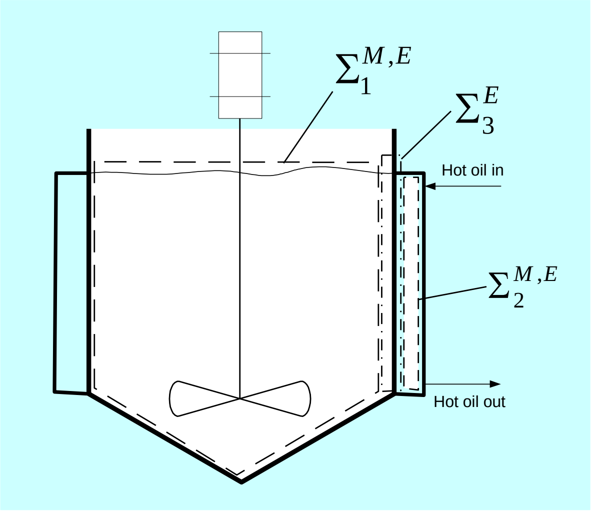
• Defining intensive variables in terms of extensive quantities and other physico-chemical properties

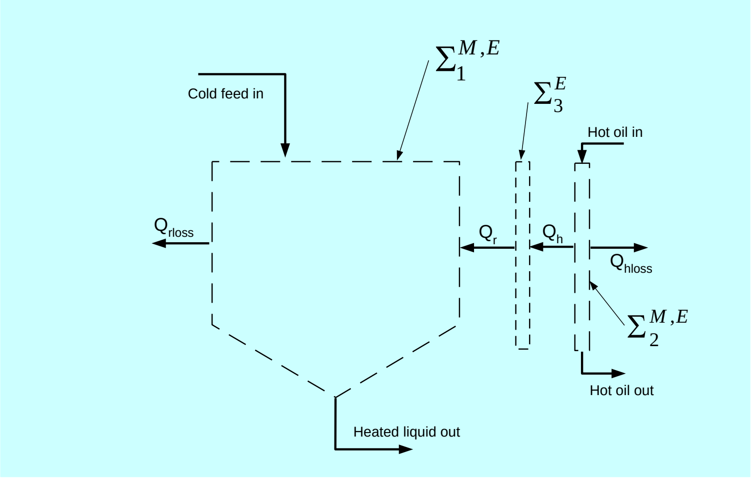
• Constraints on the system (control relations)?

Balance volumes, flows and system processes

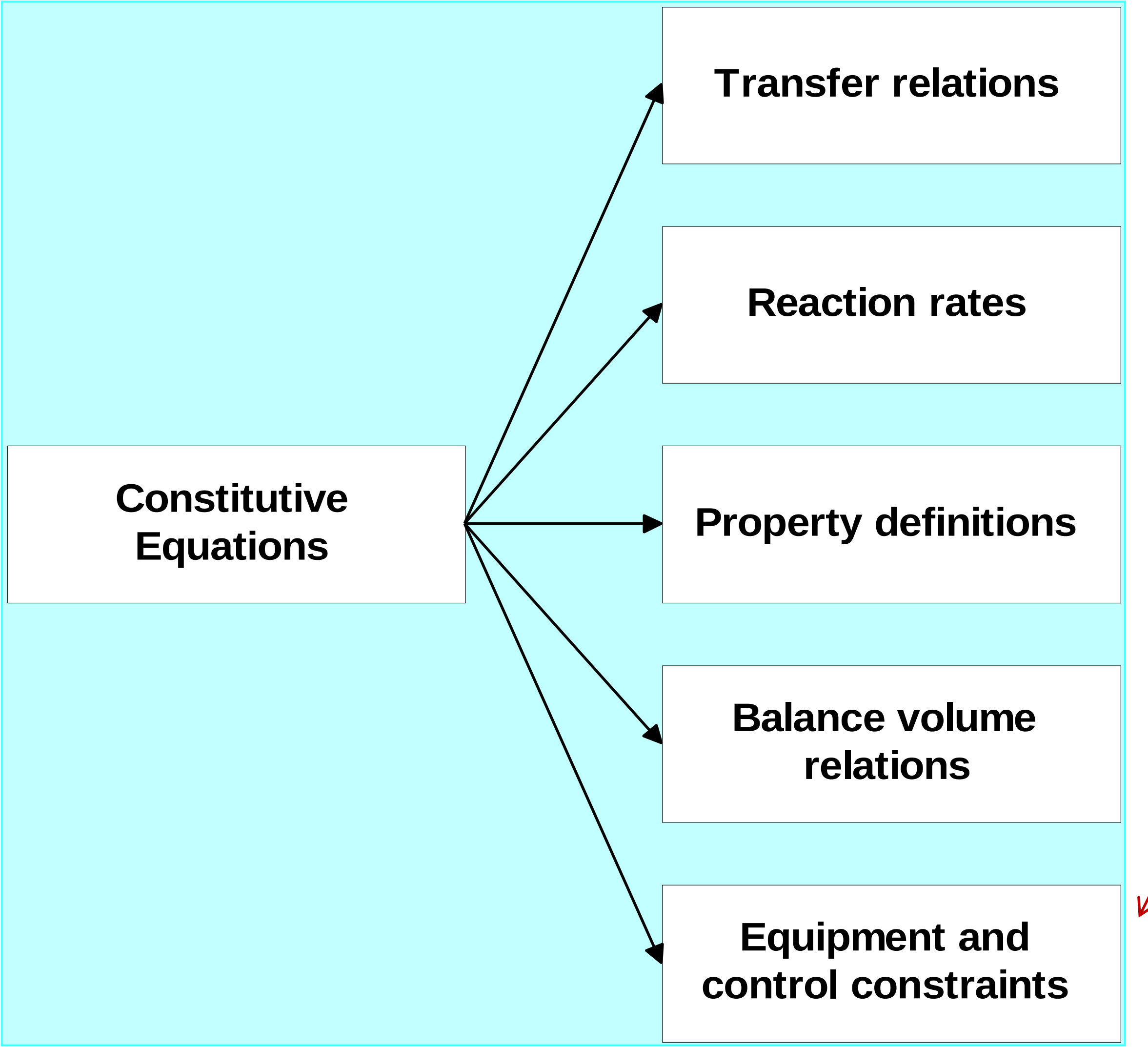








Classes of Relations



These are conditional equations and not constitutive equations

1. Transfer Relations

- General form

$$rate_{\chi}^{(p,r)} = \psi^{(p,r)}\left(\varsigma^{(p)} - \kappa^{(r)}\right)$$

- Particular forms
  - mass transfer $j = K_G\left(C_G^* - C_G\right)$
  - heat transfer $q_{CV} = UA\Delta T$

2. Reaction rates

- Reaction rate

  (batch reactor only)

$$r_i = \frac{1}{V}\frac{dn_i}{dt}$$

- General reaction expression

$$r_A = k_A f\left(C_A^{\alpha}, C_B^{\beta}, \ldots\right)$$

$$k_A = k_0 e^{-\frac{E}{RT}}$$

3. Thermodynamic relations

- Property relations (density, viscosity, …)

$$\rho_L = f(P, T, x_i)$$

- Equilibrium relations (control/conditional equation)
  - Raoult's law
  - Isofugacity criteria (same model for each phase)
  - Gamma-Phi (different models for each phase)

Models for Thermodynamic properties

- Enthalpy

$$h(T) = h(T_R) + \int_{T_R}^{T} c_p(T)dT$$

- linear

$$h(T) = c_p T$$

$$h(T) = c_p T + \lambda_{VAP}$$

- nonlinear

$$c_p = a_0 + a_1 T + a_2 T^2 + \ldots$$

$$h(T) = h(T_0) + \int_{T_0}^{T} c_p(T)dT$$

Models for Thermodynamic properties

- Equations of state
  - ideal gas

$$PV = nRT$$

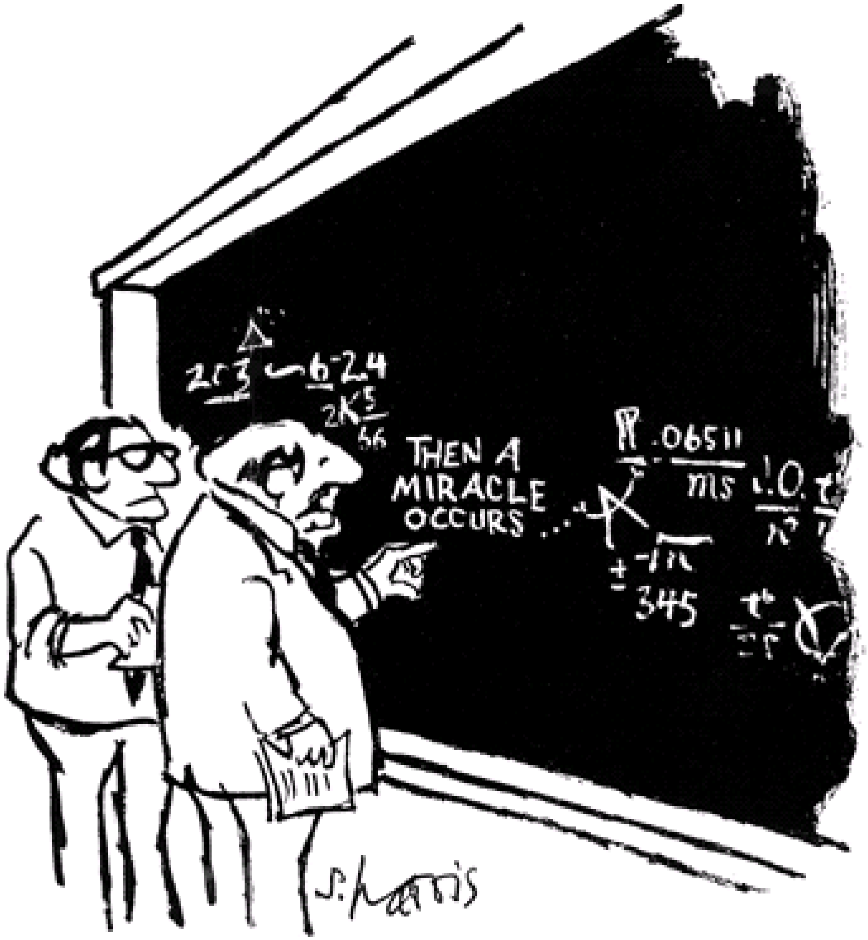
  - cubic EoS

$$P = f(V,T)$$

    - SRK
    - Peng Robinson

- Ge Models (NRTL, UNIQUAC, UNIFAC, ….)

How do constitutive relations arise ?



"I think you should be more explicit here in step two."

Constitutive model developers perform miracles everyday!

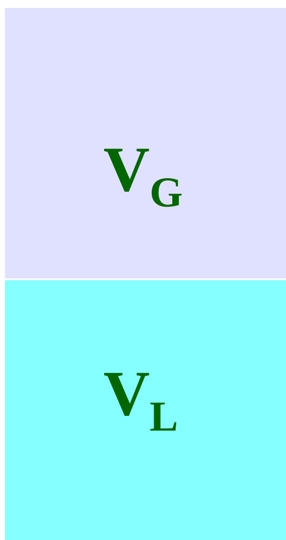
- **Add one or more parameters (regress them with available experimental data)**
- **Use another model to generate the missing data**

.....

Develop a better theory!

4. Balance volume relations

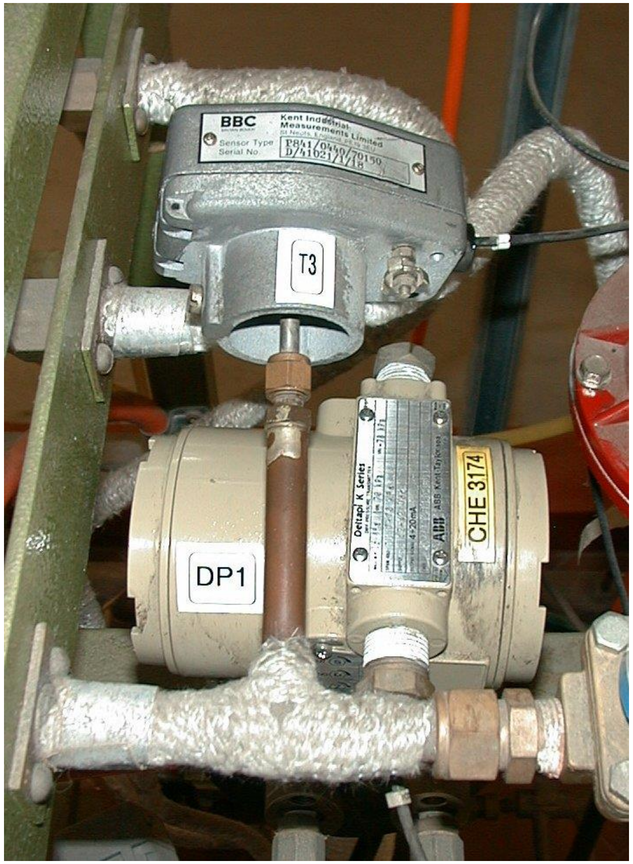
❖ Relations between phases (control/conditional equations)

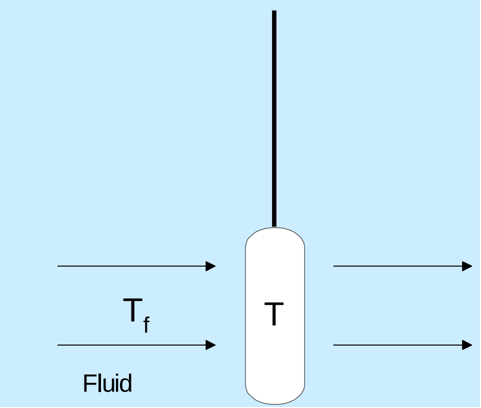


$$V_G = V - V_L$$

5. Equipment and Control

❖ Sensors





$$\frac{dU}{dt} = \frac{d(Mc_pT)}{dt} = \tilde{U}A(T_f - T)$$

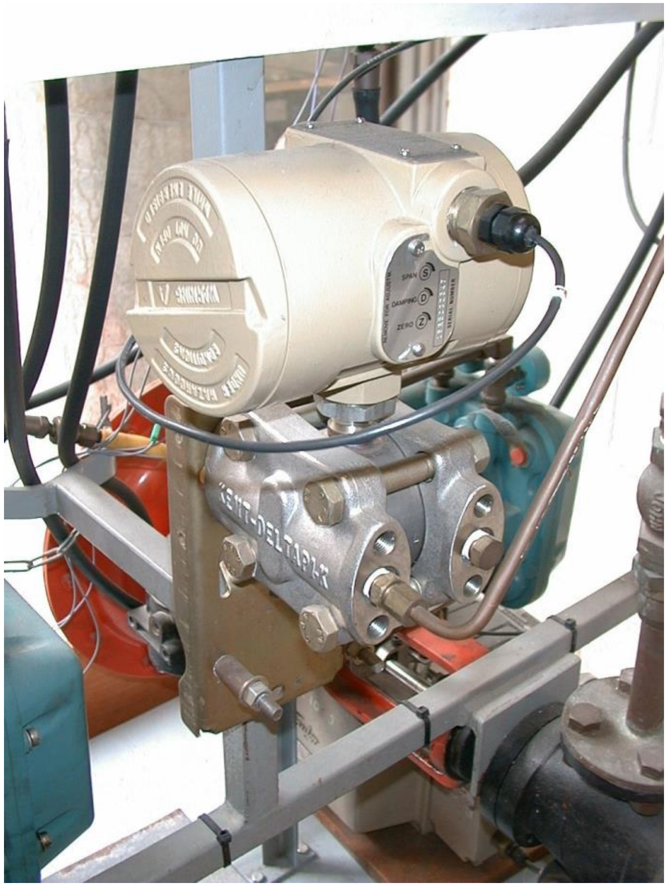
$$\frac{dT}{dt} = \frac{\tilde{U}A}{Mc_p}(T_f - T)$$

$$\frac{dT}{dt} = \frac{(T_f - T)}{\tau}$$

What is the unit of $\tilde{U}$?

5. Equipment & Control: Control Elements

Transmitters (4-20mA, 20-100kPa) – calculate the measured (controlled) variable signal



$$O_p = O_{p_{\min}} + (I_p - z_0)G$$

I_p is the input signal

z_0 is the zero

G is the gain

5. Equipment & Control: Controllers

Traditional (P, PI, PID)

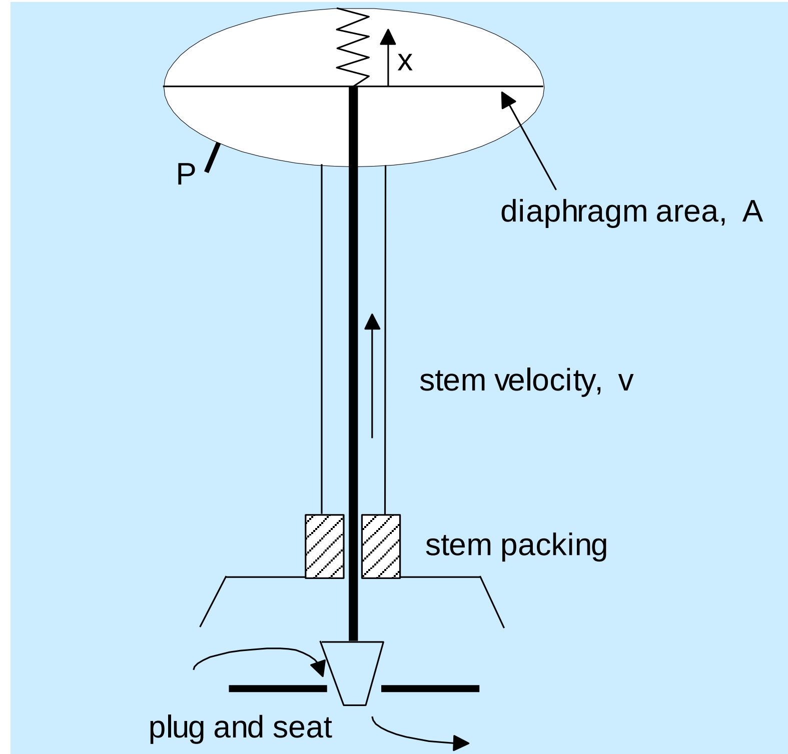
$$O_C = B + K_C(S_P - O_P) = B + K_C\varepsilon$$

$$O_C = B + K_C\varepsilon + \frac{K_C}{\tau_I}\int \varepsilon dt$$

$$O_C = B + K_C\varepsilon + \frac{K_C}{\tau_I}\int \varepsilon dt + K_C\tau_D\frac{d\varepsilon}{dt}$$

O_c = u; B = u*; S_p = y*; O_p = y

Actuators on valves



$$\tau^2 \frac{d^2 S}{dt^2} + 2\xi\tau \frac{dS}{dt} + S = G_a I$$

S = stem movement (0 - 1)

G_a = actuator gain

τ, ξ = time constant and damping factor

Note: $I = O_c$

5. Equipment & Control: Valves

- Static valves

$$F = C_V \sqrt{\Delta P}$$

- Control valves
  - characteristics

$$F = C_V c(S) \sqrt{\Delta P}$$

$c(S) = S$	linear
$c(S) = a^{S-1}$	equal percentage
$c(S) = \sqrt{S}$	square root

Modelling exercise – 2b: Constitutive models

Problem-I (home exercise)

1. Write* the reaction rate models for compounds A and B for the following reaction system:

   $$A \leftrightarrow B \rightarrow C;\ 2A \rightarrow D$$

   $$k_{1f} = 0.01;\ k_{1b} = 5.0;\ k_{2f} = 10.0,\ k_{3f} = 100$$

2. Write* a model for pure component vapour pressure as a function of temperature
3. Write* the model for estimating component liquid activity coefficients as a function of liquid composition and temperature

*** Provide derivation details & model description**
Select any property model for I-2 and I-3