Modeling & Simulation in Chemical Engineering

(CHE-F418)

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Pre-requisites for the Course

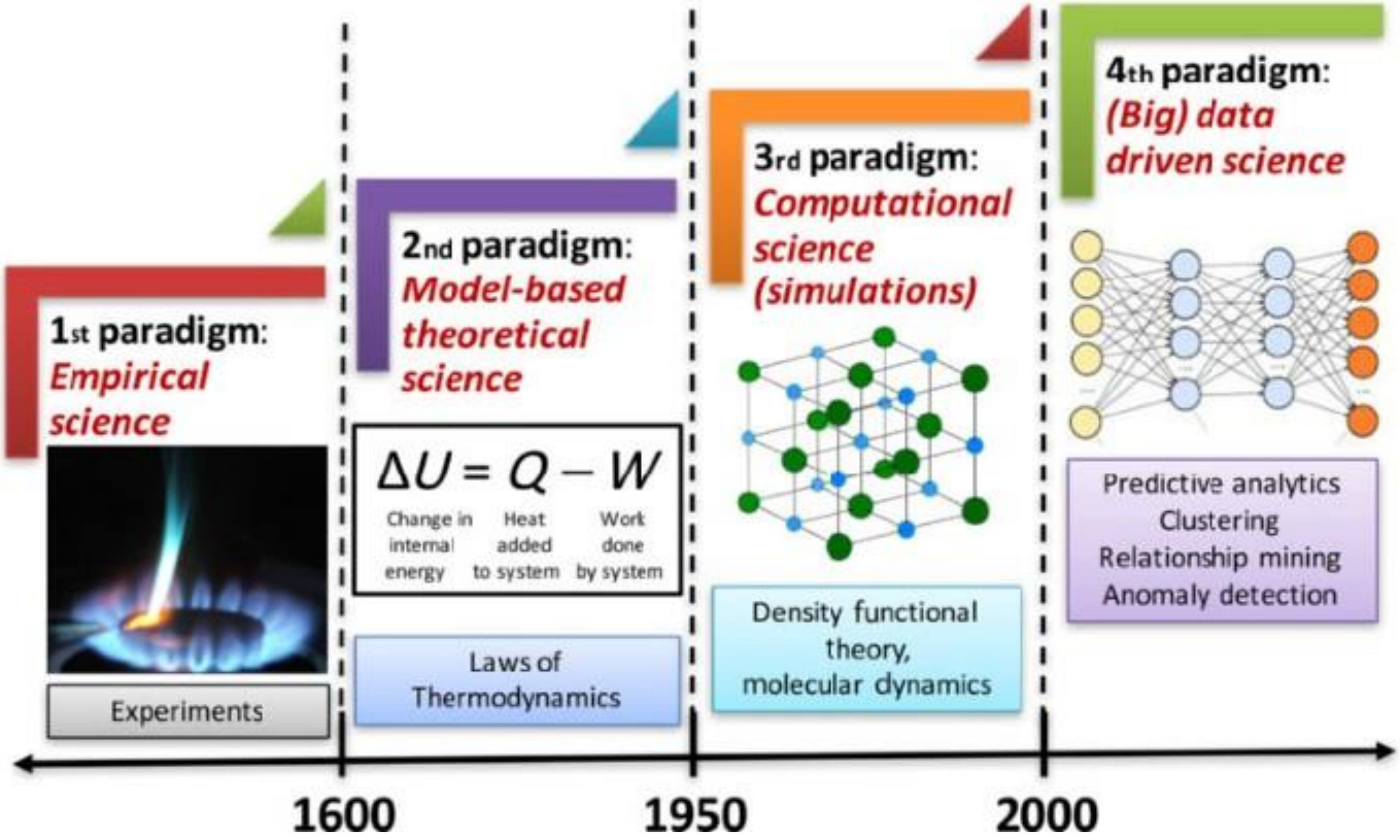
- Chemical Engineering Principles
- Numerical Methods in Chemical Engineering (Solvers & Optimizers)

- Thermodynamics
- Reactor kinetics
- Transport phenomena

    1. Heat transfer
    2. Mass transfer
    3. Fluid dynamics

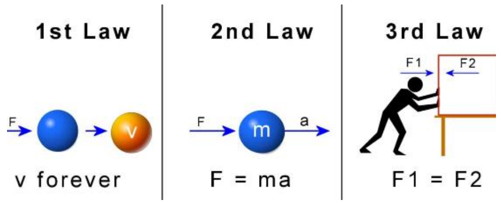
Module 1: Introduction to Modeling & Simulations

Evolution of Modeling



Breakthrough Phenomena (Phenomenological Model)

<u>Newton's Law of Motion, 1687</u>



<u>Einstein's Theory of Relativity, 1905</u>

$$t' = \frac{t}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$t' = change\ in\ time$$
$$t = rest\ time$$
$$v = velocity$$
$$c = speed\ of\ light$$

<u>Sadi Carnot's second law of TD, 1824</u>

dS = dQ/T

<u>Boyle's experiment, 1646</u>

PV= constant

Joule's, 1846

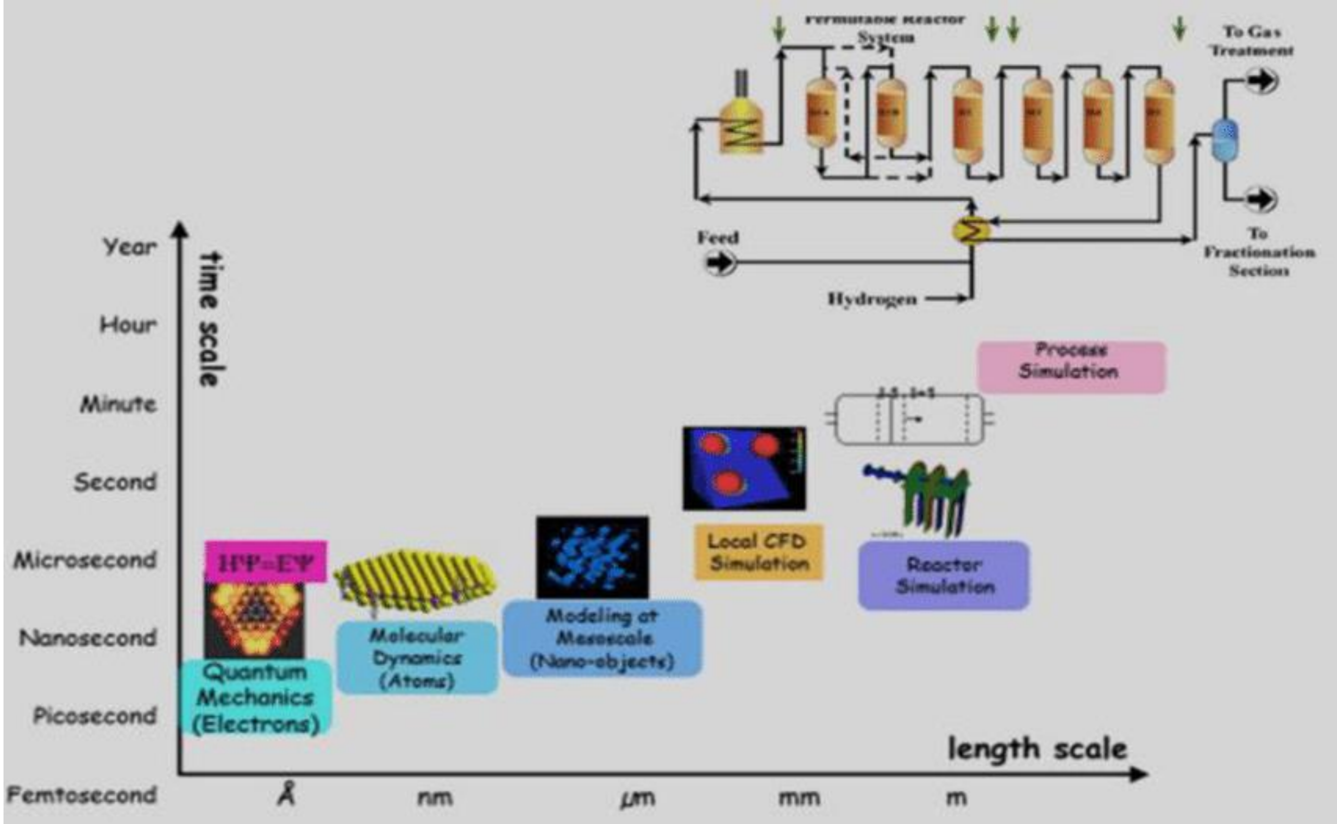
Q ~ W

dU = Q+W

<u>Black Holes, 2008</u>

"Debatable"

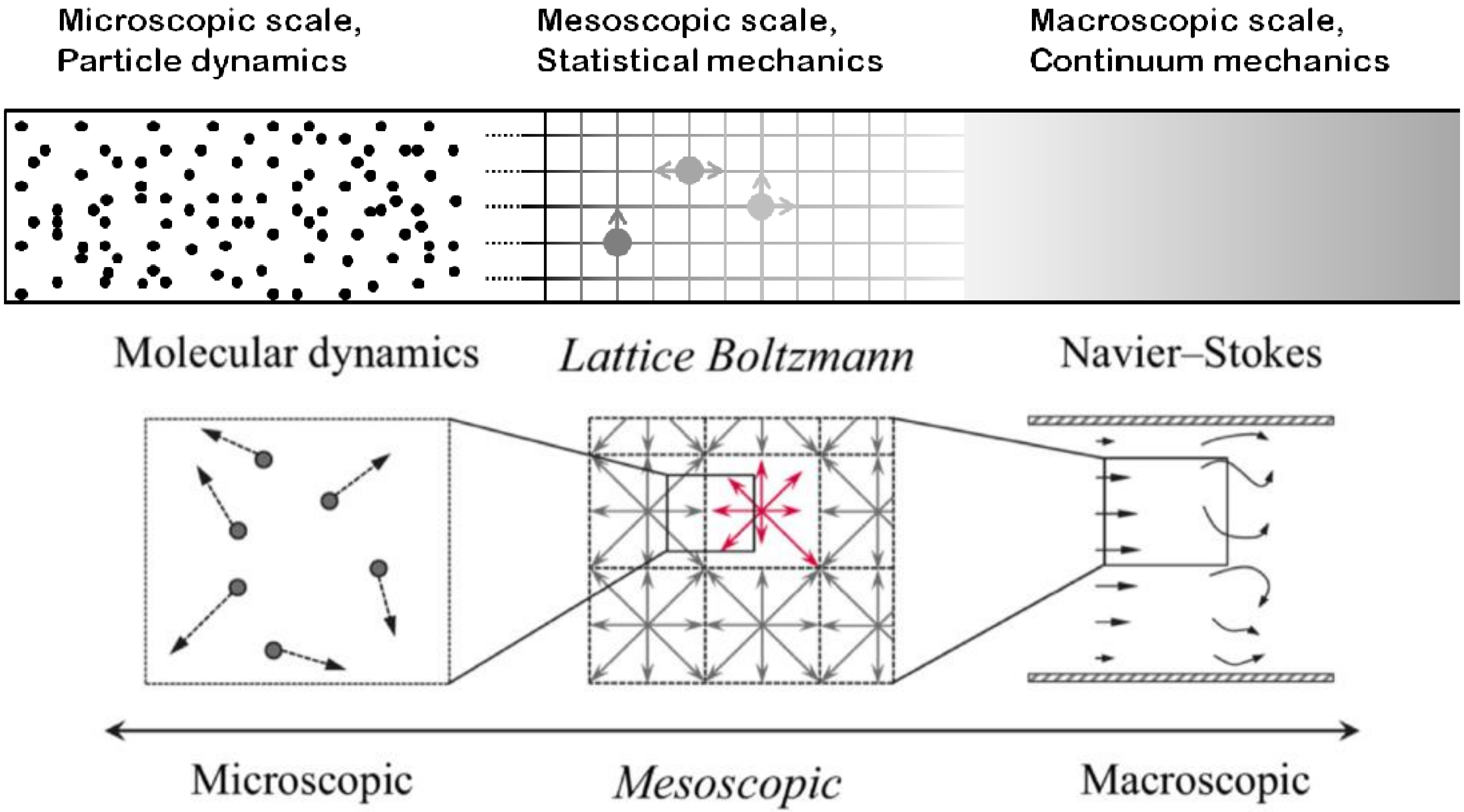
Multiscale Modeling



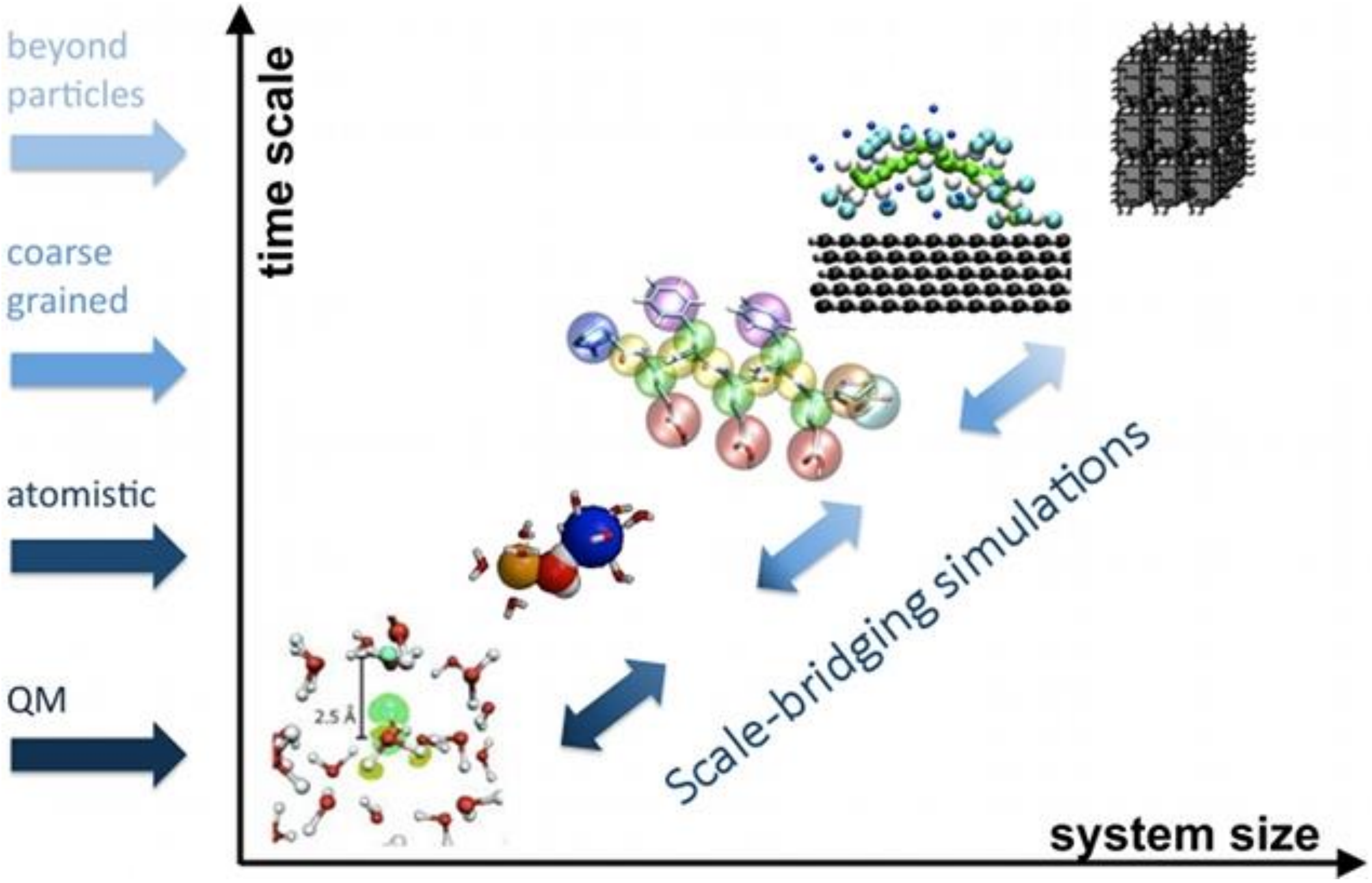
- Thermodynamics
- Reaction Engineering
- Transport Phenomena

(Flow profiles: velocity, pressure, temp, concentration)

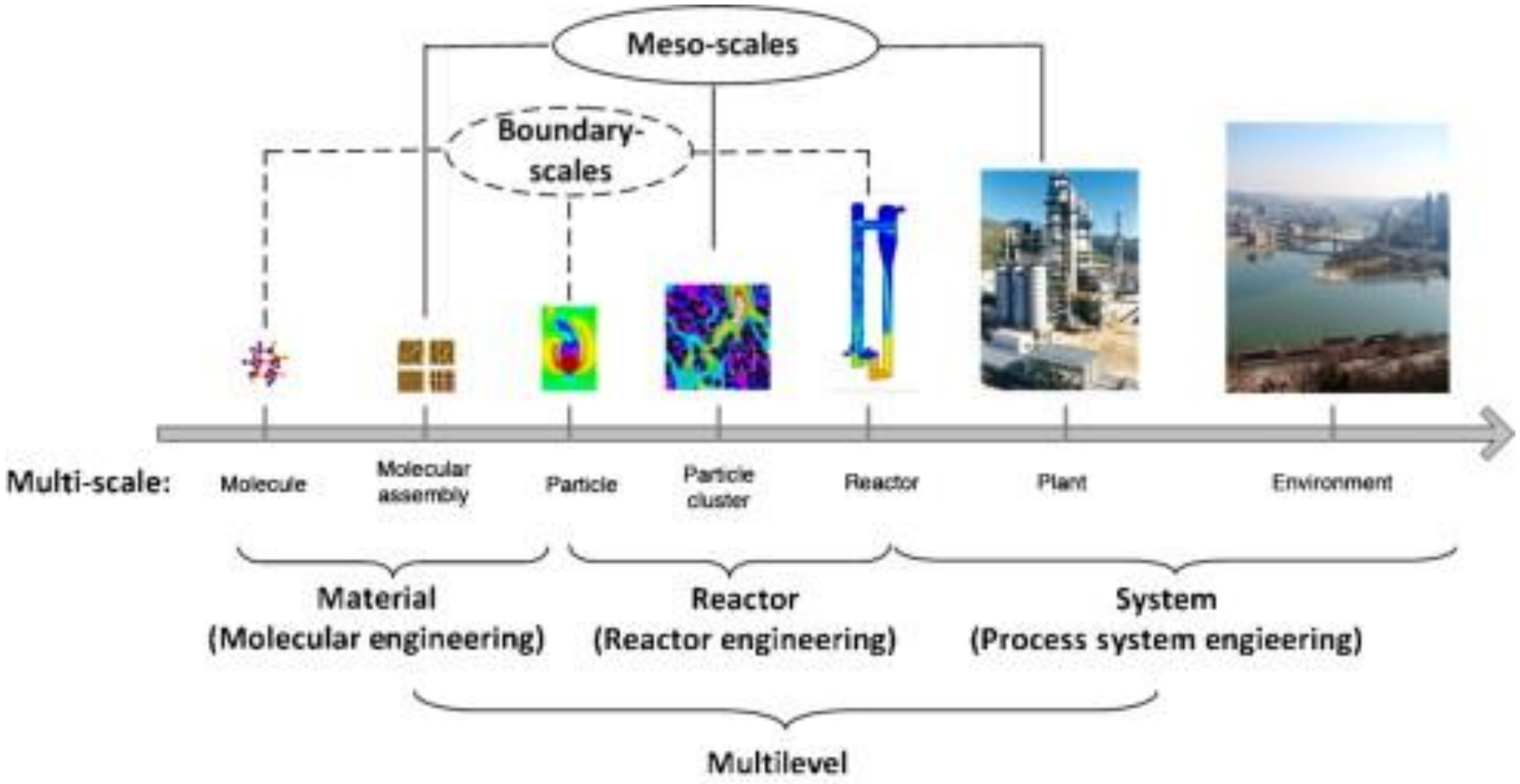
Physics of Modeling



Materials Modeling_Applications



Multiscale Modeling_Applications



Mathematical Modeling?

"Mathematical representation of any physical/real/existing systems"

Comprising of,

- ***Set of equations (algebraic or integral or differential)***
- ***Set of variables (dependent/response & independent/predictor)***

"DOF analysis (model evaluation)"

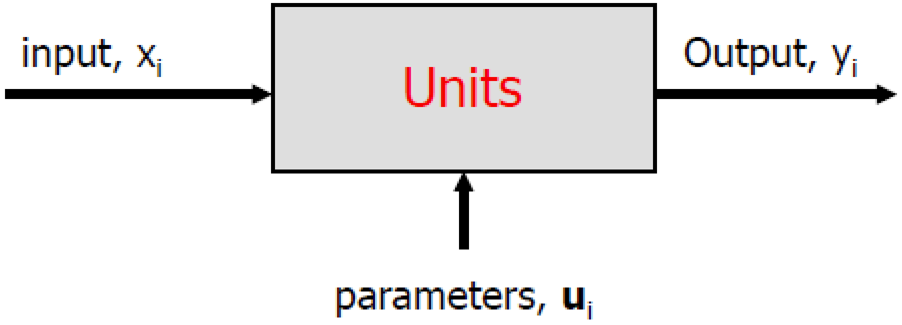
General form of a Mathematical System

$$\frac{d}{dt}x(t) = f(x, p)$$

where:

- x is the state variables
- p is a set of parameters
- f is a nonlinear vector-valued function
- t is the independent variable

Mathematical Modeling



i.e.: $f_i(x_i, y_i, \mathbf{u}_i) = 0$, then, $y_i = g_i(x_i, \mathbf{u}_i)$

$f_i(x_i, y_i, \mathbf{u}_i) = 0 \downarrow$ fixed

$y_i = g_i(x_i, \mathbf{u}_i) \downarrow$ calculated

$$NE = n \left\{ \begin{array}{l} f_1(x_1, x_2, \ldots, x_m) = 0 = \overbrace{r_1}^{\text{residuals}} \\ f_2(x_1, x_2, \ldots, x_m) = 0 = r_2 \\ \vdots \\ \underbrace{f_n(x_1, x_2, \ldots, x_m)}_{NV = m} = 0 = r_n \end{array} \right.$$

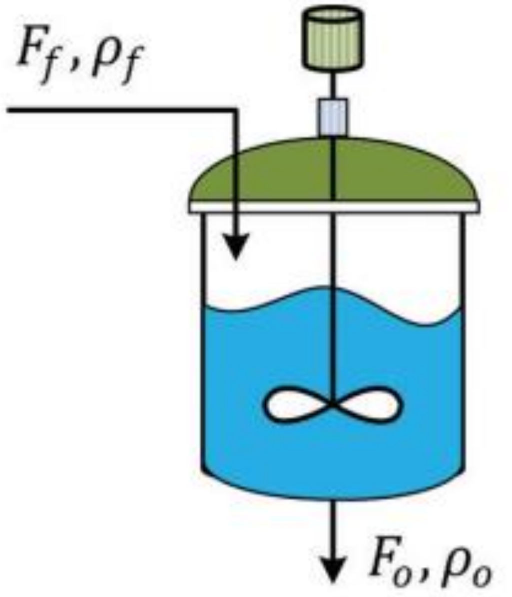
DOF = (NV - NE)

For model simulation,	NV= NE	*(well-specified)*
	NV>NE	*(under-specified)*
	NV < NE	*(over-specified)*

*If NV>NE, the remaining NV – NE = ***NP variables*** (design variables) have to be selected and fixed (as model parameters).

DOF analysis of a non-reacting system

Consider the perfectly mixed storage tank shown below. A liquid stream with volumetric rate F_f and density ρ_f flow into the tank. The outlet stream has volumetric rate F_o and density ρ_o. Our objective is to develop a mathematical model for the variations of the tank holdup, that is, the volume (V) of the fluid in the tank.
Carry out the DOF analysis for the system.



Overall mass balance

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

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

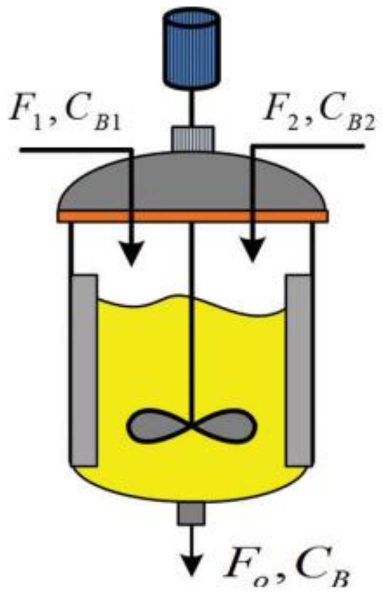
$$F_o = \alpha\sqrt{L}$$

DOF = (N_V - N_E)

N_V= 02 (L, F_o) & N_E= 02

DOF = 0 (model specified)

DOF analysis of a reacting system



$$A + B \rightarrow C$$

$$r\left(\frac{\text{mol}}{\text{m}^3\ \text{s}}\right) = \frac{k_1 C_B}{(1 + k_2 C_B)^2}$$

Overall mass balance

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

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

Component-mass balance

$$V\frac{dC_B}{dt} = F_1\left(c_{B1} - c_B\right) + F_2\left(c_{B2} - c_B\right) - rV$$

DOF = (N_V - N_E)

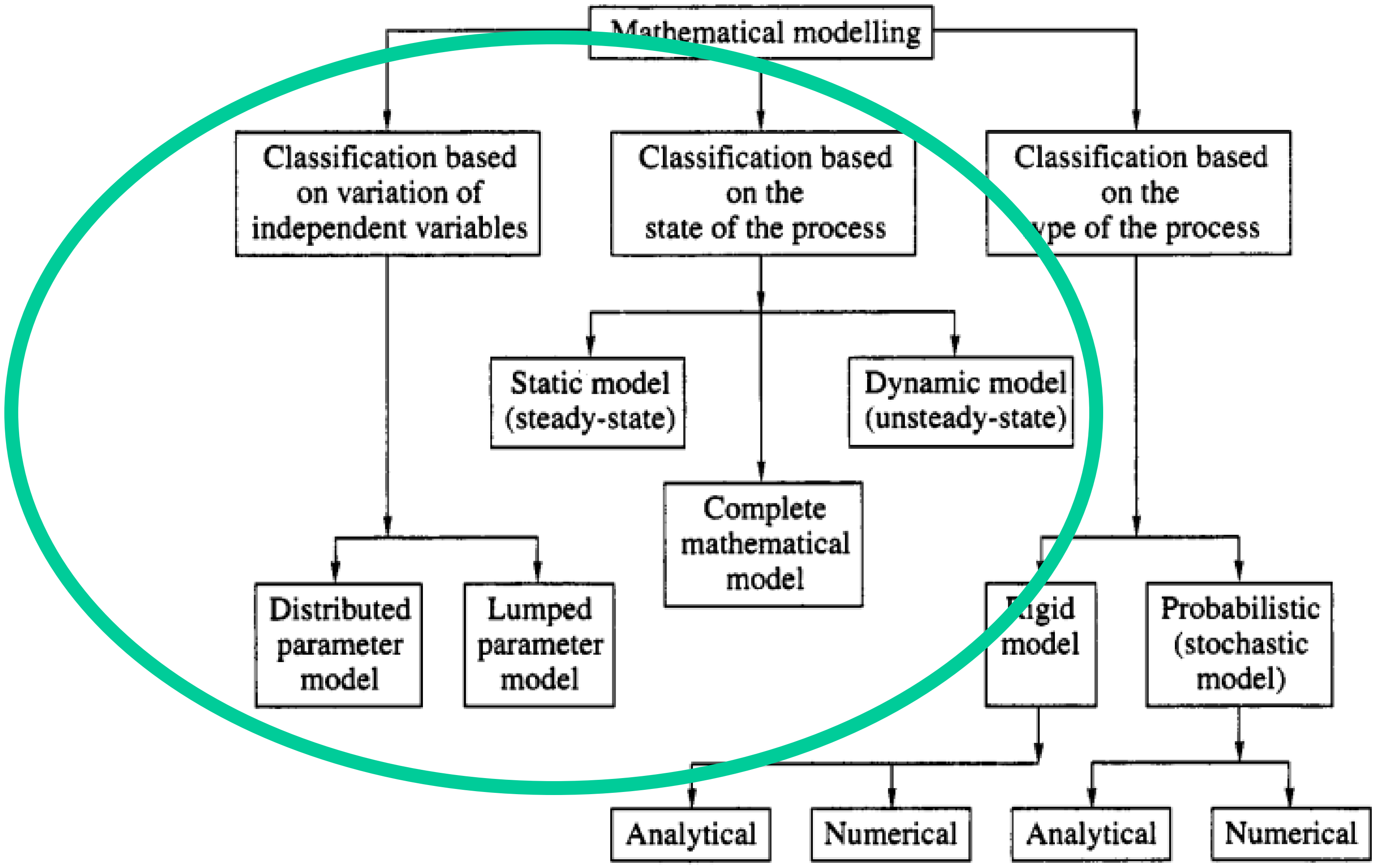
N_V= 03 (L, F_o, C_B) & N_E= 03

DOF = 0 (model specified)

Note: *Reactant A is assumed to be in excess & not involved in the reaction.*

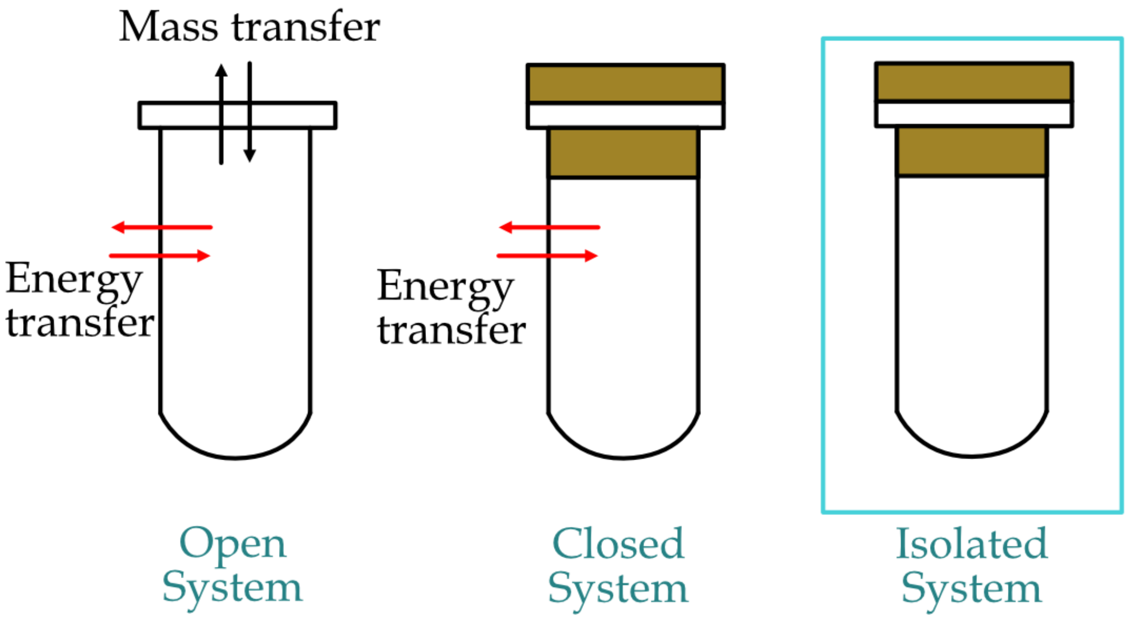
Module 2: Classification of Modeling & Simulations

Classification_Mathematical Modeling



Classification_Model System (Process)

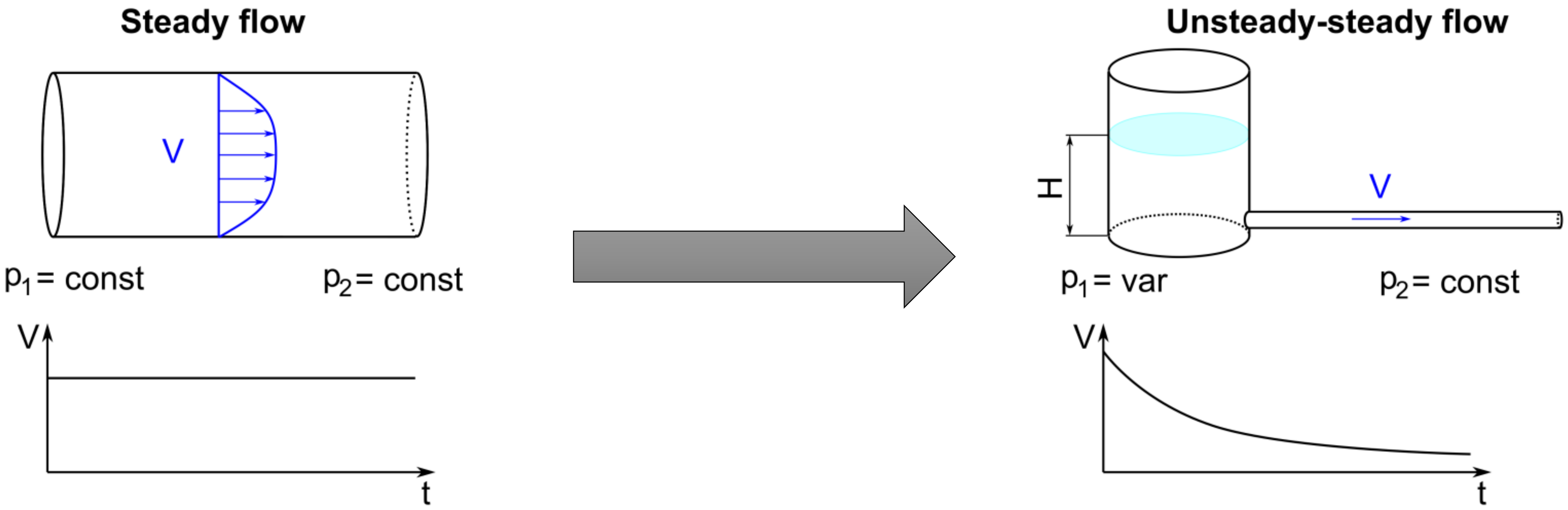
- ➢Open-System (continuous process)
- ➢Closed-system (batch process)
- ➢Isolated-system



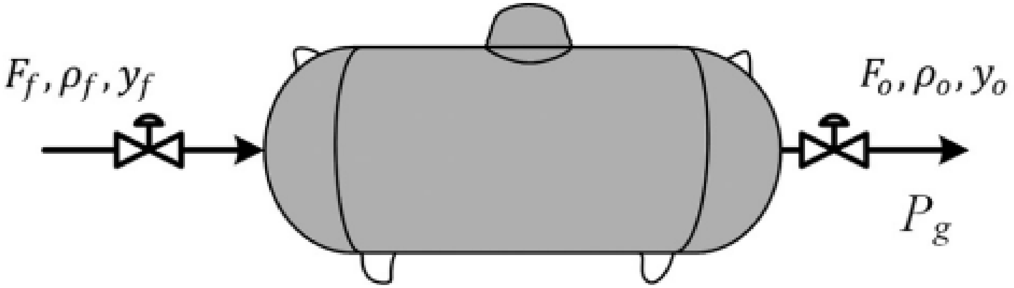
Classifications of Models: Based on Model Behavior

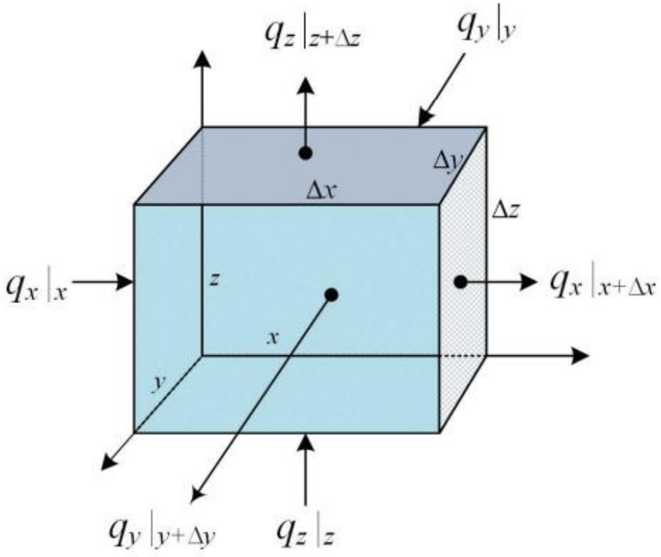
- Steady Vs Unsteady Model
- Stationary vs Transient Model
- Static Vs Dynamic Model
- Lumped (time, 0-D) Vs Distributed Model (time, 1-D, 2-D & 3-D)
- Deterministic (rigid) Vs Stochastic (probabilistic) Model

Steady Vs Unsteady Model



Lumped Vs Distributed Model





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

$$\overbrace{\rho C_p \frac{\partial T}{\partial t}}^{\text{accum.}} = \overbrace{-\rho C_p\left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z}\right)}^{\text{transport by bulk flow}} + \overbrace{k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)}^{\text{transport by thermal diffusion}} + \overbrace{\Phi}^{\text{gen.}}$$

"Set of ODE equations"

↓

Lumped Model

"Set of PDE equations"

↓

Distributed Model

Lumped Vs Distributed Model

- **Lumped Model:** No spatial (x, y, z) variation in temperature, pressure and concentration. only variation is with time.
  (*e.g. reaction engineering problems, **ODE in nature***)

or

"The states (T, P, concentration) in lumped parameter systems are concentrated in single point and are not spatially distributed"

- **Distributed Model:** Both time and spatial variation in flows/states (Temp, pressure and conc.)
  (*e.g. fluid flow, mass and heat transport, **PDE in nature***)

Chemical Engineering_Fundamental Laws

Steady-state model

Unsteady-state model

Fourier's law of heat conduction

$$\frac{Q}{A} = -k\left(\frac{dT}{dx}\right)$$

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{\dot{q}}{k} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$$

Fick's first law of diffusion

$$q_m = J = -D\left(\frac{dc}{dx}\right)$$

$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z}}^{\text{Convection}}\right) + \overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}^{\text{Diffusion}} + \overbrace{R_A}^{\text{reaction}}$$

Newton's law of viscosity

$$\tau = -\mu\left(\frac{dv}{dx}\right)$$

$$\rho\frac{\partial v_x}{\partial t} + \rho\left(v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z}\right) = \mu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right) - \frac{\partial p}{\partial x} + \rho g_x$$

Module 3: Development & Validation of Model

Steps involved in Modeling & Simulations

- Model Development
- Model Solving
- Model Analysis
- Model Optimization
- Model Validation

* ***Model:*** Fundamental/data-driven model

Approach to Modeling

- Empirical modeling (theoretical modeling)
- Fundamental (First-Principles) based modeling
- Data-driven modeling

Approach to Data Modeling

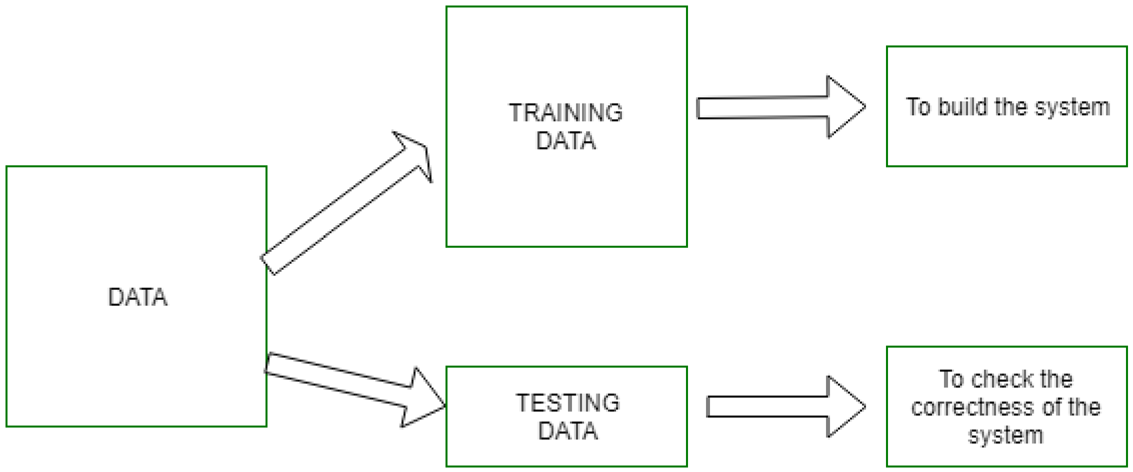
- Collection of data
- Understanding data types (i.e. variables)
- Data reconciliation and identifying outliers
- Data processing
- Model development, error analysis, optimization

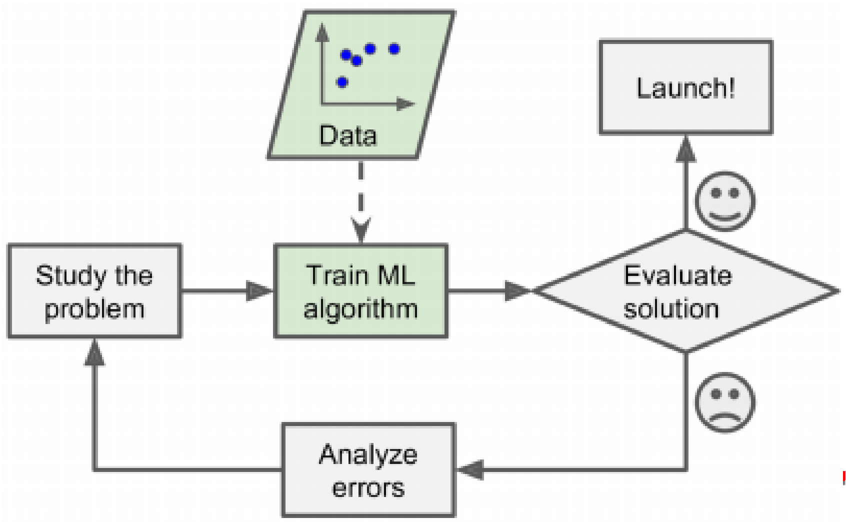
Input
$(V_1, V_2, V_3....V_n)$ → ***Function*** → **$(V_1, V_2, V_3....V_n)$**
Output

$f\,(V_1, V_2, V_3....V_n) = 0$

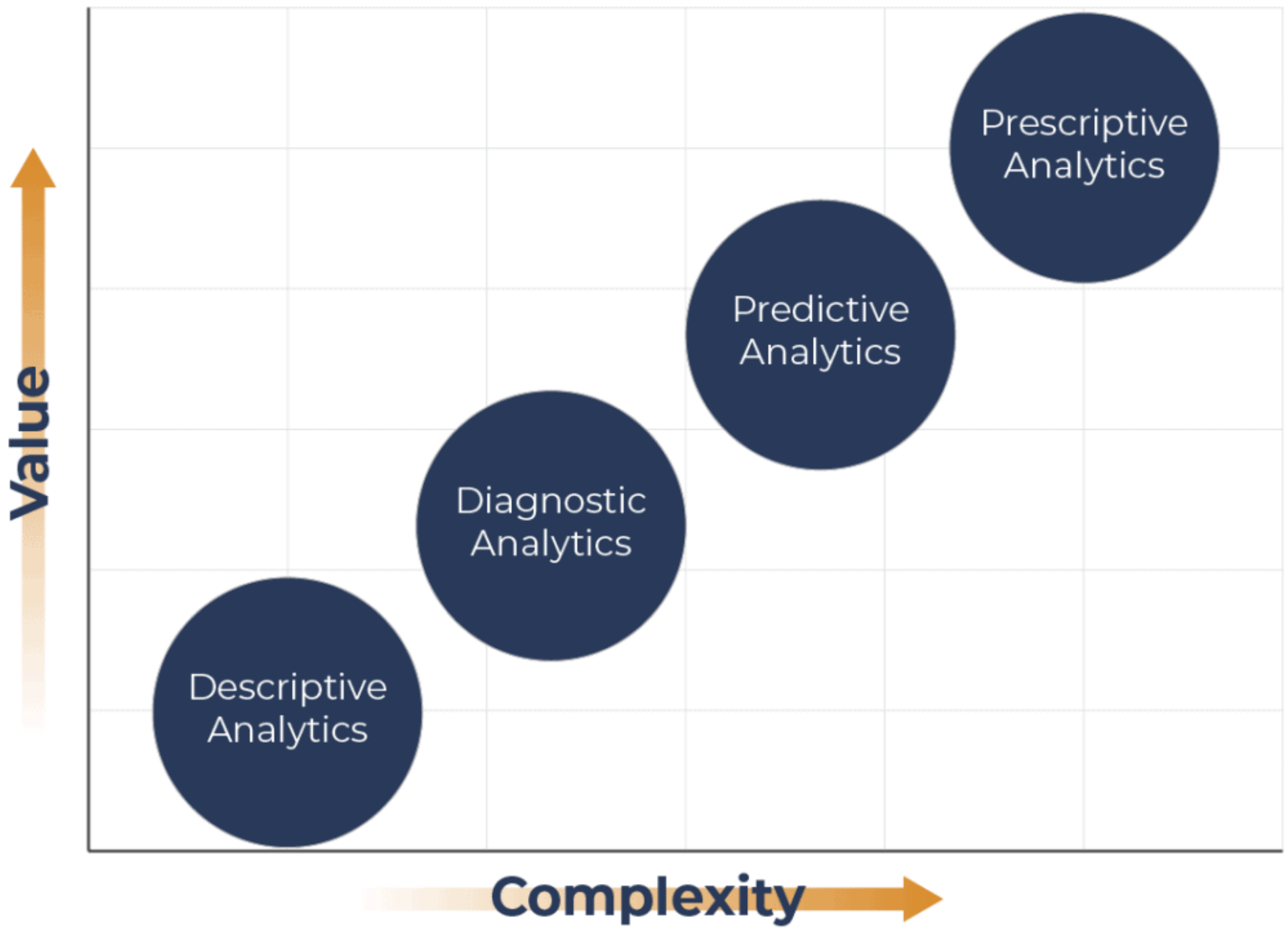
$V_1 = f(V_2, V_3....V_n)$

$V_2 = f(V_1, V_3, ...V_n)$ ....so on

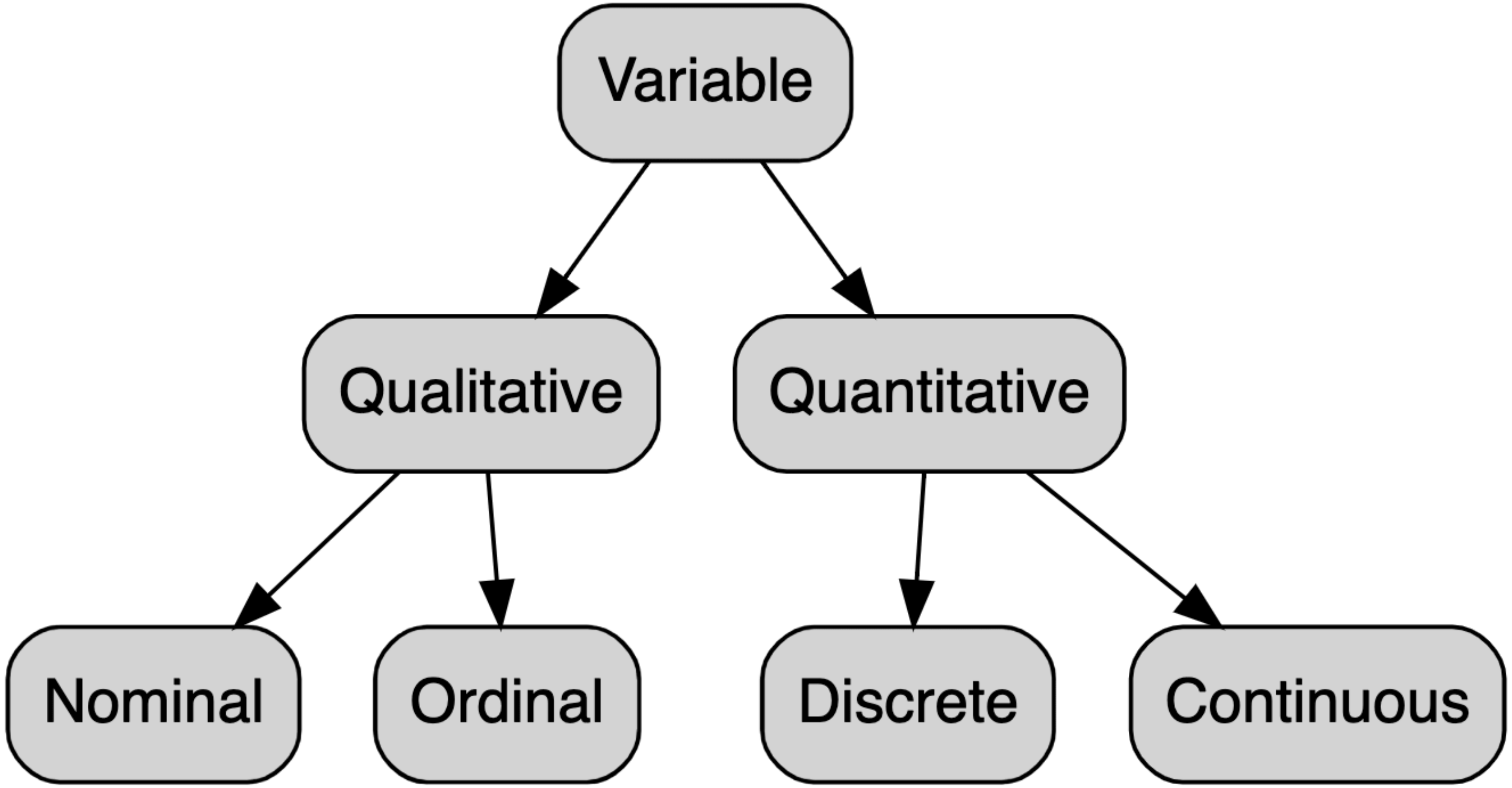




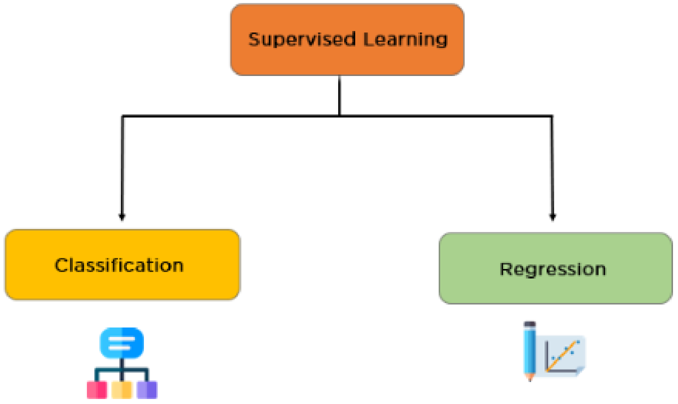
Approach to Data Analytics/Modeling

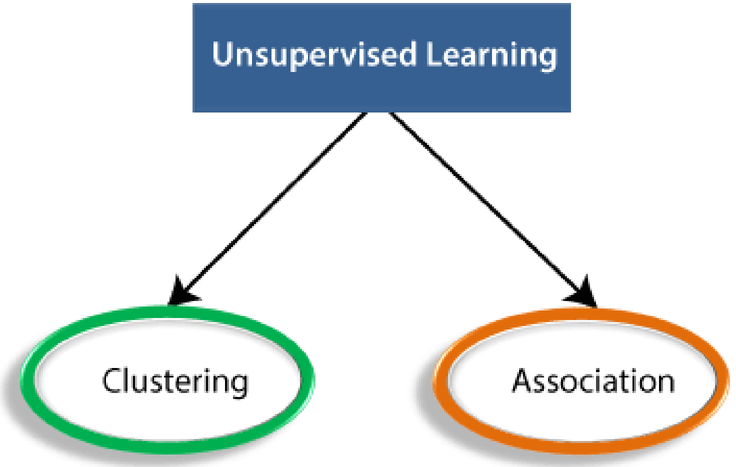


Variable-types



Machine Learning Algorithm





Machine Learning Algorithms *(sample)*

	Unsupervised	Supervised
Continuous	• Clustering & Dimensionality Reduction ◦ SVD ◦ PCA ◦ K-means	• Regression ◦ Linear ◦ Polynomial • Decision Trees • Random Forests
Categorical	• Association Analysis ◦ Apriori ◦ FP-Growth • Hidden Markov Model	• Classification ◦ KNN ◦ Trees ◦ Logistic Regression ◦ Naive-Bayes ◦ SVM

Data-Model Types

Linear Regression Model:

$$Y = \beta o + \beta_1 * x_1 + \beta_2 * x_2 + \beta_3 * x_3 + \ldots. \beta_n * x_n$$

Nonlinear Regression Model:

$$Y = \beta_1 * x_1^2 + \beta_2 * x_1 x_2 + \beta_3^2 * x_3 + \ldots\ldots \beta^2{}_n * x_n$$

ANN model: **"Black-box model"**

Analysis of Data-Model (KPIs)

Performance Indicator	Equation
Coefficient of determination (R^2)	$R^2 = 1 - \frac{\sum_{i=1}^{n}(H_{i,m} - H_{i,c})^2}{\sum_{i=1}^{n}(H_{i,m} - \overline{H_m})^2}$
Root mean square error (*RMSE*)	$RMSE = \left[\frac{1}{n}\sum_{i=1}^{n}(H_{i,c} - H_{i,m})^2\right]^{1/2}$
Mean percentage error (MPE)	$MPE(\%) = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{H_{i,c} - H_{i,m}}{H_{i,m}}\right) \times 100$
Mean absolute percentage error (MAPE)	$MPE(\%) = \frac{1}{n}\sum_{i=1}^{n}\left\lvert\left(\frac{H_{i,c} - H_{i,m}}{H_{i,m}}\right)\right\rvert \times 100$

t-value:
Higher the t-value, the greater the confidence & high reliability of the predictive power of coefficient.

p-value:
Lower the p-value, the greater the confidence & high reliability of the predictive power of coefficient

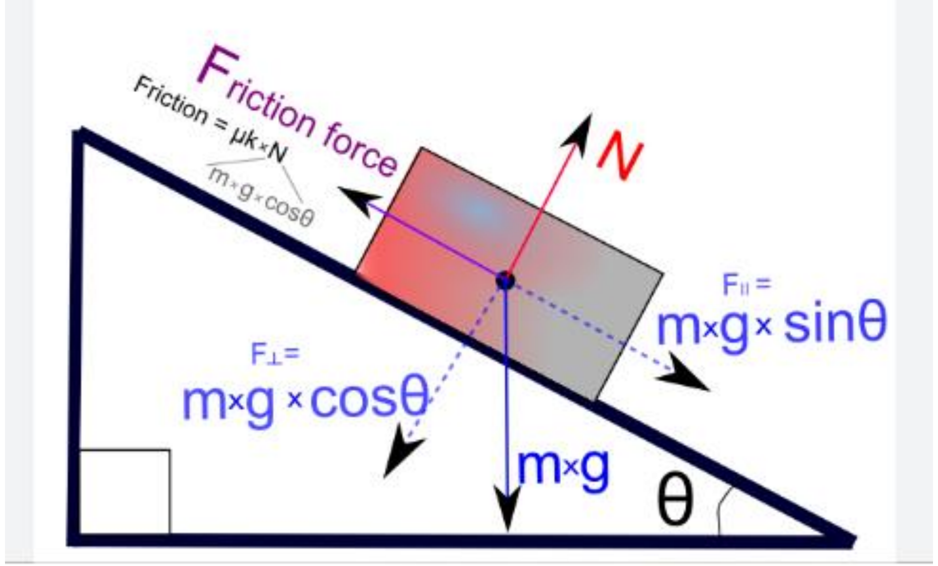
CL = [1- (p-value)]

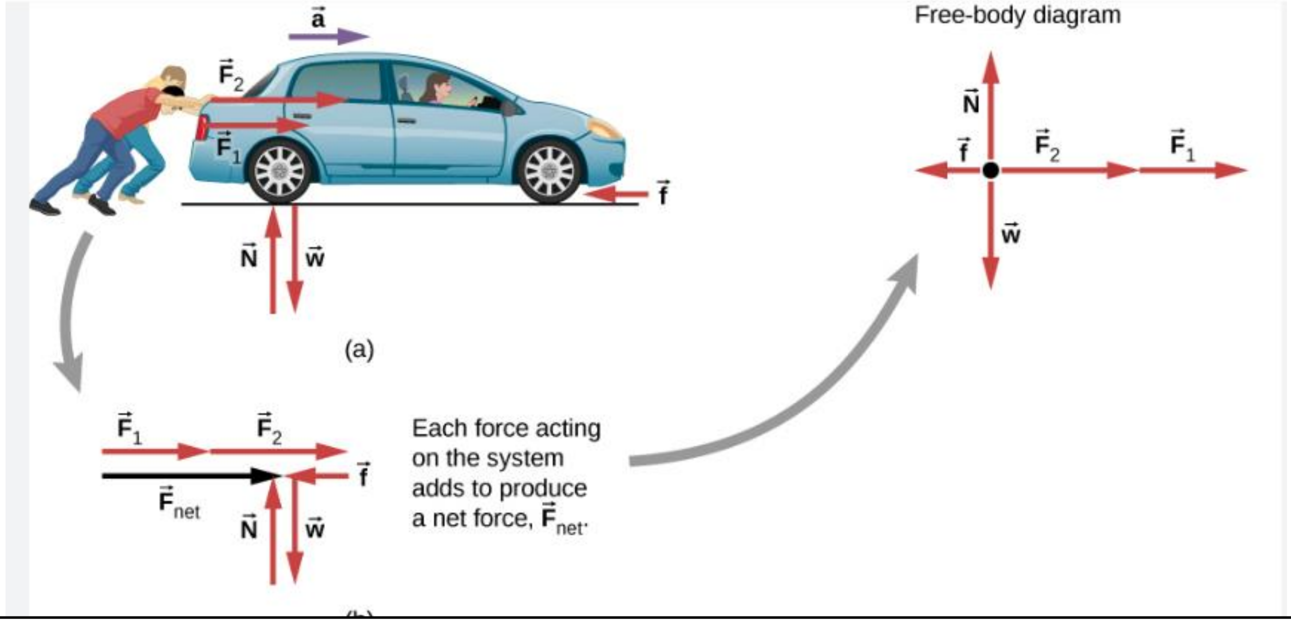
Standard deviation (σ) & standard error (SE):

SE = (σ/n)

F-value: null vs alternate hypothesis

Approach to Fundamental Modeling





- Force/Momentum Balance
- Mass Balance
- Energy Balance
- Charge Balance
- Entropy Balance

- *Simply, by applying laws of conservation to a model system (CV: open/closed)*

- *Model type: Lumped or Distributed (0-D to 3-D)*
- *Lumped: ODE systems (steady/unsteady state)*
- *Distributed: PDE systems (unsteady/steady state)*

Generalized Balance Equation

$$\text{in} - \text{out} + \text{generation} - \text{consumption} = \text{accumulation}$$

Note: Applicable to momentum-balance, mass-balance and energy-balance for any chemical engineering systems

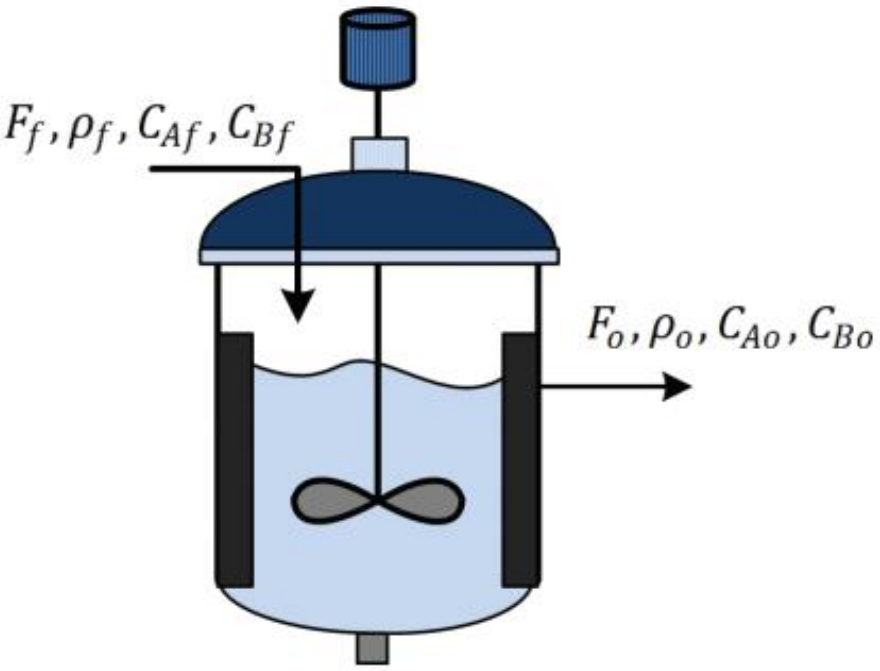
Module 4: Modeling of Chemical Engineering Systems: Reaction Engineering

Mass/Mole Balance Equation

$$\left\{\begin{matrix}\text{Rate of}\\ \text{accumulation}\end{matrix}\right\} = \left\{\begin{matrix}\text{Rate of mass}\\ \text{in}\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of mass}\\ \text{out}\end{matrix}\right\}$$

$$\left\{\begin{matrix}\text{Rate of}\\ \text{accumulation}\\ \text{of moles of A}\end{matrix}\right\} = \left\{\begin{matrix}\text{Rate of}\\ \text{moles of}\\ A\ \text{in}\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of}\\ \text{moles of}\\ A\ \text{out}\end{matrix}\right\} + \left\{\begin{matrix}\text{Rate of}\\ \text{generation of}\\ \text{moles of}\ A\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of}\\ \text{consumptions}\\ \text{of moles of}\ A\end{matrix}\right\}$$

Isothermal CSTR Model with single reaction



$$A \rightarrow B,\ r = kc_A.$$

Overall mass-balance

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

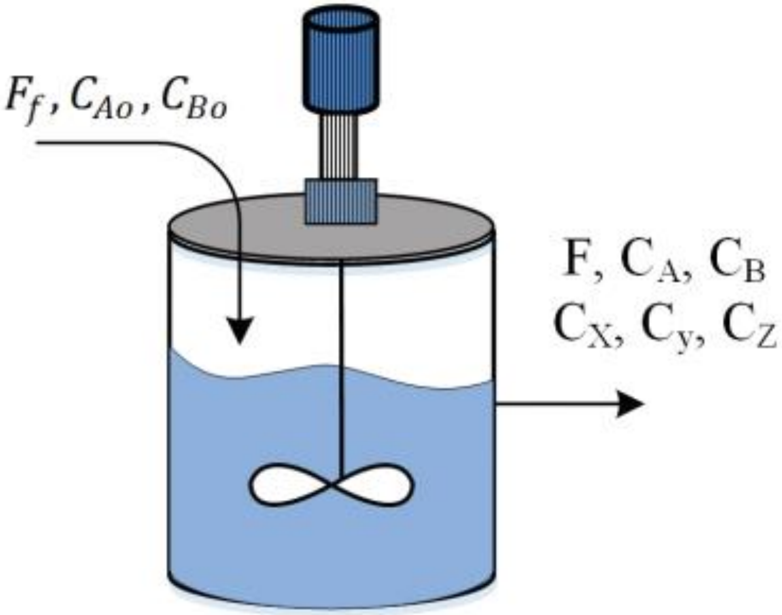
Component mass-balance

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

$$V\frac{dC_A}{dt} = F_f(C_{Af} - C_A) + r_A V$$

Note: Since the system is well mixed, concentration C_A and C_B is equal to the effluent concentration C_{Ao} and C_{Bo}.

CSTR Model with multiple reactions



$$A + B \xrightarrow{k_1} X$$

$$B + X \xrightarrow{k_2} Y$$

$$B + Y \xrightarrow{k_3} Z$$

Component wise mass-balance

$$\frac{dC_A}{dt} = \frac{(F_0 C_{Ao} - FC_A)}{V} - k_1 C_A C_B$$

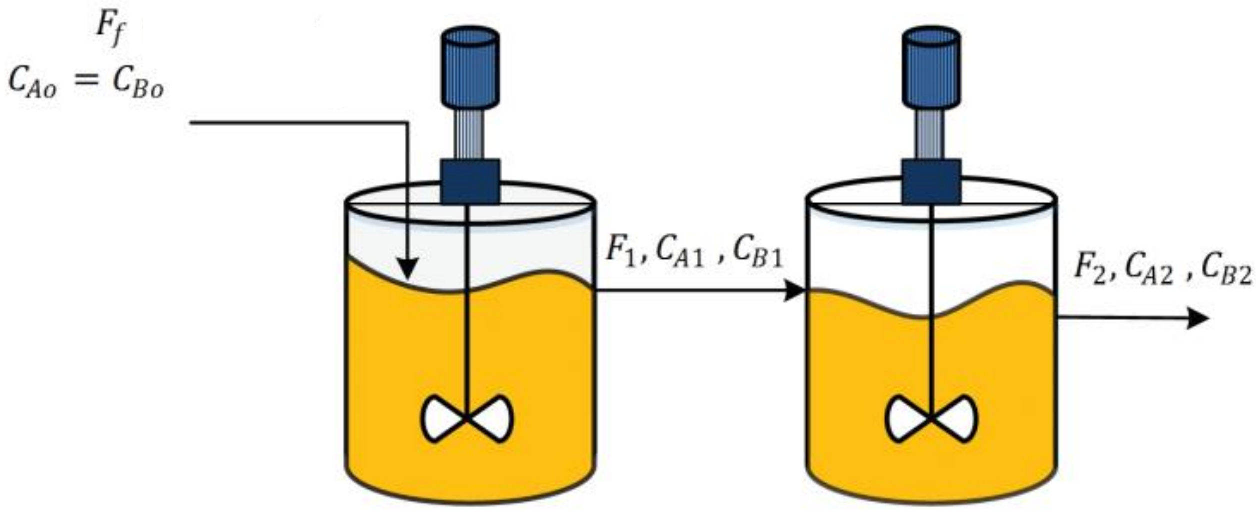
$$\frac{dC_B}{dt} = \frac{(F_0 C_{Bo} - FC_B)}{V} - k_1 C_A C_B - k_2 C_X C_B - k_3 C_Y C_B$$

$$\frac{dC_X}{dt} = \frac{(F_0 C_{Xo} - FC_X)}{V} + k_1 C_A C_B - k_2 C_X C_B$$

$$\frac{dC_Y}{dt} = \frac{(F_0 C_{Yo} - FC_Y)}{V} + k_2 C_X C_B - k_3 C_Y C_B$$

$$\frac{dC_Z}{dt} = \frac{(F_0 C_{Zo} - FC_Z)}{V} + k_3 C_Y C_B$$

CSTR-in-Series Model



Component mass-balance for each tank

Tank 1

$$\frac{dC_{A1}}{dt} = \frac{F_f}{V_1}(C_{A0} - C_{A1}) - kC_{A1}C_{B1}$$

$$\frac{dC_{B1}}{dt} = \frac{F_f}{V_1}(C_{B0} - C_{B1}) - kC_{A1}C_{B1}$$

Tank 2

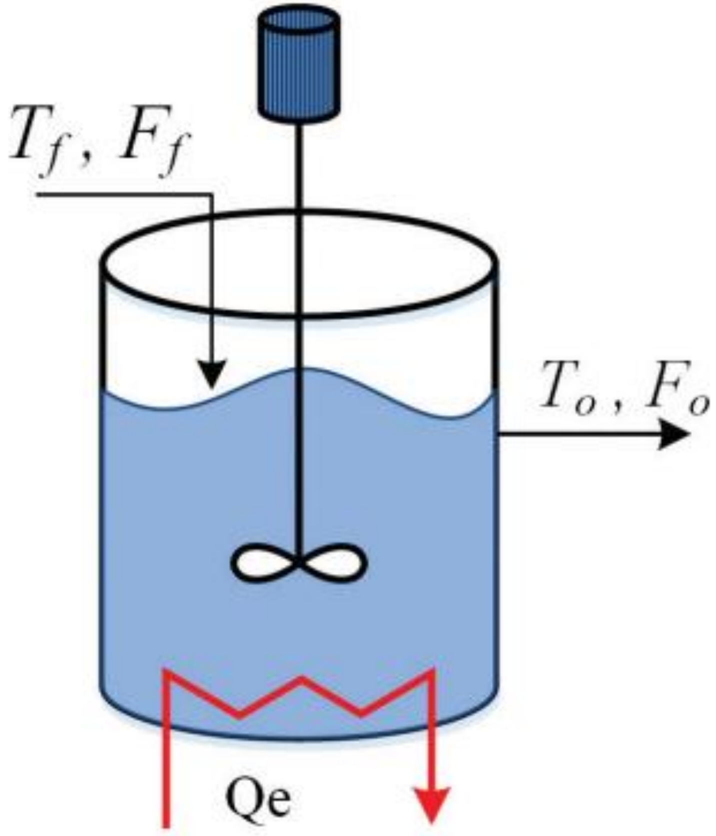
$$\frac{dC_{A2}}{dt} = \frac{F_f}{V_2}(C_{A1} - C_{A2}) - kC_{A2}C_{B2}$$

$$\frac{dC_{B2}}{dt} = \frac{F_f}{V_2}(C_{B1} - C_{B2}) - kC_{A2}C_{B2}$$

Energy Balance Equation

$$\left\{\begin{matrix}\text{Rate of}\\ \text{Accumulation}\\ \text{of energy}\end{matrix}\right\} = \left\{\begin{matrix}\text{Rate of}\\ \text{energy}\\ \text{input}\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of}\\ \text{energy}\\ \text{output}\end{matrix}\right\} + \left\{\begin{matrix}\text{Rate of}\\ \text{energy}\\ \text{generated}\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of}\\ \text{energy}\\ \text{consumed}\end{matrix}\right\} \pm \left\{\begin{matrix}\text{Rate of energy}\\ \text{exchanged}\\ \text{with the}\\ \text{surrounding}\end{matrix}\right\}$$

Non-isothermal CSTR Model



Overall mass-balance

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

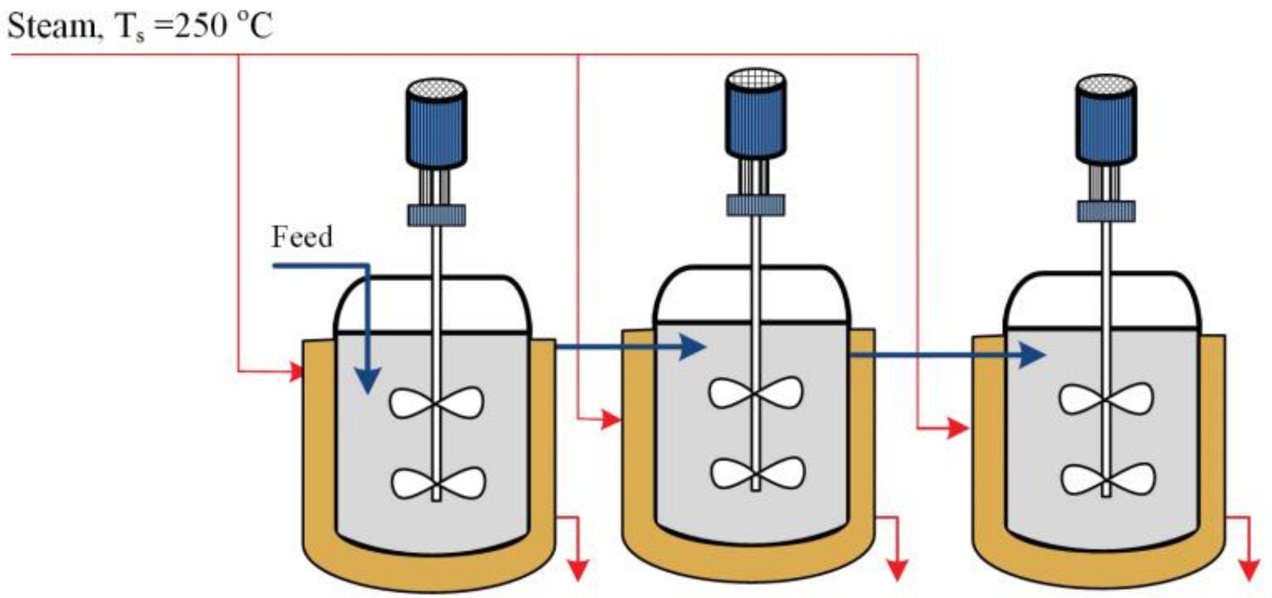
Component mass-balance

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

Energy-balance

$$\rho C_p V\frac{dT}{dt} = \rho F_f C_p\left(T_f - T\right) + \left(-\Delta H_r\right)V_r - Q_c$$

Heated Stirred Tank-in-Series Model



Energy-balance equation for each tank

$$\frac{dT_1}{dt} = \frac{\dot{m}}{m}(T_o - T_1) + \frac{UA}{mC_p}(T_s - T_1)$$

$$\frac{dT_2}{dt} = \frac{\dot{m}}{m}(T_1 - T_2) + \frac{UA}{mC_p}(T_s - T_2)$$

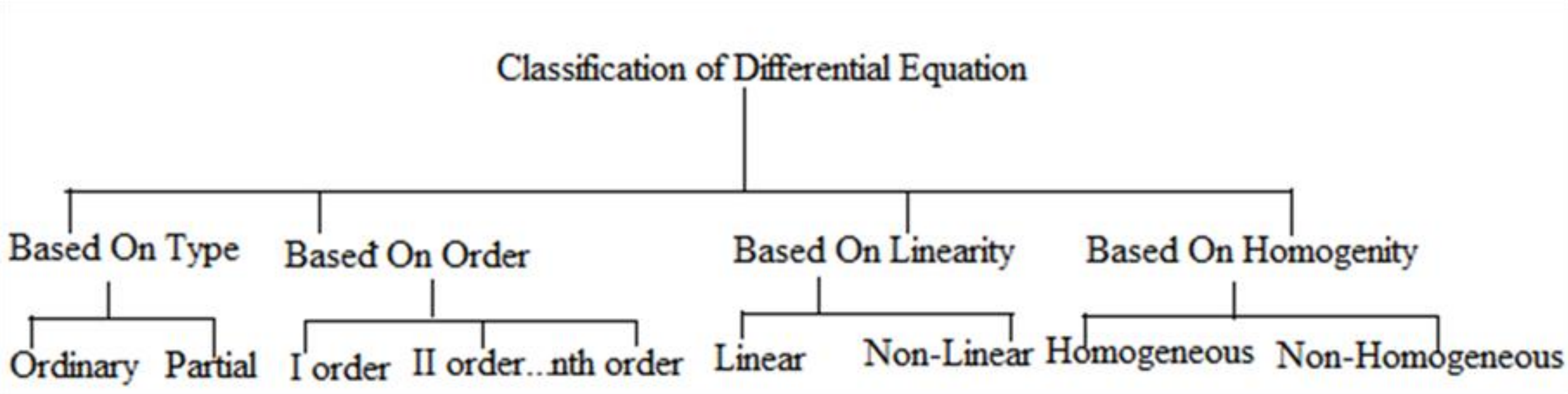
$$\frac{dT_3}{dt} = \frac{\dot{m}}{m}(T_2 - T_3) + \frac{UA}{mC_p}(T_s - T_3)$$

$$\frac{dm}{dt} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}}$$

$$\frac{d\left(mC_p(T_1 - T_{\text{ref}})\right)}{dt} = \dot{m}C_p(T_0 - T_1) - \dot{m}C_p(T_1 - T_{\text{ref}}) + UA(T_s - T_1)$$

Module 5: Solving System of Ordinary Differential Equations (ODEs)

Classification of ODEs



Major emphasis is on ***first-order, linear, non-homogeneous*** type of ODEs (***most common in reaction engineering***)

$$\frac{dy}{dx} + Py = Q$$

Where, y= state-variable, dependent (**e.g., T, C_A Pressure, Velocity**)
x= independent-variable (**e.g. time, volume, length**)
P & Q are either constant or function of x

Solution of ODEs

Exact methods:

- General solution of linear differential equation
- Method of separation of variables
- Method of integrating factors (IFs)

Numerical methods (iterative methods):

- **Euler's method (backwards & forward differentiation methods)**
- **Runge-Kutta method (2^{nd}/4^{th} order) {modified Euler's method}**
- **Heun's methods**

ODE Solving using RK-2nd/4th order method

$$\frac{dy}{dx} = f(x,y)$$

IC: $y(x_0) = y_o$

Taylor's series for complete solution of model at intial condition ($x = x_0$) (good for higher order derivatives),

$$y(x) = y(x_0) + y'(x_0)(x - x_0) + \frac{1}{2!}y''(x_0)(x - x_0)^2 + \ldots + \frac{1}{n!}y^n(x_0)(x - x_0)^n$$

Solution (Runge-Kutta Method),

$$y_{i+1} = y_i + \frac{h}{2}(k_1 + k_2)$$ *(RK-2nd order)*

$$y_{i+1} = y_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$ *(RK-4th order)*

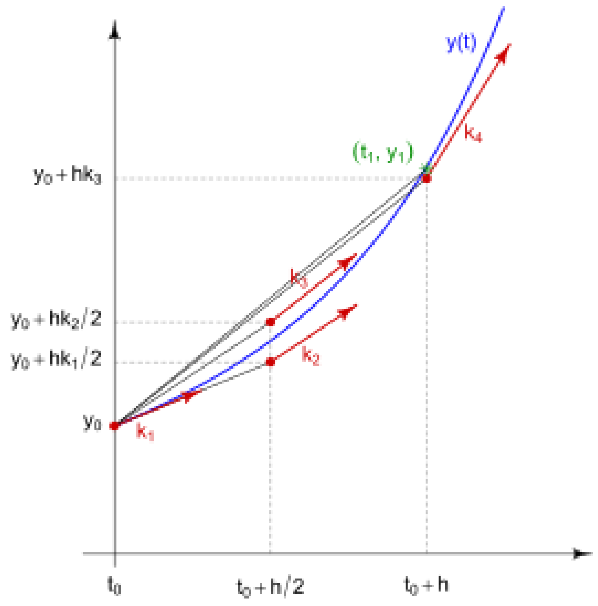
Where,

$$k_1 = f(x_i, y_i)$$

$$k_2 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_1\right)$$

$$k_3 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}k_2\right)$$

$$k_4 = f(x_i + h, y_i + k_3 h)$$



***Note**: Runge–Kutta methods are a family of implicit/explicit iterative Euler method, used in **temporal discretization** for the approximate solutions of simultaneous nonlinear equations.*

Problem Statements: Initial Value Problem

Use the second-order Runge-Kutta method (RK2) to solve the following ODE:

$$\frac{dy}{dx} = 2x + y^2 x$$

where $y(0) = 2$

Solve for $h = 0.1$ and compute $y(0.1)$.

Note: *Solve the ODE numerically and also using R ("**desolve**") or MATLAB ("**ode45**")*

Solution of ODEs: IVP (initial value problem)

$$\frac{dy}{dx} + Py = Q$$

y(x=0)= yo , initial condition

P & Q are model parameters (constants) or function of x

ODEs are solved analytically & also using numerical methods algorithms available in **R or MATLAB** (e.g. ***desolve, ode-45, ode-23***)

$$V\frac{dC_A}{dt} = F_f(C_{Af} - C_A) + r_A V$$

$$\frac{dT_1}{dt} = \frac{\dot{m}}{m}(T_o - T_1) + \frac{UA}{mC_p}(T_s - T_1)$$

Classical examples of ODEs (mass & energy balance eqn) in reaction engineering **(lumped-parameter models)**

Problem Statements on IVP

(Applications in Chemical Engineering)

Problem Statement_IVP_Fluidized Packed Bed Catalytic Reactor

The irreversible gas phase catalytic reaction

$$A \rightarrow B$$

is to be carried out in a fluidized packed bed reactor. Material and energy balances for this reactor yield

$$\frac{dP}{d\tau} = P_e - P + H_g\left(P_p - P\right)$$

$$\frac{dT}{d\tau} = T_e - T + H_T\left(T_p - T\right) + H_W\left(T_W - T\right)$$

$$\frac{dP_p}{d\tau} = \frac{H_g}{A}\left\{P - P_p\left(1+K\right)\right\}$$

$$\frac{dT_p}{d\tau} = \frac{H_T}{C}\left\{\left(T - T_p\right) + FKP_p\right\}$$

$$K = 6\times10^{-4}\exp\left(20.7 - \frac{1000}{T_p}\right)$$

where
- T (°R) is the temperature of the reactant
- P (atm) is the partial pressure of the reactant
- T_p (°R) is the temperature of the reactant at the surface of the catalyst
- P_p (atm) is the partial pressure of the reactant at the surface of the catalyst
- K is the rate constant (dimensionless)
- τ is time (dimensionless)
- and the subscript e is the inlet condition

The parameters and constants used in the model equations are

$$H_g = 320,\quad T_e = 600,\quad H_T = 266.67,\quad H_W = 1.6,\quad T_W = 720,\quad F = 8000,\quad A = 0.17142,$$
$$C = 205.74,\quad P_e = 0.1$$

Solve the differential equations from $\tau = 0$ to 1500 and plot the changes of dependent variables. Initial conditions are $P(0) = 0.1$, $T(0) = 600$, $P_p = 0$, and $T_p = 761$.

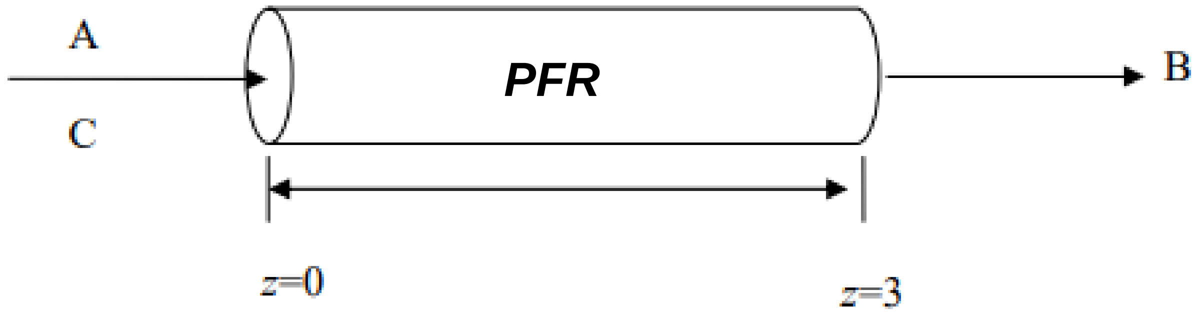
Problem Statement_IVP_Biochemical Reaction

A biological process involving the growth of a biomass from substrate can be represented as

$$\frac{dB}{dt} = \frac{kBS}{K+S}, \quad \frac{dS}{dt} = -\frac{0.75kBS}{K+S}$$

where B and S are the biomass and substrate concentrations, respectively. Solve these differential equations from $t = 0$ to 20. At $t = 0$, S and B are 5 and 0.05, respectively. The reaction kinetics are $k = 0.3$ and $K = 0.000001$.

Problem Statement_IVP_Isothermal Plug Flow Reactor



$$u\frac{dC_A}{dz} = -2kC_A^2$$
$$u\frac{dC_B}{dz} = 2kC_A^2$$
$$u\frac{dC_C}{dz} = 0$$

With the following initial values:

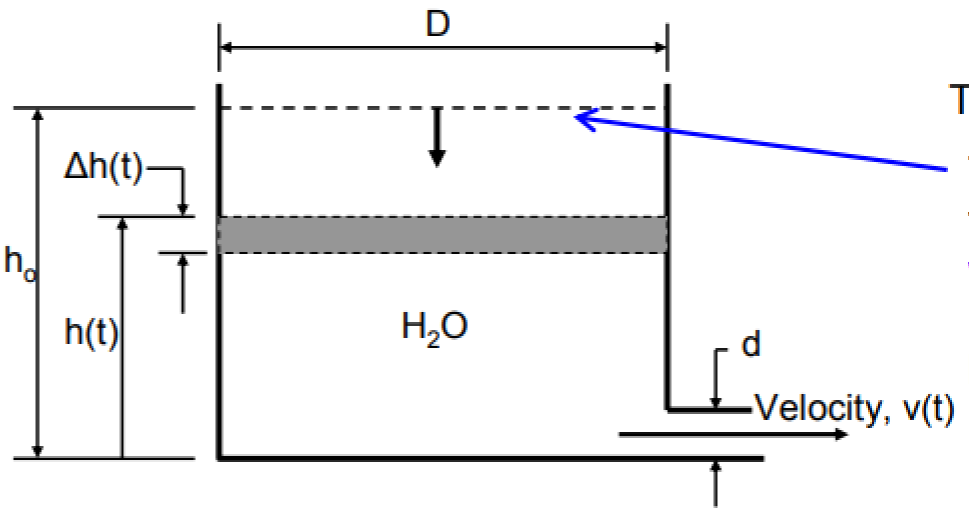
$$C_A(0) = 2\text{kmol/m}^3,\ \ C_B(0) = 0,\quad C_C(0) = 2\text{kmol/m}^3$$

$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x\frac{\partial C_A}{\partial x} + v_y\frac{\partial C_A}{\partial y} + v_z\frac{\partial C_A}{\partial z}}^{\text{Convection}}\right) + \overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}^{\text{Diffusion}} + \overbrace{R_A}^{\text{reaction}}$$

PDE form for a PFR is converted to ODEs

If $u = 0.5m/s$, $k = 0.3m^3/kmol\ s$, and reactor length $z = 3m$. Solve the differential equations and plot the concentration of each species along the reactor length

Problem Statement_IVP_Fluid Flow



The given initial water level in the tank is h_o

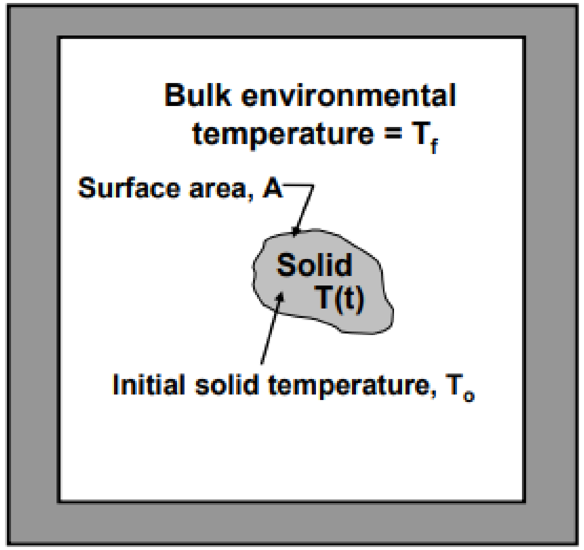
The water level keeps dropping after the tap exit is opened, and the reduction of water level is CONTINUOUS with time t

Let the water level at time t be h(t)

$$\frac{dh(t)}{dt} = -\sqrt{2g}\left(\frac{d^2}{D^2}\right)\sqrt{h(t)}$$

Tank diameter, D = 12" = 1 ft.
Drain pipe diameter, d = 1" = 1/12 ft.
Initial water level in the tank, h_o = 12" = 1 ft.
Gravitational acceleration, g = 32.2 ft/sec.

Problem Statement_IVP_Unsteady State Heat Transfer



$$\frac{dT(t)}{dt} = -\alpha A\left[T(t) - T_f\right]$$

$T_o = 80^oC$, $T_f = 5^oC$, $\alpha = 0.002/m^2\text{-}s$ and $A = 0.2\ m^2$

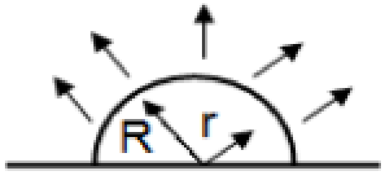
Solve the differential equation and find out the time required to reach the steady-state conditions.

The ***steady state heat-conduction*** can be also represented in ODE form and solved using IVP methods.

$$q(r) = -k\frac{dT(r)}{dr}$$

Problem Statement_IVP_Mass Transfer

A hemispherical droplet of liquid water, lying on a flat surface, evaporates by molecular diffusion through still air surrounding the droplet. The droplet initially has a radius R. As the liquid water slowly evaporates, the droplet shrinks slowly with time, but the flux of the water vapor is at a nominal steady state. The temperature of the droplet and the surrounding still air are kept constant. The air contains water vapor at an infinitely long distance from the droplet's surface.



$$N_A = -cD_{AB}\frac{dy_A}{dr} + y_A(N_A + N_B)$$

$$N_B = 0$$

$$N_A = -\frac{cD_{AB}}{(1-y_A)}\frac{dy_A}{dr}$$

Basic assumptions:

1. Steady state conditions
2. No chemical reaction
3. Constant pressure and temperature
4. One dimensional mass transfer (r direction)
5. $N_{Air} = 0$

Solve the first order differential equation of IVP and find out the graphically show the variation of mole-fraction of liquid-water with r.
at r=0, $y_A(0) = 0.8$,

Data given,
$c = 5$ mol/m^3. $D_{AB} = 10^{-2}$ m^2/s, $N_A = 20$ mol /m^2.s

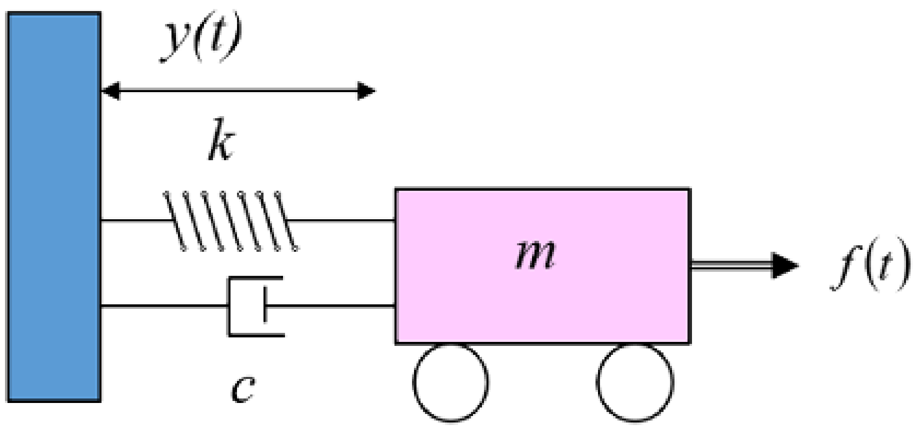
Unsteady state diffusion can be also represented in ODE form (specific) and solved using IVP.

$$\nabla \cdot \mathbf{N}_A + \frac{\partial c_A}{\partial t} - R_A = 0 \qquad \frac{\partial c_A}{\partial t} = D_{AB}\frac{\partial^2 c_A}{\partial z^2}$$

Second order Differential Equation

$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = f(x)$$

Spring-mass-damper response theory



Sum of forces acting on suspension

$$F_m + F_d + F_k = f(t)$$

$$\frac{m}{g_c}\frac{d^2y}{dt^2} + c\frac{dy}{dt} + ky = f(t)$$

Mass acceleration

$$F_m = ma; \quad a = \frac{dv}{dt}; \quad v = \frac{dy}{dt} \quad \Rightarrow \quad a = \frac{d^2y}{dt^2}$$

$$F_m = \frac{m}{g_c}\frac{d^2y}{dt^2}$$

Damping force

$$F_d = c\frac{dy}{dt}; \quad c[=]damping\ coefficient\ \frac{lb_f}{ft/sec}$$

Spring force

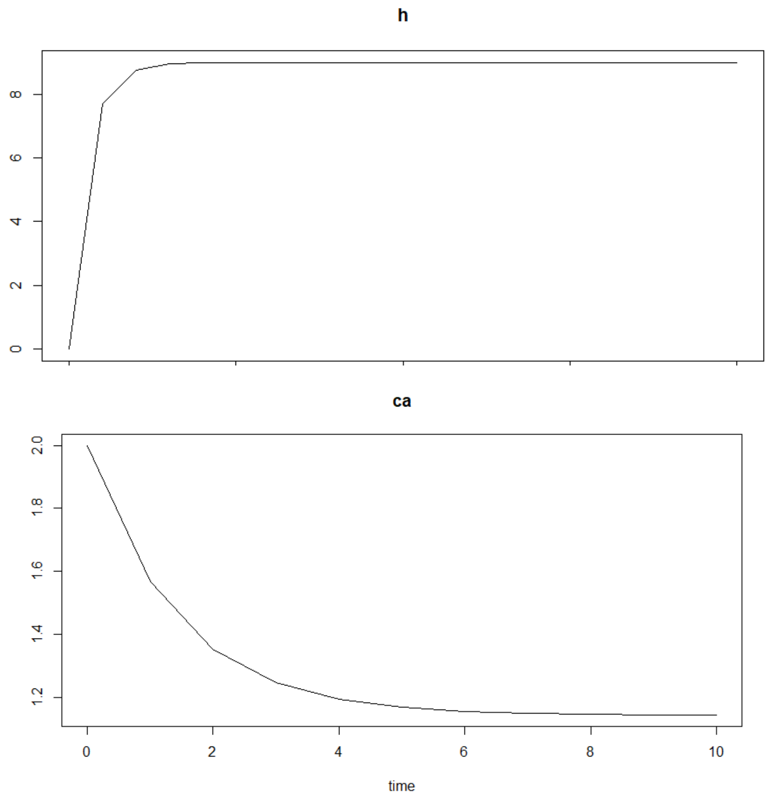
$$F_k = ky; \quad k[=]spring\ constant\ \frac{lb_f}{ft}$$

Driving bump force

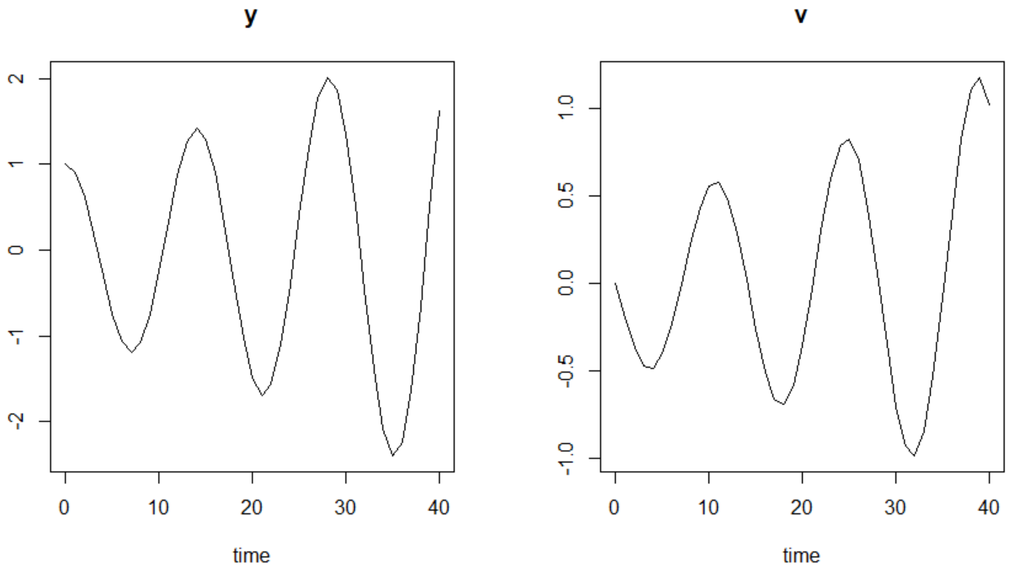
$$f(t)[=]bump\ force \quad lb_f$$

Graphical Representations_ODEs

$$\frac{dy}{dx} + Py = Q$$



$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = f(x)$$



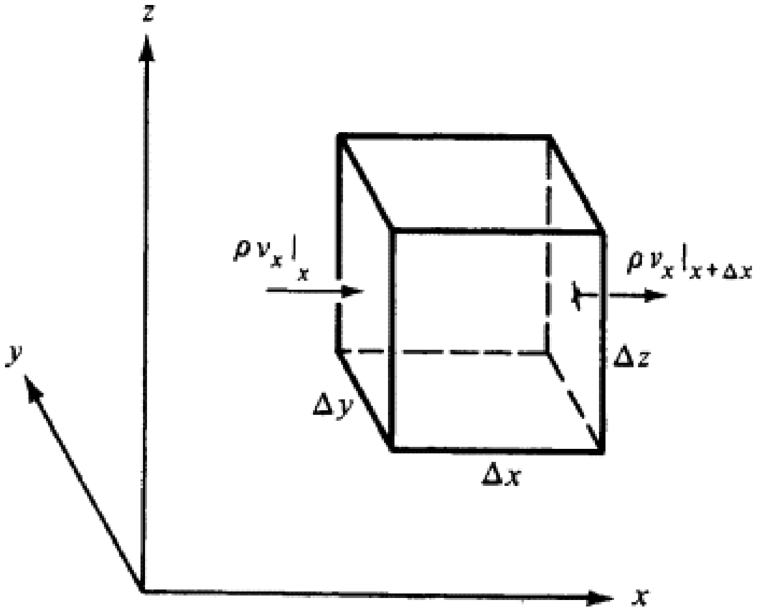
Module 6: Modeling of Transport Processes

(Fluid flow, heat transfer & mass-transfer with & without reaction)

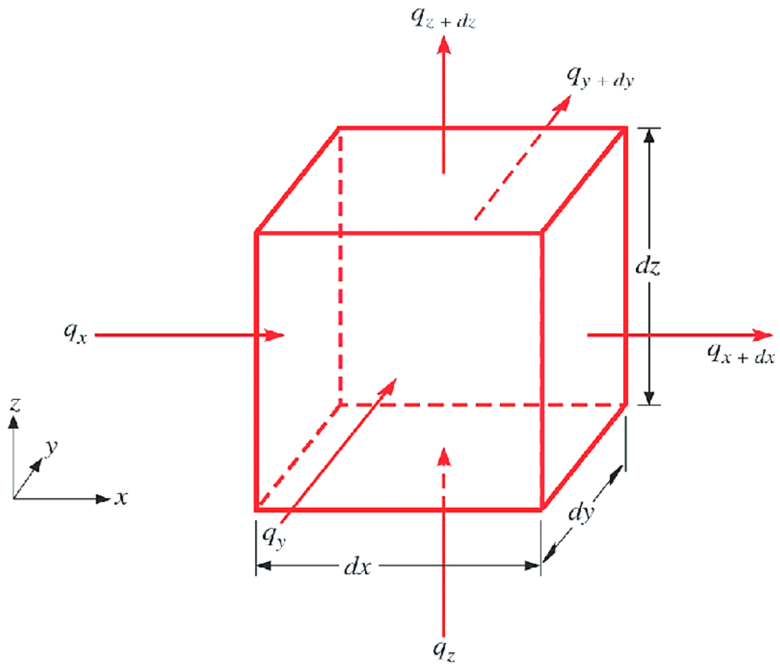
Distributed-Parameter Model

Distributed parameter systems vary continuously from one point to another, and the system state variables vary in space and in time. The mathematical description of a distributed system includes ***partial differential equations.***

“Microscopic balances in distributed parameter systems”



“Control-volume (Δx.Δ.yΔz)”



Summary_Fundamental Modeling

Lumped-parameter models

- Model is homogeneous and consistent throughout entire CV.
- Independent variables: only time & 0-D

Applications:
Reacting systems (CSTR, Batch reactors)

Mass and energy balance of lumped systems forms set of ***ODEs***

Distributed-parameter models

- Model is heterogeneous and inconsistent throughout entire CV.
- Independent variables: time & space (1-D to 3-D)

Applications:
- Reacting systems (PFR)
- Mass transport (diffusion)
- Fluid dynamics (momentum transport)
- Energy transport (heat transfer)

Mass and energy balance of distributed systems forms set of ***PDEs***

Distributed-Parameter Model Development

- 1-D model development (mass & energy balance & momentum Balance, both steady & unsteady state model)……"refer to class notes"

- 2-D model development (mass & energy balance & momentum balance)

- 3-D model development (mass & energy balance & momentum balance)

Model Equations: Distributed Parameter Model

$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z}}^{\text{Convection}}\right) + \overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}^{\text{Diffusion}} + \overbrace{R_A}^{\text{reaction}}$$

"Mass Balance Equation"

$$\overbrace{\rho C_p \frac{\partial T}{\partial t}}^{\text{accum.}} = \overbrace{-\rho C_p\left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z}\right)}^{\substack{\text{transport by}\\ \text{bulk flow}}} + \overbrace{k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)}^{\substack{\text{transport by thermal}\\ \text{diffusion}}} + \overbrace{\Phi}^{\text{gen.}}$$

"Energy Balance Equation"

$$\overbrace{\rho \frac{\partial v_x}{\partial t}}^{\text{accum.}} = \overbrace{-\rho\left(v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z}\right)}^{\text{transport by bulk flow}} + \overbrace{\mu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right)}^{\text{transport by viscous forces}} \overbrace{- \frac{\partial P}{\partial x} + \rho g_x}^{\text{generation}}$$

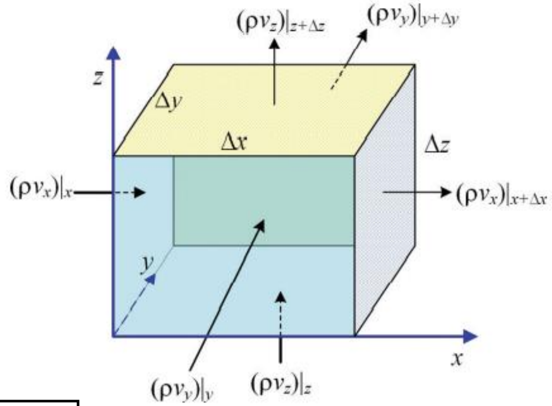
"Momentum Balance Equation"

Mass Balance

1. **Total continuity equation** applies the law of conservation of mass to **the total mass of the system**.
2. **Component continuity equation** applies the law of conservation of **mass to an individual component**.

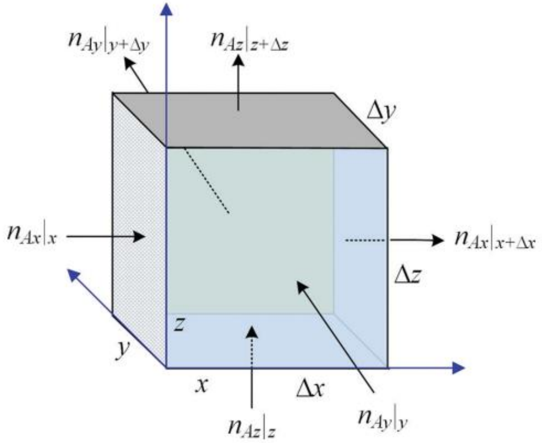
Overall mass-balance (Total Continuity equation)

$$\begin{Bmatrix}\text{Rate of}\\\text{accumulation}\end{Bmatrix}=\begin{Bmatrix}\text{Rate of mass}\\\text{in}\end{Bmatrix}-\begin{Bmatrix}\text{Rate of mass}\\\text{out}\end{Bmatrix}$$

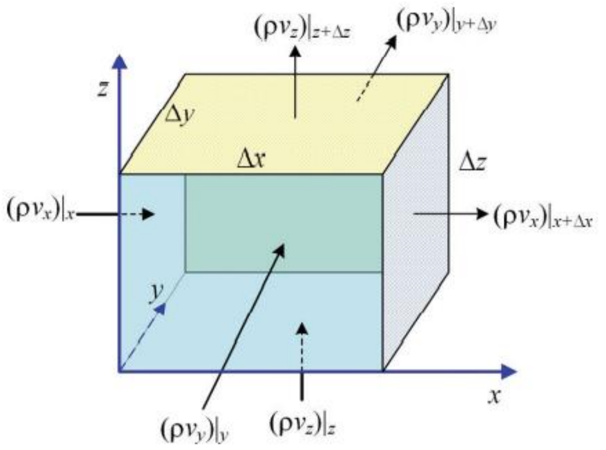


Component mass-balance (Component Continuity Equation)

$$\begin{Bmatrix}\text{Rate of}\\\text{accumulation}\\\text{of moles of A}\end{Bmatrix}=\begin{Bmatrix}\text{Rate of}\\\text{moles of}\\A\text{ in}\end{Bmatrix}-\begin{Bmatrix}\text{Rate of}\\\text{moles of}\\A\text{ out}\end{Bmatrix}+\begin{Bmatrix}\text{Rate of}\\\text{generation of}\\\text{moles of }A\end{Bmatrix}-\begin{Bmatrix}\text{Rate of}\\\text{consumptions}\\\text{of moles of }A\end{Bmatrix}$$



Total Continuity Equation



Direction	In	Out	(In – Out) × Area
x	$\rho v_x \Delta y \Delta z\big\rvert_x$	$\rho v_x \Delta y \Delta z\big\rvert_{x+\Delta x}$	$\left(\rho v_x\big\rvert_x - \rho v_x\big\rvert_{x+\Delta x}\right)\Delta y \Delta z$
y	$\rho v_y \Delta x \Delta z\big\rvert_y$	$\rho v_y \Delta x \Delta z\big\rvert_{y+\Delta y}$	$\left(\rho v_y\big\rvert_y - \rho v_y\big\rvert_{y+\Delta y}\right)\Delta x \Delta z$
z	$\rho v_z \Delta x \Delta y\big\rvert_z$	$\rho v_z \Delta x \Delta y\big\rvert_{z+\Delta z}$	$\left(\rho v_z\big\rvert_z - \rho v_z\big\rvert_{z+\Delta z}\right)\Delta x \Delta y$

$$\left\{\begin{matrix}\text{Rate of}\\ \text{accumulation}\end{matrix}\right\} = \left\{\begin{matrix}\text{Rate of mass}\\ \text{in}\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of mass}\\ \text{out}\end{matrix}\right\}$$

$$\left[\rho v_x\big\rvert_x \Delta y \Delta z + \rho v_y\big\rvert_y \Delta x \Delta z + \rho v_z\big\rvert_z \Delta x \Delta y\right]$$

$$-\left[\rho v_x\big\rvert_{x+\Delta x} \Delta y \Delta z + \rho v_y\big\rvert_{y+\Delta y} \Delta x \Delta z + \rho v_z\big\rvert_{z+\Delta z} \Delta x \Delta y\right] = \frac{dm}{dt}$$

$$\text{Accumulation} = \frac{\partial m}{\partial t} = \frac{\partial \rho \Delta x \Delta y \Delta z}{\partial t} = \Delta x \Delta y \Delta z \frac{\partial \rho}{\partial t}$$

Total Continuity Equation

$$\frac{\rho v_x|_x - \rho v_x|_{x+\Delta x}}{\Delta x} + \frac{\rho v_y|_y - \rho v_y|_{y+\Delta y}}{\Delta y} + \frac{\rho v_z|_z - \rho v_z|_{z+\Delta z}}{\Delta z} = \frac{d\rho}{dt}$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho v_x}{\partial x} - \frac{\partial \rho v_y}{\partial y} - \frac{\partial \rho v_z}{\partial z}$$

For incompressible fluid, constant density, steady state flow

$$0 = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}$$

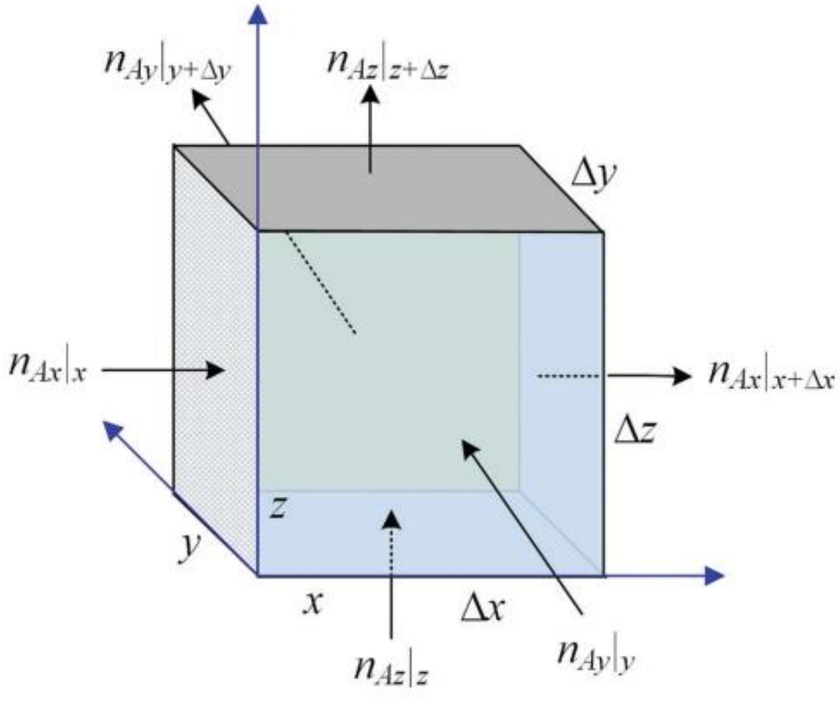
Component Continuity Equation

1. Mass continuity equation (mass units)
2. Molar continuity equation (molar units)

$$\text{in} - \text{out} + \text{generation} - \text{consumption} = \text{accumulation}$$

$$\text{Accumulation of component } A = \frac{\partial m_A}{\partial t} = \frac{\partial \rho_A \Delta x \Delta y \Delta z}{\partial t} = \Delta x \Delta y \Delta z \frac{\partial \rho_A}{\partial t}$$

$$\text{Rate of production of } A \text{ (generation)} = r_A \, \Delta x \Delta y \Delta z$$



Direction	In	Out	(In – Out) × Area
x	$n_{Ax}\Delta y\Delta z\big\|_x$	$n_{Ax}\Delta y\Delta z\big\|_{x+\Delta x}$	$\left(n_{Ax}\big\|_x - n_{Ax}\big\|_{x+\Delta x}\right)\Delta y\Delta z$
y	$n_{Ay}\Delta x\Delta z\big\|_y$	$n_{Ay}\Delta x\Delta z\big\|_{y+\Delta y}$	$\left(n_{Ay}\big\|_y - n_{Ay}\big\|_{y+\Delta y}\right)\Delta x\Delta z$
z	$n_{Az}\Delta x\Delta y\big\|_z$	$n_{Az}\Delta x\Delta y\big\|_{z+\Delta z}$	$\left(n_{Az}\big\|_z - n_{Az}\big\|_{z+\Delta z}\right)\Delta x\Delta y$

Component Continuity Equation

$$\left\{ n_{Ax}\big|_x (\Delta y \Delta z) + n_{Ay}\big|_y (\Delta x \Delta z) + n_{Az}\big|_z (\Delta x \Delta y) \right\}$$
$$- \left\{ n_{Ax}\big|_{x+\Delta x} (\Delta y \Delta z) + n_{Ay}\big|_{y+\Delta y} (\Delta x \Delta z) + n_{Az}\big|_{z+\Delta z} (\Delta x \Delta y) \right\}$$
$$+ \left\{ r_A (\Delta x \Delta y \Delta z) \right\} = (\Delta x \Delta y \Delta z) \frac{d\rho_A}{dt}$$

$$\frac{n_{Ax}\big|_x - n_{Ax}\big|_{x+\Delta x}}{\Delta x} + \frac{n_{Ay}\big|_y - n_{Ay}\big|_{y+\Delta y}}{\Delta y} + \frac{n_{Az}\big|_z - n_{Az}\big|_{z+\Delta z}}{\Delta z} + r_A = \frac{d\rho_A}{dt}$$

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial n_{Ax}}{\partial x} + \frac{\partial n_{Ay}}{\partial y} + \frac{\partial n_{Az}}{\partial y} = r_A}$$

Component Continuity Equation

1. Mass continuity equation (mass units)
2. Molar continuity equation (molar units)

$$n_{Ax} = \rho_A v_x + j_{Ax}$$

(Diffusive & convective terms)

$$\frac{\partial \rho}{\partial t} + \frac{\partial n_{Ax}}{\partial x} + \frac{\partial n_{Ay}}{\partial y} + \frac{\partial n_{Az}}{\partial y} = r_A$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho_A v_x)}{\partial x} - \frac{\partial(\rho_A v_y)}{\partial y} - \frac{\partial(\rho_A v_z)}{\partial z} - \frac{\partial j_{Ax}}{\partial x} + \frac{\partial j_{Ay}}{\partial y} + \frac{\partial j_{Az}}{\partial z} + r_A$$

$$j_{Au} = -\rho D_{AB} \frac{\partial w_A}{\partial u}$$

mass fraction $w_A = \rho_A/\rho$.

Component Continuity Equation

$$\frac{\partial \rho_A}{\partial t} = -\rho_A\left(\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}\right)-\left(v_x\frac{\partial \rho_A}{\partial x}+v_y\frac{\partial \rho_A}{\partial y}+v_z\frac{\partial \rho_A}{\partial z}\right)$$

$$+\left(\frac{\partial}{\partial x}\left(\frac{\partial \rho D_{AB} w_A}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\partial \rho D_{AB} w_A}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\partial \rho D_{AB} w_A}{\partial z}\right)\right)+r_A$$

$$\frac{\partial \rho_A}{\partial t} = -\left(v_x\frac{\partial \rho_A}{\partial x}+v_y\frac{\partial \rho_A}{\partial y}+v_z\frac{\partial \rho_A}{\partial z}\right)+D_{AB}\left(\frac{\partial^2 \rho_A}{\partial x^2}+\frac{\partial^2 \rho_A}{\partial y^2}+\frac{\partial^2 \rho_A}{\partial z^2}\right)+r_A$$

$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x\frac{\partial C_A}{\partial x}+v_y\frac{\partial C_A}{\partial y}+v_z\frac{\partial C_A}{\partial z}}^{\text{Convection}}\right)+\overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2}+\frac{\partial^2 C_A}{\partial y^2}+\frac{\partial^2 C_A}{\partial z^2}\right)}^{\text{Diffusion}}+\overbrace{R_A}^{\text{reaction}}$$

Summary_Conservation of Mass (Diffusion Equation)

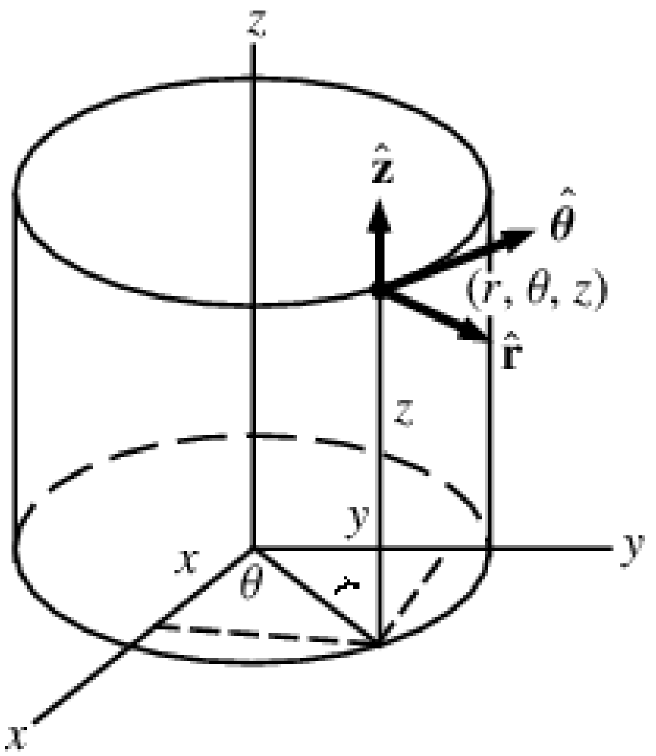
$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z}}^{\text{Convection}}\right) + \overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}^{\text{Diffusion}} + \overbrace{R_A}^{\text{reaction}}$$

Equation of Change: Cylindrical Systems

Total Continuity Equation

$$\rho\left(\frac{1}{r}\frac{\partial r v_r}{\partial r}+\frac{1}{r}\frac{\partial v_\theta}{\partial \theta}+\frac{\partial v_z}{\partial z}\right)=0$$

- *Radial-change in state*
- *Axial-change in state*
- *Angular-change in state*

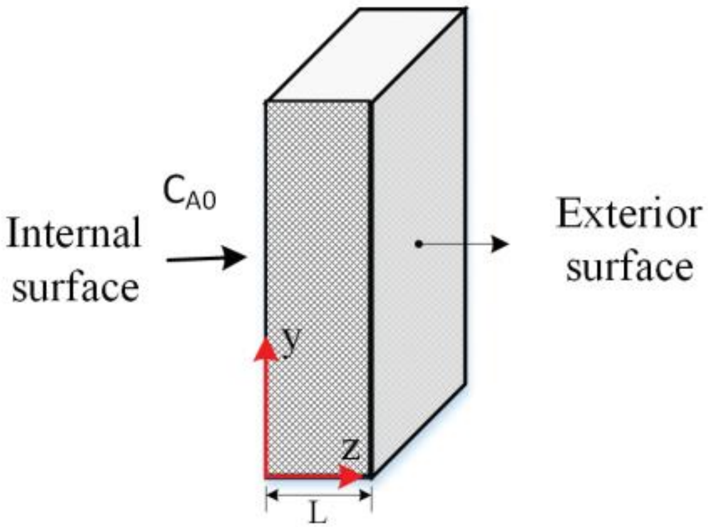


Component Continuity Equation

$$\frac{\partial C_A}{\partial t}=-\left(v_r\frac{\partial C_A}{\partial r}+v_\theta\frac{1}{r}\frac{\partial C_A}{\partial \theta}+v_z\frac{\partial C_A}{\partial z}\right)$$

$$+D_A\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2}+\frac{\partial^2 C_A}{\partial z^2}\right)+R_A$$

Problem Statement: Mass Transfer with Diffusion



Diffusion with chemical reaction inside a slab catalyst

$$\underbrace{\frac{\partial C_A}{\partial t}}_{\text{accum.}} = -\left(\underbrace{v_x\frac{\partial C_A}{\partial x} + v_y\frac{\partial C_A}{\partial y} + v_z\frac{\partial C_A}{\partial z}}_{\text{Convection}}\right) + \underbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}_{\text{Diffusion}} + \underbrace{R_A}_{\text{reaction}}$$

Assumptions:

- Steady state.
- Transportation of gas takes place by diffusion only.
- Diffusion in x and y directions are negligible.
- Diffusivity of gas in the membrane tube is constant.

Steady state | $(v_x = 0)$ | $(v_y = 0)$ | $(v_z = 0)$ | Neglect diffusion in x and y

$$\cancel{\frac{\partial C_A}{\partial t}} = -\left(\cancel{v_x\frac{\partial C_A}{\partial x}} + \cancel{v_y\frac{\partial C_A}{\partial y}} + \cancel{v_z\frac{\partial C_A}{\partial z}}\right) + D_{AB}\left(\cancel{\frac{\partial^2 C_A}{\partial x^2}} + \cancel{\frac{\partial^2 C_A}{\partial y^2}} + \frac{\partial^2 C_A}{\partial z^2}\right) + R_A$$

$$D_A\frac{d^2 C_A}{dz^2} + R_A = 0$$

$$R_A = -kC_A$$

Problem Statement: Mass Transfer with Diffusion

$$D_A \frac{d^2C_A}{dz^2} + R_A = 0$$

$$\frac{d^2C_A}{dz^2} - \alpha^2 C_A = 0 \qquad \alpha^2 = k/D_A.$$

$$C_A = C_1 e^{\alpha z} - C_2 e^{-\alpha z}$$

B.C.1: at $z = 0$, $C_A = C_{Ao}$

B.C.2: at $z = L$, $\dfrac{dC_A}{dz} = 0$

From B.C.1:

$$C_{Ao} = C_1 - C_2$$

From B.C.2:

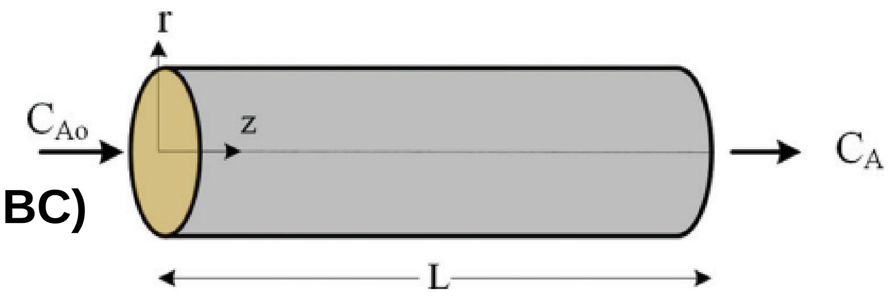
$$0 = C_1 \alpha e^{\alpha L} + C_2 \alpha e^{-\alpha L}$$

$$C_2 = -C_1 e^{2\alpha L} \qquad C_1 = \frac{C_{Ao}}{1+e^{2\alpha L}} \qquad C_2 = -\frac{C_{Ao}}{1+e^{2\alpha L}} e^{2\alpha L}$$

$$C_A = \frac{C_{Ao}}{1+e^{2\alpha L}} e^{\alpha z} + \frac{C_{Ao}\, e^{2\alpha L}}{1+e^{2\alpha L}} e^{-\alpha z}$$

$$\boxed{C_A = \frac{C_{Ao}}{1+e^{2\alpha L}} \left\{ e^{\alpha z} + e^{2\alpha L} e^{-\alpha z} \right\}}$$

Problem Statement: PFR (Diffusion with reaction)



B.C.1: at $z = 0$, $C_A = C_{A0}$ (inlet concentration of A) **(Dirichlet BC)**

B.C.2: at $z = L$, $dC_A/dz = 0$ (convective flux at the exit of the reactor) **(Neumann BC)**

$$\frac{\partial C_A}{\partial t} = -\left(v_r \frac{\partial C_A}{\partial r} + v_\theta \frac{1}{r}\frac{\partial C_A}{\partial \theta} + v_z \frac{\partial C_A}{\partial z}\right)$$

$$+ D_A\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2} + \frac{\partial^2 C_A}{\partial z^2}\right) + R_A$$

$$\boxed{0 = -\left(v_z \frac{dC_A}{dz}\right) + D_{AB}\left(\frac{d^2 C_A}{dz^2}\right) - kC_A}$$

(Convection, diffusion & Reaction)

Note: Dirichlet BCs assume the solution to the variable. In Neumann BCs, a solution is assumed for the derivative of the variable.

PFR (Diffusion with reaction)

$$0 = -\left(v_z \frac{dC_A}{dz} \right) + D_{AB} \left(\frac{d^2 C_A}{dz^2} \right) - kC_A$$

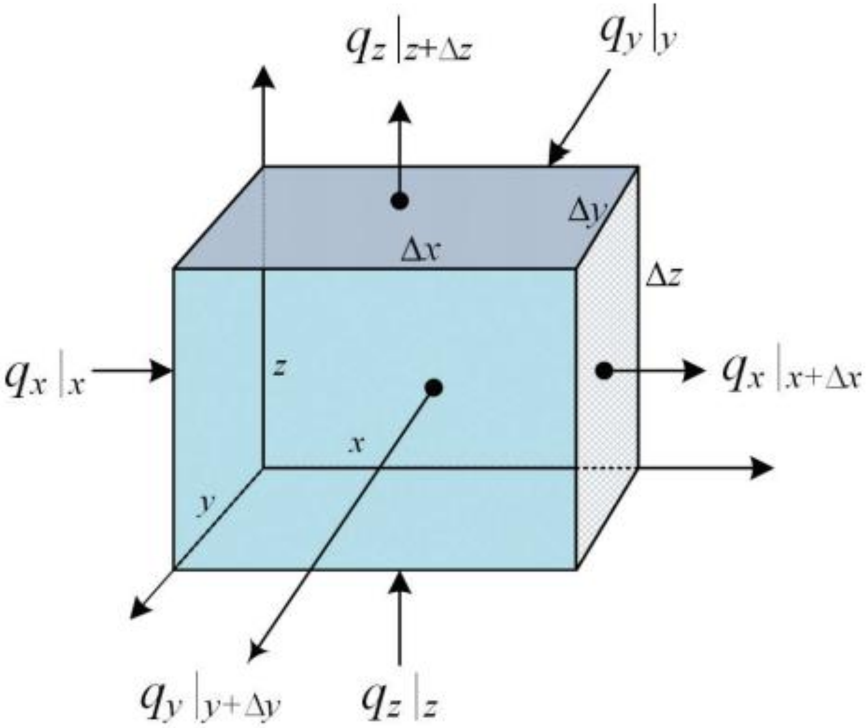
Assumption 1: **The convective term is much larger than diffusive term (since no catalyst bed)**

$$v_z \frac{dC_A}{dz} = -kC_A$$ **(R_A= -kC_A)**

$$\frac{dF_A}{dV} = R_A$$ **(performance equation of a PFR)**

Assumption 2: **The convective term is negligible compared to diffusive term (for a catalytic bed)**

Energy Balance



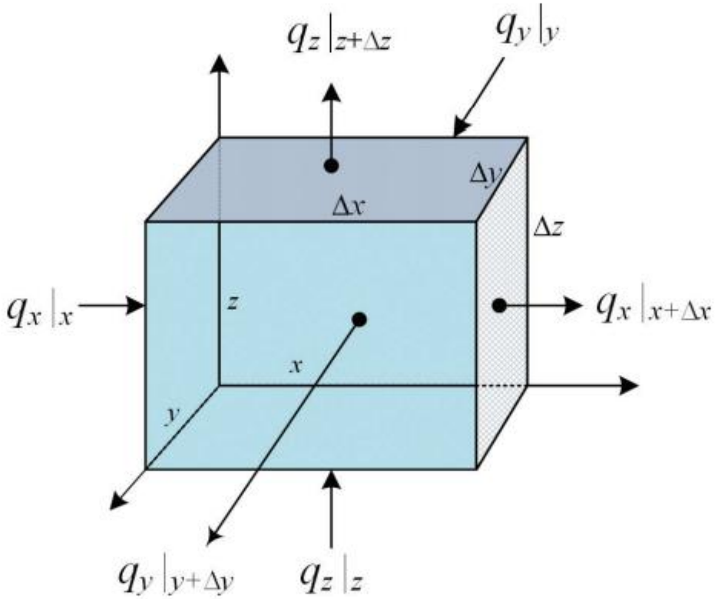
$$\begin{Bmatrix}\text{Rate of}\\ \text{Accumulation}\\ \text{of energy}\end{Bmatrix} = \begin{Bmatrix}\text{Rate of}\\ \text{energy}\\ \text{input}\end{Bmatrix} - \begin{Bmatrix}\text{Rate of}\\ \text{energy}\\ \text{output}\end{Bmatrix} + \begin{Bmatrix}\text{Rate of}\\ \text{energy}\\ \text{generated}\end{Bmatrix} - \begin{Bmatrix}\text{Rate of}\\ \text{energy}\\ \text{consumed}\end{Bmatrix} \pm \begin{Bmatrix}\text{Rate of energy}\\ \text{exchanged}\\ \text{with the}\\ \text{surrounding}\end{Bmatrix}$$

Total **"energy flux"** is the **sum of heat flux and bulk flux**,

$$E = q + \rho v C_p T \, .$$

Energy Balance

Direction	In	Out
x	$\left(q_x + \rho v_x C_p T\right)\Big\|_x$	$\left(q_x + \rho v_x C_p T\right)\Big\|_{x+\Delta x}$
y	$\left(q_y + \rho v_y C_p T\right)\Big\|_y$	$\left(q_y + \rho v_y C_p T\right)\Big\|_{y+\Delta y}$
z	$\left(q_z + \rho v_z C_p T\right)\Big\|_z$	$\left(q_z + \rho v_z C_p T\right)\Big\|_{z+\Delta z}$



Input

$$\left(q_x + \rho v_x C_p T\right)\Big|_x \Delta y \Delta z + \left(q_y + \rho v_y C_p T\right)\Big|_y \Delta x \Delta z + \left(q_z + \rho v_z C_p T\right)\Big|_z \Delta x \Delta y$$

output

$$\left(q_x + \rho v_x C_p T\right)\Big|_{x+\Delta x} \Delta y \Delta z + \left(q_y + \rho v_y C_p T\right)\Big|_{y+\Delta y} \Delta x \Delta z + \left(q_z + \rho v_z C_p T\right)\Big|_{z+\Delta z} \Delta x \Delta y$$

Energy Balance

$$\frac{\partial(\rho C_p T)}{\partial t} = -\frac{\partial(\rho v_x C_p T)}{\partial x} - \frac{\partial(\rho v_y C_p T)}{\partial y} - \frac{\partial(\rho v_z C_p T)}{\partial z} - \frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_z}{\partial z} + \Phi$$

$$\begin{aligned}\rho C_p \frac{\partial T}{\partial t} + C_p T \frac{\partial \rho}{\partial t} = {} & -\rho C_p \left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) \\ & - \rho C_p T \left(\frac{\partial \rho v_x}{\partial x} + \frac{\partial \rho v_y}{\partial y} + \frac{\partial \rho v_z}{\partial z} \right) \\ & - \frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_z}{\partial z} + \Phi\end{aligned}$$

$$\rho C_p \frac{\partial T}{\partial t} = -\rho C_p \left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) - \frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_z}{\partial z} + \Phi$$

Summary_Conservation of Energy

$$\overbrace{\rho C_p \frac{\partial T}{\partial t}}^{\text{accum.}} = \overbrace{-\rho C_p \left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right)}^{\substack{\text{transport by} \\ \text{bulk flow}}} + \overbrace{k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)}^{\substack{\text{transport by thermal} \\ \text{diffusion}}} + \overbrace{\Phi}^{\text{gen.}}$$

$$\overbrace{\rho C_p \frac{\partial T}{\partial t}}^{\text{accum.}} = \overbrace{k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)}^{\substack{\text{transport by} \\ \text{thermal diffusion}}} + \overbrace{\Phi}^{\text{gen.}}$$

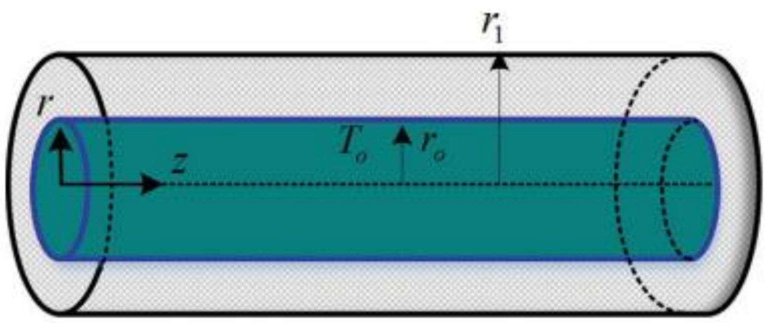
Equation of Change: Cylindrical Systems

Energy Balance Equation

$$\rho C_p \frac{\partial T}{\partial t} = -\rho C_p \left(v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) +$$

$$k \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right) + Q$$

Problem Statement: Heat Diffusion in a Packed Bed Reactor



Chemical reactor with packed bed of catalyst

- Steady state
- Neglect of convective heat
- Neglect of the temperature gradients in the axial and angular direction

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left(v_r \frac{\partial T}{\partial r} + v_\theta \frac{1}{r}\frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right) + \Phi_H$$

No convective heat

Steady state $\qquad v_r = v_\theta = v_z = 0$

Temperature gradients in the axial and angular direction is neglected

$$\rho C_p \cancel{\frac{\partial T}{\partial t}} + \rho C_p \left(\cancel{v_r \frac{\partial T}{\partial r}} + \cancel{v_\theta \frac{1}{r}\frac{\partial T}{\partial \theta}} + \cancel{v_z \frac{\partial T}{\partial z}} \right) = k \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r} \right) + \cancel{\frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2}} + \cancel{\frac{\partial^2 T}{\partial z^2}} \right) + \Phi_H$$

Problem Statement: Heat Diffusion in a Packed Bed Reactor

$$0 = k\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)\right) + Q$$

$$\frac{d}{dr}\left(r\frac{dT}{dr}\right) = -\frac{Q}{k}r$$

$$r\frac{dT}{dr} = -\frac{Q}{2k}r^2 + C_1$$

$$T = -\frac{Q}{4k}r^2 + C_1 lnr + C_2$$

B.C.1 : $r = r_o,\ dT/dr = 0,$

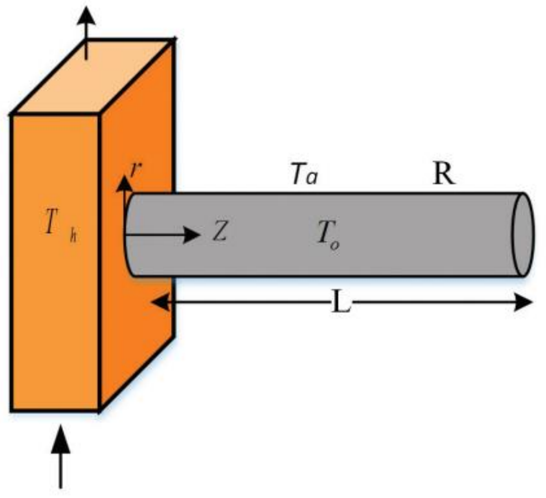
$$C_1 = -\frac{Q}{2k}r_o^2$$

B.C.2: $r = r_o,\ T = T_o.$

$$C_2 = T_0 + \frac{Q}{4k}r_o^2 - \frac{Q}{2k}r_o^2 lnr_o$$

$$\boxed{T = \frac{Qr_o^2}{4k}\left\{1 - \left(\frac{r}{r_o}\right)^2 + 2ln\left(\frac{r}{r_o}\right)\right\} + T_0}$$

Problem Statement: Heat Conduction Through a Fin



Assumptions:

1. Steady state condition
2. No convective heat flow
2. If the radius of the rod is very small compared to rod length so the radial temperature gradient is neglected

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left(v_r \frac{\partial T}{\partial r} + v_\theta \frac{1}{r}\frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right) + \Phi_H$$

$$\rho C_p \frac{\partial T}{\partial t} = k \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right) + Q$$

$$0 = k \left(0 + \frac{\partial^2 T}{\partial z^2} \right) + Q$$

BC 1: at z=0, $T = T_H$
BC 2: at z= L, dT/dz = 0
or at z=L, $T= T_a$

Heat Conduction Through a Fin

$$0 = k\left(0 + \frac{\partial^2 T}{\partial z^2}\right) + Q$$

$$Q = h\frac{A_s}{V_b}(T - T_a) = h\frac{2\pi RL}{\pi R^2 L}(T - T_a)$$

$$P = 2\pi R,\ A_c = \pi R^2$$

$$m^2 = hP/(kA_c)$$

$$\theta(z) = (T - T_a)$$

$$0 = \frac{d^2\theta}{dz^2} - m^2\theta$$

$$\theta(z) = C_1 e^{mz} + C_2 e^{-mz}$$

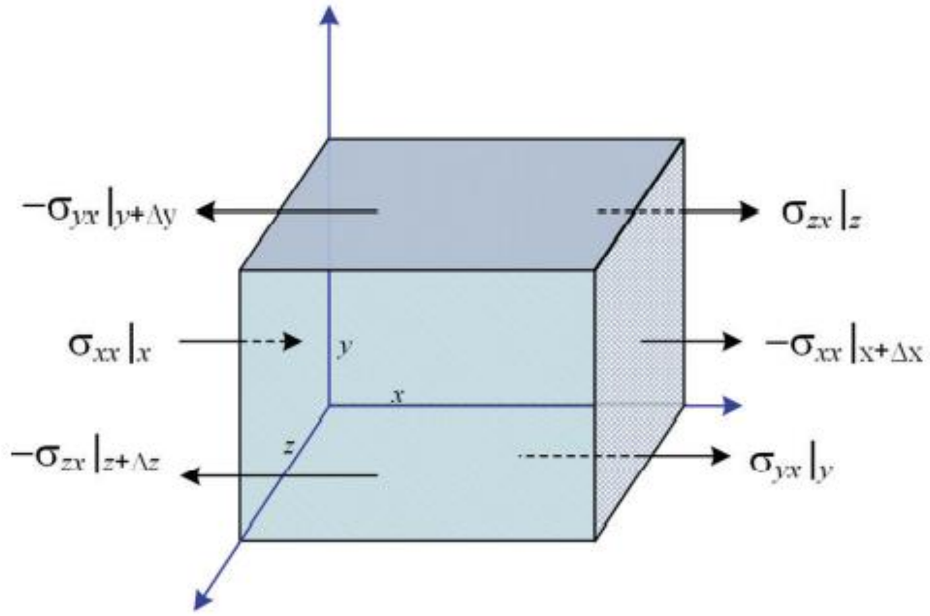
B.C.1: at $z = 0$, $\theta = \theta_h$, wall of the fin

B.C.2: at $z = L$, $d\theta/dz = 0$, thermal insulation, no heat loss from the fin axial end

$$\boxed{\frac{\theta}{\theta_h} = \frac{\cosh m(L - z)}{\cosh mL}}$$

Momentum Balance

Consider a fluid flowing with a velocity v t(, x y, , z). The flow is assumed laminar. The momentum is transferred through **convection (bulk flow)** and by **molecular transfer (velocity gradient)**



$$\left\{\begin{matrix}\text{Rate of}\\\text{accumulation}\\\text{of momentum}\end{matrix}\right\} = \left\{\begin{matrix}\text{Rate of}\\\text{momentum}\\\text{in}\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of}\\\text{momentum}\\\text{out}\end{matrix}\right\} + \left\{\begin{matrix}\text{Rate of}\\\text{momentum}\\\text{generated}\end{matrix}\right\} - \left\{\begin{matrix}\text{Rate of}\\\text{momentum}\\\text{consumed}\end{matrix}\right\}$$

$$\begin{aligned}\text{Rate of momentum accumulation} &= \text{transport rate of momentum in}\\ &\quad - \text{transport rate of momentum out}\\ &\quad + \text{sum of forces acting on element}\end{aligned}$$

Momentum Balance

convection (bulk flow)

Direction	In	Out	(In – Out) × Area
x	$(\rho v_x) v_x\vert_x$	$(\rho v_x) v_x\vert_{x+\Delta x}$	$\left((\rho v_x) v_x\vert_x - (\rho v_x) v_x\vert_{x+\Delta x}\right)\Delta y \Delta z$
y	$(\rho v_y) v_x\vert_y$	$(\rho v_y) v_x\vert_{y+\Delta y}$	$\left((\rho v_y) v_x\vert_y - (\rho v_y) v_x\vert_{y+\Delta y}\right)\Delta x \Delta z$
z	$(\rho v_z) v_x\vert_z$	$(\rho v_z) v_x\vert_{z+\Delta z}$	$\left((\rho v_z) v_x\vert_z - (\rho v_z) v_x\vert_{z+\Delta z}\right)\Delta x \Delta y$

molecular transfer (velocity gradient)

Direction	In	Out	(In – Out) × Area
x	$\tau_{xx}\vert_x$	$\tau_{xx}\vert_{x+\Delta x}$	$\left(\tau_{xx}\vert_x - \tau_{xx}\vert_{x+\Delta x}\right)\Delta y \Delta z$
y	$\tau_{yx}\vert_y$	$\tau_{yx}\vert_{y+\Delta y}$	$\left(\tau_{yx}\vert_y - \tau_{yx}\vert_{y+\Delta y}\right)\Delta x \Delta z$
z	$\tau_{zx}\vert_z$	$\tau_{zx}\vert_{z+\Delta z}$	$\left(\tau_{zx}\vert_z - \tau_{zx}\vert_{z+\Delta z}\right)\Delta x \Delta y$

Momentum Balance

$$\frac{\partial(\rho v_x)}{\partial t} = -\left(\frac{\partial(\rho v_x v_x)}{\partial x} + \frac{\partial(\rho v_x v_y)}{\partial y} + \frac{\partial(\rho v_x v_z)}{\partial z}\right)$$

$$-\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right) - \frac{\partial P}{\partial x} + \rho g_x$$

$$\tau_{xx} = -\mu\frac{\partial v_x}{\partial x},\ \tau_{yx} = -\mu\frac{\partial v_x}{\partial y},\ \tau_{zx} = -\mu\frac{\partial v_x}{\partial z}$$

$$v_x\frac{\partial \rho}{\partial t} + \rho\frac{\partial v_x}{\partial t} = -v_x\left(\frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_y)}{\partial y} + \frac{\partial(\rho v_z)}{\partial z}\right)$$

$$-\rho\left(v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right)$$

$$-\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right) - \frac{\partial P}{\partial x} + \rho g_x$$

Summary_Model Equations: Distributed Parameter Model

$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z}}^{\text{Convection}}\right) + \overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}^{\text{Diffusion}} + \overbrace{R_A}^{\text{reaction}}$$

“Mass Balance Equation”

$$\overbrace{\rho C_p \frac{\partial T}{\partial t}}^{\text{accum.}} = \overbrace{-\rho C_p\left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z}\right)}^{\text{transport by bulk flow}} + \overbrace{k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)}^{\text{transport by thermal diffusion}} + \overbrace{\Phi}^{\text{gen.}}$$

“Energy Balance Equation”

$$\overbrace{\rho \frac{\partial v_x}{\partial t}}^{\text{accum.}} = \overbrace{-\rho\left(v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z}\right)}^{\text{transport by bulk flow}} + \overbrace{\mu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right)}^{\text{transport by viscous forces}} \overbrace{- \frac{\partial P}{\partial x} + \rho g_x}^{\text{generation}}$$

“Momentum Balance Equation”

Equation of Change: Cylindrical Systems

Momentum Balance Equation

r component:

$$\rho \frac{\partial v_r}{\partial t} = -\rho\left(v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta} + \frac{v_\theta^2}{r} + v_z \frac{\partial v_r}{\partial z}\right)$$

$$+\mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial (r v_r)}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \theta^2} + \frac{2}{r^2}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial^2 v_r}{\partial z^2}\right) - \frac{\partial P}{\partial r} + \rho g_r$$

θ component:

$$\rho \frac{\partial v_\theta}{\partial t} = -\rho\left(v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{v_r v_\theta}{r} + v_z \frac{\partial v_\theta}{\partial z}\right)$$

$$+\mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial r v_\theta}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_\theta}{\partial \theta^2} + \frac{2}{r^2}\frac{\partial v_r}{\partial \theta} + \frac{\partial^2 v_\theta}{\partial z^2}\right) - \frac{1}{r}\frac{\partial p}{\partial \theta} + \rho g_\theta$$

z component

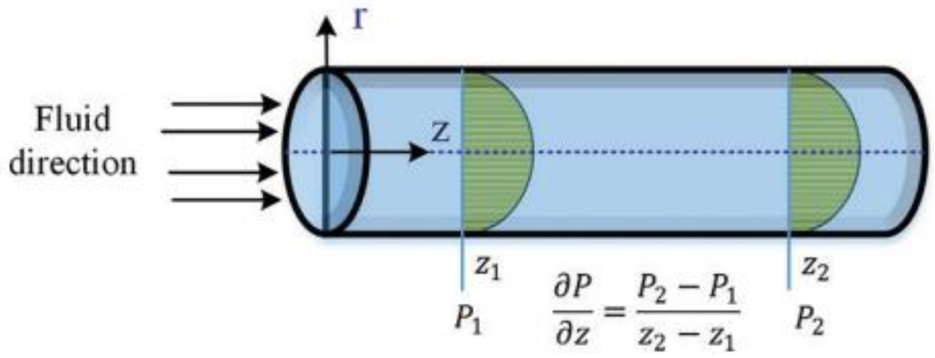
$$\rho \frac{\partial v_z}{\partial t} = -\rho\left(v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z}\right)$$

$$+\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_z^2}{\partial \theta^2} + \frac{\partial^2 v_z}{\partial z^2}\right) - \frac{\partial P}{\partial z} + \rho g_z$$

Problem Statement: Fluid Flow Through Pipe

$$\rho\frac{\partial v_z}{\partial t}+\rho\left(v_r\frac{\partial v_z}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta}+v_z\frac{\partial v_z}{\partial z}\right)$$

$$=\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_z^2}{\partial \theta^2}+\frac{\partial^2 v_z}{\partial z^2}\right)-\frac{\partial p}{\partial z}+\rho g_z$$



Velocity in the r-direction equals to zero $(v_r = 0)$

From continuity $\frac{\partial v_z}{\partial z} = 0$

From continuity $\frac{\partial v_z}{\partial z} = 0$

$$\rho\cancel{\frac{\partial v_z}{\partial t}}+\rho\left(\cancel{v_r}\frac{\partial v_z}{\partial r}+\cancel{\frac{v_\theta}{r}}\frac{\partial v_z}{\partial \theta}+v_z\cancel{\frac{\partial v_z}{\partial z}}\right)=\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\cancel{\frac{\partial^2 v_z^2}{\partial \theta^2}}+\cancel{\frac{\partial^2 v_z}{\partial z^2}}\right)-\frac{\partial p}{\partial z}+\rho \cancel{g_z}$$

Steady state

Angular velocity can be neglected $(v_\theta = 0)$

v_z does not change with θ

No gravity in the z-direction

$$0=\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)\right)-\frac{\Delta p}{\Delta z}$$

Fluid Flow Through Pipe

$$0 = \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)\right) - \frac{\Delta p}{\Delta z}$$

$$r\frac{\partial v_z}{\partial r} = \frac{\Delta p}{\mu L}\times\frac{r^2}{2} + C_1$$

$$\frac{\partial v_z}{\partial r} = \frac{\Delta p}{\mu L}\frac{r}{2} + \frac{C_1}{r}$$

$$v_z = \frac{\Delta p}{\mu L}\frac{r^2}{4} + C_1 \ln r + C_2$$

B.C.1: at $r = 0$, $dv_z/dr = 0$ (because of symmetry about the centerline)

$$C_1 = 0$$

B.C.2: at $r = R$, $v_z = 0$ (the no-slip condition at the pipe surface)

$$C_2 = -\frac{\Delta p}{4\mu L}R^2$$

$$v_z = \frac{\Delta p}{4\mu L}r^2 - \frac{\Delta p}{4\mu L}R^2$$

$$v_z = -\frac{\Delta p R^2}{4\mu L}\left[1-\left(\frac{r}{R}\right)^2\right]$$

$$v_z = \frac{(p_o - p_L)R^2}{4\mu L}\left[1-\left(\frac{r}{R}\right)^2\right]$$

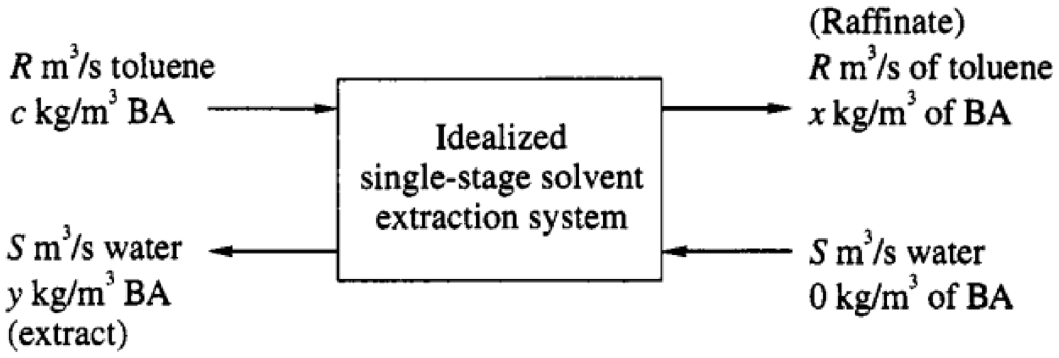
$$\boxed{v_{z,\max} = -\frac{\Delta p R^2}{4\mu L} = \frac{(p_o - p_L)R^2}{4\mu L}}$$

Problem Statements on BVP

(Applications in Chemical Engineering)

Modeling of Mass Transfer Systems

Mass Transfer System: Solvent-Extraction



Assumptions:

- Steady state process
- Two streams leaving a stage are always in equilibrium with each other

Input of BA = Rc (kg/s)

Output of BA = $Rx + Sy$ (kg/s)

$$y = mx$$

$$Rc = Rx + Sy$$

$$Rc = Rx + mSx$$

$$\therefore x = \frac{Rc}{R + mS}$$

$$y = \frac{mRc}{R + mS}$$

Fraction of BA extracted: $E = \dfrac{Sy}{Rc}$

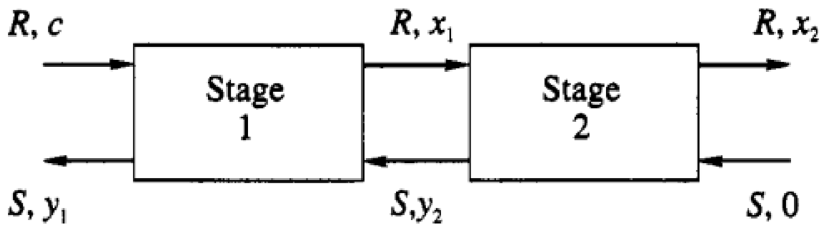
$$\frac{Sy}{Rc} = \frac{S(mRc)}{Rc(R + mS)} = \frac{mS}{R + mS}$$

$$\frac{Sy}{Rc} = \frac{1}{\left(\frac{R}{mS}\right) + 1}$$

$$\alpha = \frac{R}{mS}$$

$$E = \frac{1}{\alpha + 1}$$

Multi-stage Solvent-Extraction System



Assumptions:

- Steady state process
- The feed concentration c remains constant.
- The mixer is so efficient that the two streams leaving a stage are always in equilibrium with each other

$$\text{Stage 1: } Rc + Sy_2 = Rx_1 + Sy_1$$

$$\text{Stage 2: } Rx_1 = Rx_2 + Sy_2$$

$$y_1 = mx_1$$

$$y_2 = mx_2$$

From equation of stage-1:

$$Rc + mSx_2 = \frac{Ry_1}{m} + Sy_1$$

$$= \frac{(R + mS)}{m} y_1$$

From equation of stage-2:

$$\frac{Ry_1}{m} = Rx_2 + mSx_2$$

$$\Rightarrow y_1 = \frac{m}{R}(Rx_2 + mSx_2)$$

$$R^2c + mRSx_2 = R^2x_2 + mRSx_2 + mRSx_2 + m^2S^2x_2$$

$$R^2c = x_2(R^2 + mRS + m^2S^2)$$

$$x_2 = \frac{R^2c}{R^2 + mRS + m^2S^2}$$

Multi-stage Solvent-Extraction System

$$y_1 = \frac{mRc(R + mS)}{R^2 + mRS + m^2S^2}$$

Fraction of BA extracted (E):

$$\frac{Sy_1}{Rc} = \frac{mS(R + mS)}{R^2 + mRS + m^2S^2}$$

$$\frac{Sy_1}{Rc} = \frac{(R/mS) + 1}{(R^2/m^2S^2) + (R/mS) + 1}$$

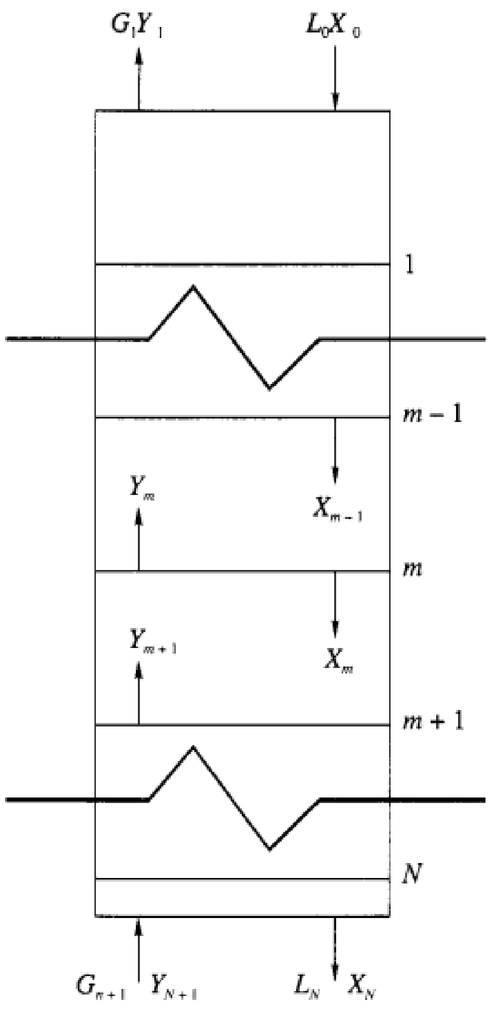
$$\alpha = \frac{R}{mS}$$

$$E = \frac{\alpha + 1}{\alpha^2 + \alpha + 1}$$

By the method of induction, for N stages,

$$E = \frac{\alpha^N - 1}{\alpha^{N+1} - 1}$$

Multi-stage Absorption System



<u>Overall mass balance over m^th plate:</u>

$$L_0 (X_m - X_{m-1}) = G_{N+1} (Y_{m+1} - Y_m)$$

<u>Overall mass balance over N^th plate:</u>

$$G_{N+1} (y_{N+1} - y_1) = L_0 (x_N - x_0)$$

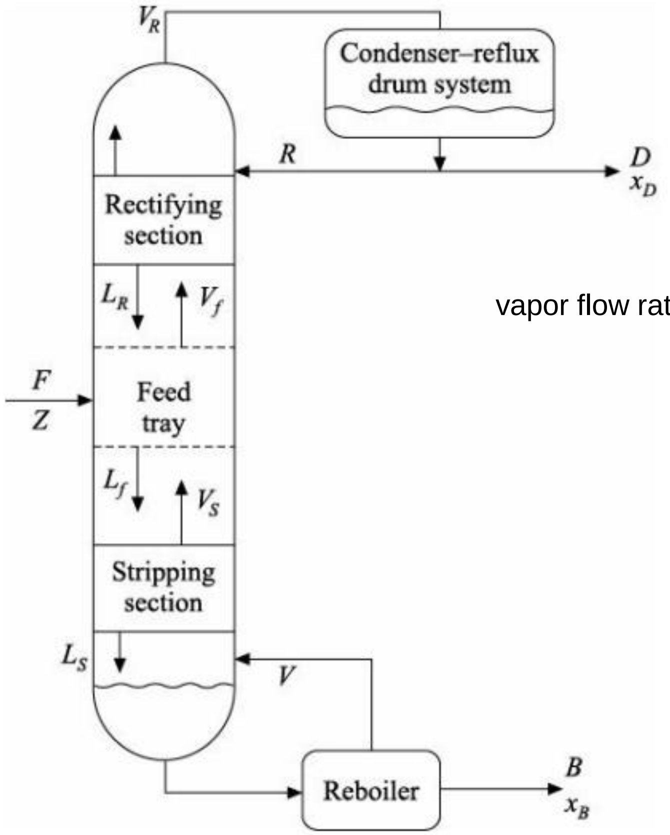
absorption factor $A = (L_0/KG_{N+1})$

equilibrium constant $K_m = y_m/x_m$,

<u>Kremser equation,</u>

$$\frac{Y_{N+1} - Y_1}{Y_{N+1} - Y_0} = \frac{A^{N+1} - A}{A^{N+1} - 1}$$

Mass Transfer System: Multistage Distillation Column



$$L_R = R$$

$$L_f = L_S = R + F$$

vapor flow rate through all trays of the column is the same,

$$V_R = V_f = V_S = V$$

$$q_F = L_F/F$$

$$1 - q_F = V_F/F.$$

Superheated vapour feed, $q_F < 0$
Saturated vapour feed, $q_F = 0$
Partially vaporized feed, $0 < q_F < 1$
Saturated liquid feed, $q_F = 1$
Subcooled liquid feed, $q_F > 1$.

Flow rate of a vapor stream leaving the feed stage (V_f):

$$V_f = V_S + V_F = V_S + F(1 - q_F)$$

$$V_f = V_R = V_S + F(1 - q_F)$$

Similarly, the flow rate of a liquid stream leaving the feed tray (L_f):

$$L_f = L_R + L_F = L_R + Fq_F$$

$$L_f = L_S = L_R + Fq_F = R + Fq_F$$

Overall & component mass balance:

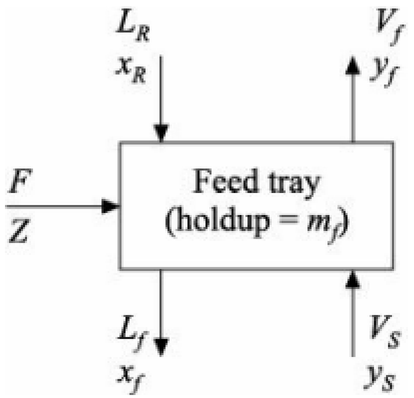
$$F = D + B$$

$$x_F*F = x_D*D + x_B*B$$

$$D = (x_f - x_B)/(x_D - x_b) *F$$

Mass Transfer System: Multistage Distillation Column

saturated liquid feed ($q_F = 1$)



Total continuity equation

$$\dot{m}_f = L_R + F + V_S - L_f - V_f$$

Component continuity equation

$$\dot{m}_f \dot{x}_f = L_R x_R + FZ + V_S y_S - L_f x_f - V_f y_f$$

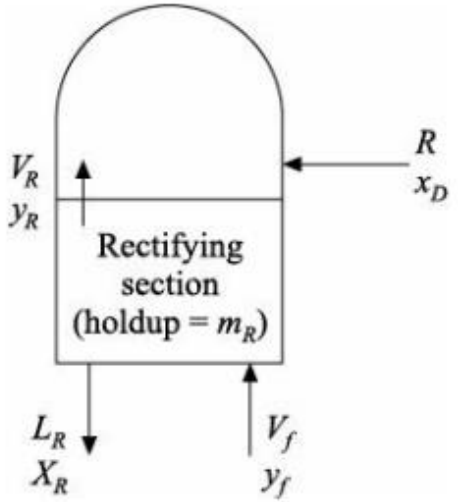
$$L_f = L_R + F.$$

$$V_S = V_f = V,$$

$$\dot{x}_f = \frac{1}{m_f}[L_R(x_R - x_f) + F(Z - x_f) + V(y_S - y_f)]$$

Note: similar steps can be followed for top trays and bottom trays

Mass Transfer System: Rectifying & Stripping Section



Total continuity equation

$$\dot m_R = R + V_f - L_R - V_R$$

Component continuity equation

$$\dot m_R \dot x_R = R x_D + V_f y_f - L_R x_R - V_R y_R$$

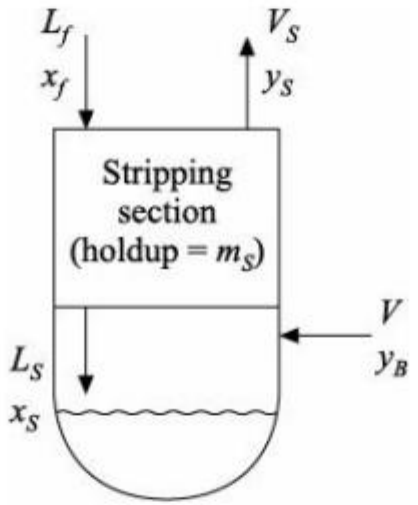
$$L_R = R$$

$$\dot x_R = \frac{1}{m_R}[R(x_D - x_R) + V(y_f - y_R)]$$

$$V_R = V_f = V_S = V$$

Total continuity equation

$$\dot m_S = L_f + V - L_S - V_S$$



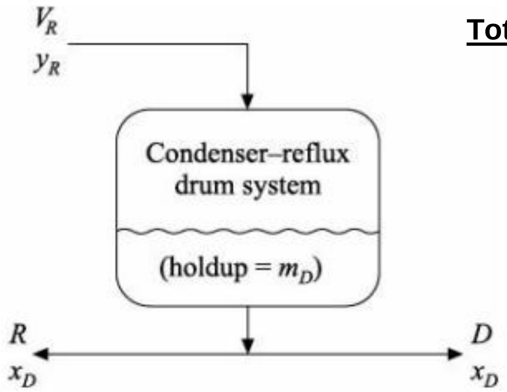
Component continuity equation

$$\dot m_S \dot x_S = L_f x_f + V y_B - L_S x_S - V_S y_S$$

$$L_f = L_S,\ V_S = V$$

$$\dot x_S = \frac{1}{m_S}[L_S(x_f - x_S) + V(y_B - y_S)]$$

Mass Transfer System: Condenser & Reboiler



Total continuity equation

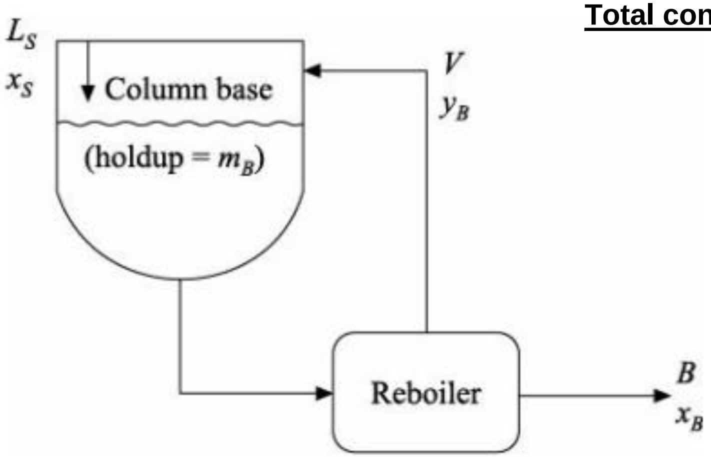
$$V = R + D$$

$$\dot{m}_D = \frac{dm_D}{dt} = V_R - R - D$$

Component continuity equation

$$\dot{m}_D \dot{x}_D = \frac{d(m_D x_D)}{dt} = V_R y_R - (R + D)x_D$$

$$\dot{x}_D = \frac{V}{m_D}(y_R - x_D)$$



Total continuity equation

$$B = L_S - V.$$

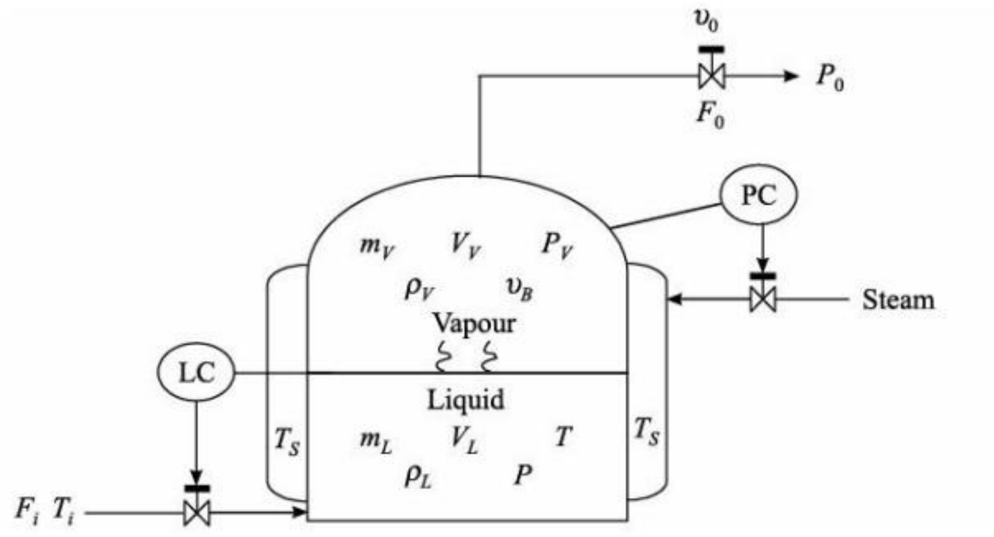
$$\dot{m}_B = L_S - B - V$$

Component continuity equation

$$\dot{m}_B \dot{x}_B = L_S x_S - B x_B - V y_B$$

$$\dot{x}_B = \frac{1}{m_B}[L_S x_S - B x_B - V y_B]$$

Heat-Transfer System: Evaporator



Mass balance (liquid phase)

$$\frac{dm_L}{dt} = \frac{d(\rho_L V_L)}{dt} = F_i \rho_L - \upsilon_B$$

Mass balance (vapor phase)

$$\upsilon_0 = K_V \sqrt{P_V (P_V - P_0)}$$

$$\frac{dm_V}{dt} = \frac{d(\rho_V V_V)}{dt} = \upsilon_B - F_0 \rho_V$$

Energy balance (liquid phase)

$$\frac{d(\rho_L V_L C_p T)}{dt} = F_i \rho_L C_p T_i - \upsilon_B(\lambda + C_p T) + Q$$

Energy balance (vapor-phase)

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

$$T_L = T_V = T$$

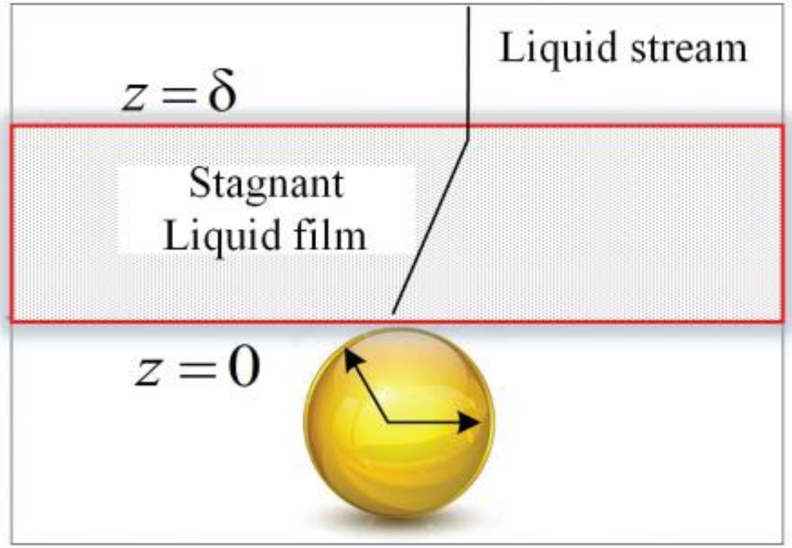
$$P_{steam} = \exp\left(11.6859 - \frac{3822.3186}{227.47 + T_S}\right)$$

$$P_V V_V = \frac{m_V RT}{MW}$$

$$V_V = V - V_L$$

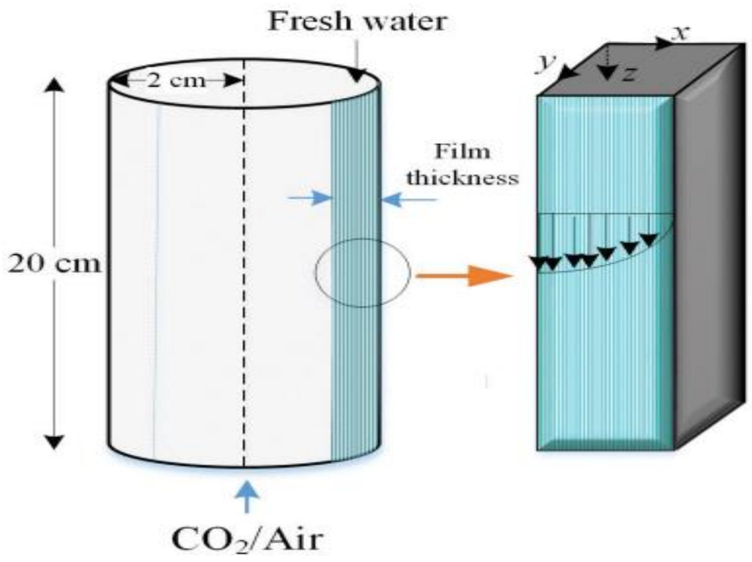
Mass Transport (Extraction)_Boundary Value Problem

Soybean oil, one of the most widely consumed cooking oils, is a vegetable oil extracted from the seeds of the soybean. Processed soybean oil is used as a base for printing inks and oil paints. In this example, a spherical soybean particle having an average diameter 2.00 mm and density $\rho = 577\,\mathrm{kg/m^3}$ is considered as a sample of an extraction process (Figure The soybean flakes contain 20% soybean oil that is to be leaked out by pure hexane solvent. The hexane solvent is flowing over the spherical particles under turbulent flow conditions. Assume a stagnant film of thickness $\delta = 0.5\,\mathrm{mm}$ around the spherical particles through which soybean oil is leached out into the bulk stream. The soybean oil density is $917\,\mathrm{kg/m^3}$, and viscosity is $\mu = 0.05$ Pa.s. The average molecular weight of soybean oil methyl esters is 292.2. The effective diffusivity is $D_{\mathrm{eff}} = 1.0 \times 10^{-11}\ \mathrm{m^2/s}$. Determine the concentration profile.



Mass Transport (Absorption)_Boundary Value Problem

Global warming is caused by the emission of greenhouse gases. Most of the emitted greenhouse gases is carbon dioxide (CO_2). In this example, carbon dioxide is being absorbed from air via a wetted wall column. The column is provided with fresh water at the top of the column, and air containing 5 mole percent CO_2 is supplied at the bottom, as described in Figure Water is flowing downward at a very low velocity of 7.96×10^{-6} m/s. The change in gas composition may be neglected due to the state of the air. The gas phase resistance to mass transfer is negligible. It is acceptable to neglect axial diffusion. Develop an expression for the carbon dioxide concentration in water.



Modeling of Heat-Transfer Systems

Heat Transport_Boundary Value Problem

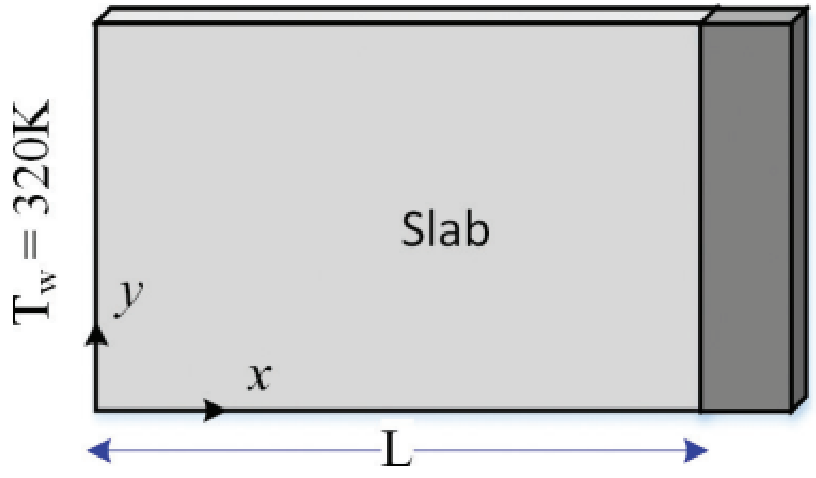
A thin slab of construction insulation material is subjected to a heat source that causes volumetric heating to vary along the length of it; see Figure

$$q = q_o \left[1 - \frac{x}{L} \right]$$

where:

q_o has a constant value of 1.8×10^5 W/m^3
slab length L is 0.06 m

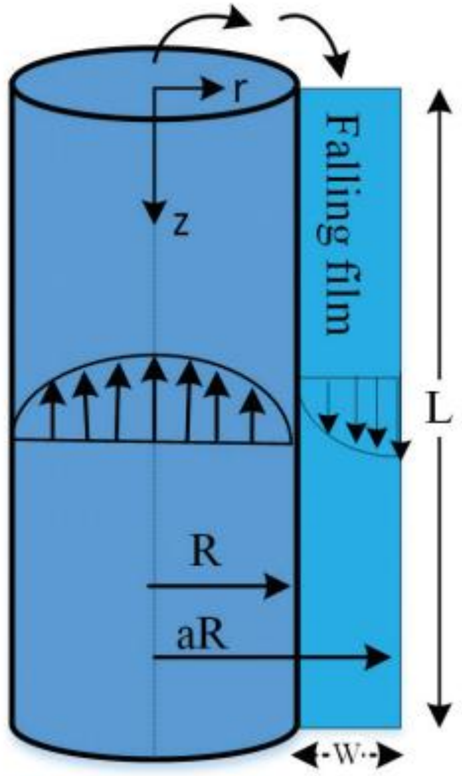
The thermal conductivity of the slab material is 0.6 W/m.K. The boundary at $x = L$ is perfectly insulated, while the surface at $x=0$ is maintained at a constant temperature of 320 K. The slab density is 1900 kg/m^3, and the specific heat capacity is 840 J/(kg . K). Develop an expression for the temperature distribution $T(x)$ in the slab. Determine an expression for the temperature profile $T(r)$, within the thin slab. What is the value of the temperate near the adiabatic wall [3]?



Modeling of Fluid-Flow Systems

Fluid Transport_Boundary Value Problem

In a gas absorption experiment, a fluid flows upward through a small circular tube and then fluid flows downward in laminar flow on the outside of the circular tube (Figure   Determine the velocity distribution in the falling film, and neglect end effects. Assume the following: width, 0.1cm; height, 1cm; inlet fluid velocity, 4.35 cm/s; $R = 0.1$ cm.



There are several assumptions that can be made to shorten the problem form:

- Steady state system.
- The flow is only in z-direction.

Summary_Model Equations: Distributed Parameter Model

$$\overbrace{\frac{\partial C_A}{\partial t}}^{\text{accum.}} = -\left(\overbrace{v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z}}^{\text{Convection}} \right) + \overbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2} \right)}^{\text{Diffusion}} + \overbrace{R_A}^{\text{reaction}}$$

$$\overbrace{\rho C_p \frac{\partial T}{\partial t}}^{\text{accum.}} = \overbrace{-\rho C_p \left(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right)}^{\substack{\text{transport by} \\ \text{bulk flow}}} + \overbrace{k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)}^{\substack{\text{transport by thermal} \\ \text{diffusion}}} + \overbrace{\Phi}^{\text{gen.}}$$

$$\overbrace{\rho \frac{\partial v_x}{\partial t}}^{\text{accum.}} = \overbrace{-\rho \left(v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right)}^{\text{transport by bulk flow}} + \overbrace{\mu \left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right)}^{\text{transport by viscous forces}} \overbrace{- \frac{\partial P}{\partial x} + \rho g_x}^{\text{generation}}$$

Module 7: Solving Set of Equations & Convergences Problems

(PDEs, ODEs and Linear Equations)

Classification of PDEs

If linear second-order differential equation

$$A\frac{\partial^2 u}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}+D\frac{\partial u}{\partial x}+E\frac{\partial u}{\partial y}+Fu=0$$

where A, B, C, D, E, and F are real constants, is said to be

hyperbolic if $B^2-4AC>0$

parabolic if $B^2-4AC=0$

elliptic if $B^2-4AC<0$

Type	*Example*	
Hyperbolic	Wave equation:	$\frac{\partial^2 u}{\partial t^2}=v^2\frac{\partial^2 u}{\partial x^2}$
Parabolic	Diffusion equation:	$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right)$
Elliptic	Poisson equation:	$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=\rho(x,y)$

Classify the following equations:

$$(a)\,3\frac{\partial^2 u}{\partial x^2}=\frac{\partial u}{\partial y}\qquad (b)\,\frac{\partial^2 u}{\partial x^2}=\frac{\partial^2 u}{\partial y^2}\qquad (c)\,\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0$$

Our focus is on "***parabolic type of PDEs***",
e.g**.: Heat-conduction equation, diffusion equation and Navier-Stokes (NS) equation**

Solution of PDEs: BVP (boundary value problem)

$$A\frac{\partial^2 u}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}+D\frac{\partial u}{\partial x}+E\frac{\partial u}{\partial y}+Fu=G$$

- ***Linear, Second-order, non-homogeneous PDEs.***
  where, *u = dependent variable (Temp, Conc, Velocity, Press)*
  x,y = *independent variable (time, space)*
  A, B…G *are either function of x & y or constants*

Note: *If G=0, it is homogeneous, else non-homogeneous*

Solution: BVPs

1. Initial conditions (ICs)
2. Boundary conditions (BCs) (**e.g.,** Dirichlet or Neumann BC)

Diffusion equation: $$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right)$$

Classical examples of PDEs (mass & energy balance eqn) in transport phenomena **(distributed-parameter models)**

PDEs are solved analytically & using numerical method algorithms available in **R or Matlab** (e.g. ***Reactran, pdepe***)

General Mathematical Solution

Equation	Solution
$\dfrac{dy}{dx} = \dfrac{f(x)}{g(y)}$	$\int g\, dy = \int f\, dx + C_1$
$\dfrac{dy}{dx} + f(x)y = g(x)$	$y = e^{-\int f\, dx}\left(\int e^{\int f\, dx} g\, dx + C_1\right)$
$\dfrac{d^2y}{dx^2} + a^2y = 0$	$y = C_1 \cos ax + C_2 \sin ax$
$\dfrac{d^2y}{dx^2} - a^2y = 0$	$y = C_1 \cosh ax + C_2 \sinh ax$ or
	$y = C_3e^{+ax} + C_4e^{-ax}$
$\dfrac{1}{x^2}\dfrac{d}{dx}\left(x^2\dfrac{dy}{dx}\right) + a^2y = 0$	$y = \dfrac{C_1}{x}\cos ax + \dfrac{C_2}{x}\sin ax$

General Mathematical Solution

$$\cosh x = \tfrac{1}{2}(e^{x} + e^{-x});$$

$$\sinh x = \tfrac{1}{2}(e^{x} - e^{-x})$$

$$\frac{d \cosh x}{dx} = \sinh x; \qquad \frac{d \sinh x}{dx} = \cosh x$$

$$\int \cosh x \, dx = \sinh x; \qquad \int \sinh x \, dx = \cosh x$$

$$2 \sinh x \cosh y = \sinh(x+y) + \sinh(x-y)$$

$$2 \cosh x \sinh y = \sinh(x+y) - \sinh(x-y)$$

$$2 \cosh x \cosh y = \cosh(x+y) + \cosh(x-y)$$

$$2 \sinh x \sinh y = \cosh(x+y) - \cosh(x-y)$$

General Solution of ODEs & PDEs

Non-homogeneous, linear, 2nd order differential equation

$$P(x)\frac{d^2y}{dx^2} + Q(x)\frac{dy}{dx} + R(x)y = G(x)$$

Homogeneous, linear, 2nd order differential equation

$$P(x)\frac{d^2y}{dx^2} + Q(x)\frac{dy}{dx} + R(x)y = 0$$

If $y_1(x)$ and $y_2(x)$ are both solutions of the linear homogeneous equation (2) and c_1 and c_2 are any constants, then the function

$$y(x) = c_1y_1(x) + c_2y_2(x)$$

is also a solution of Equation 2.

General Solution of ODEs & PDEs

innovate achieve lead

$$ay'' + by' + cy = 0$$

$$ar^2e^{rx} + bre^{rx} + ce^{rx} = 0$$

$$(ar^2 + br + c)e^{rx} = 0$$

$y = e^{rx}$ (where r is a constant)

$$y' = re^{rx}$$

$$y'' = r^2e^{rx}$$

$$r_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \qquad r_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

If the roots r_1 and r_2 of the auxiliary equation $ar^2 + br + c = 0$ are real and unequal, then the general solution of $ay'' + by' + cy = 0$ is

$$y = c_1e^{r_1x} + c_2e^{r_2x}$$

PDEs_Classical Examples

***U=* T, P, C, V (state-variables)**
***X=* t, x, y, z (independent-variables)**

$$A\frac{\partial^2 u}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}+D\frac{\partial u}{\partial x}+E\frac{\partial u}{\partial y}+Fu=G$$

- ***First-order PDEs***
- ***Second order PDEs (parabolic, hyperbolic, elliptical)***

Possible set of equations (functional form),

- *Diffusion through a porous medium* ***(e.g., flow through membranes, filters, diffusion of gas in air, absorption of gas in liquid, mass transfer processes)***
- *Diffusion plus reaction in catalyst bed* ***(e.g., PFR, both isothermal & non-isothermal, reaction engineering)***
- *Thermal diffusion* ***(e.g., heat conduction in a slab)***
- *Convective flows (i.e. bulk flow of fluid)* ***(e.g., heat-flow in heat-exchangers, fluid flow in a tank***)
- *Bulk fluid flow/ molecular transfer (i.e. velocity gradient)* ***(e.g., flow through a pipe***)

Note: *Any equation (PDEs) can be of transient-type or steady-state type with or without generation terms* ***(reaction or heat or mass)***

Methods for Solving of PDEs

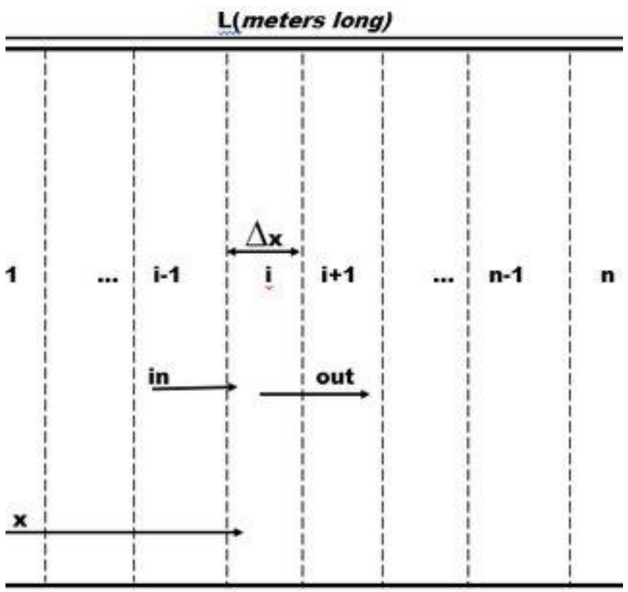
Exact methods:

- Separation of variables
- Transforming PDEs to ODEs
- Laplace transform (t-domain to variable "s")
- Fourier transform (t-domain to frequency)
- Gradient discretization method

Numerical methods (iterative methods):

- Finite difference method (FDM)
- Finite element method (FEM)
- Finite volume method (FVM)
- Methods of line **(Crank-Nicolsan Algorithm)**

Finite Difference Method (FDM)



$$\left(\frac{dy}{dx}\right)_i = \frac{(y_i - y_{i-1})}{h}$$ (Backward finite difference scheme)

$$\left(\frac{dy}{dx}\right)_i = \frac{(y_{i+1} - y_i)}{h}$$ (Forward finite difference scheme)

$$\left(\frac{dy_1}{dx}\right)_i = \frac{(y_{i+1} - y_{i-1})}{2h}$$

(by central finite difference scheme)

$$\left(\frac{d^2y}{dx^2}\right)_i = \frac{(y_{i+1} - 2y_1 + y_{i-1})}{h^2}$$

Problem Statements: Finite Difference Methods

➢ ***Dirichlet BC***

Question ①

$$\frac{d^2y}{dx^2} - 2 = 0 \quad (0 < x < 1) \; ; \; (2^{nd} \text{ order ODE})$$

@ $x = 0 \; ; \; y = 0$; (1) compute y at $x = 0.5$ i.e. → at node (2)

@ $x = 1, \; y = 0$ (2) make 2-parts. (3-nodes)

➢ ***Neumann BC***

Question ②

$$\frac{d^2y}{dx^2} - 2 = 0 \quad (0 < x < 1)$$

@ $x = 0, \; y = 0$ (Dirichlet BC)

@ $x = 1, \; \frac{dy}{dx} = 1$ (Neumann BC)

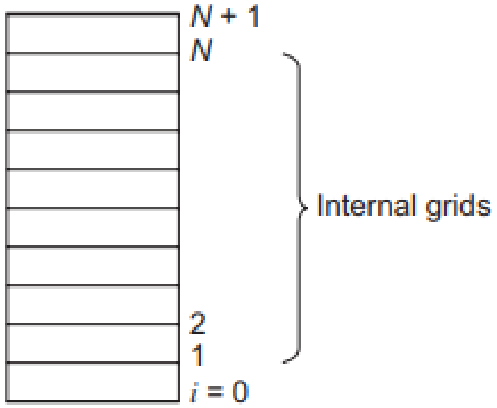
Problem Statement: Diffusion Equation_MOL

$$\frac{\partial c}{\partial t} = \left(\frac{1}{P}\right)\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} - kc^2$$

BC 1: (at $x = 0$): $\left(\frac{\partial c}{\partial x}\right)_{x=0} = P(c\ (x = 0) - 1)$

BC 2: at $x = 1$; $\frac{\partial c}{\partial x} = 0$

Initial condition: $c(0, x) = g(x)$

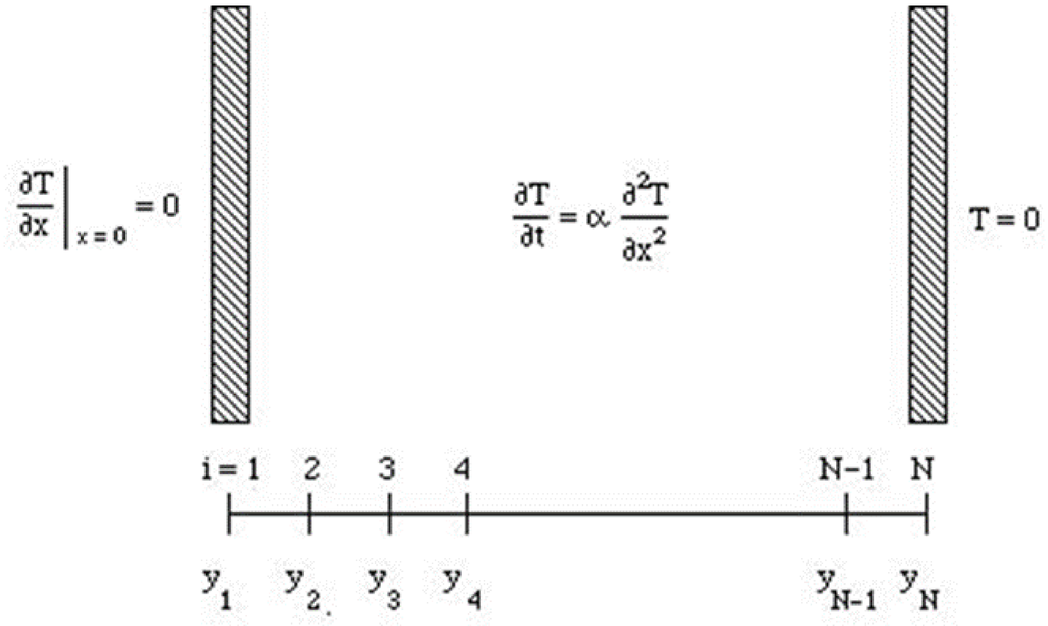


For $i = 1$; $$\left(\frac{dc_1}{dt}\right) = \left(\frac{1}{P}\right)\left[\frac{(c_2 - 2c_1 + c_0)}{h^2}\right] - \left[\frac{(c_2 - c_0)}{(2h)}\right] - kc_1^2$$

For $i = 2, N - 1$, $$\left(\frac{dc_i}{dt}\right) = \left(\frac{1}{P}\right)\left[\frac{(c_{i+1} - 2c_i + c_{i-1})}{h^2}\right] - \left[\frac{(c_{i+1} - c_{i-1})}{(2h)}\right] - kc_i^2$$

For $i = N$, $$\left(\frac{dc_N}{dt}\right) = \left(\frac{1}{P}\right)\left[\frac{(c_{N+1} - 2c_N + c_{N-1})}{h^2}\right] - \left[\frac{(c_{N+1} - c_{N-1})}{(2h)}\right] - kc_N^2$$

1-D & Transient Heat Equation: Methods of Line



Finite difference method mostly applies in FTCS:

FTCS: "forward in time and center in space"

Problem Statement: Heat Conduction through rod

Case 1: *Steady-state model (1-D, PDE, with/without source term)*

Case 2: *Transient model (1-D, PDE, with/without source term)*

Solving PDE (Diffusion & Heat Equation) Computationally

- *R (using "ReacTran" tool)*
- *Matlab (using "pdepe" tool)*
- *COMSOL (in-built PDE equations, ICs & BCs needed)*

1D-PDE (Diffusion-Equation) solving using "R"

Consider a one-dimensional PDE type diffusion-reaction model in a packed-bed reactor of length 10 meter. The boundary conditions for the system are given below. Use **R-solver** to predict the concentration change with time and space and also produce the concentration profile. Make100 nodes to carry out the spatial discretization.

BC:

$$\frac{\partial C}{\partial x}_{x=0} = 0$$

$$C_{x=10} = C_{ext}$$

$$\boxed{\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D \cdot \frac{\partial C}{\partial x}\right) - Q}$$

The model parameters are:

```
D    <- 1    # diffusion constant
Q    <- 1    # uptake rate
Cext <- 20
```

Solution:

Use "ReacTran" module available in R-software

1D-PDE solving using “ReacTran”

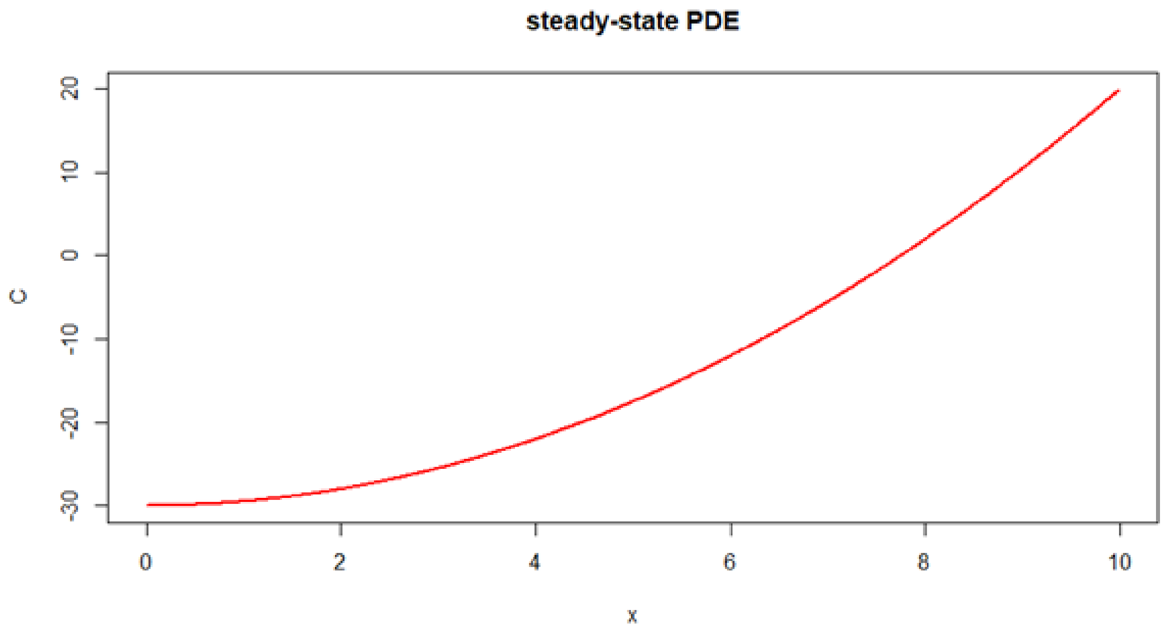
```r
# solving heat-conduction equation in R [parabolic, one-dimensional PDE (heat-diffusion equation)]
library(ReacTran)
?ReacTran
Grid <- setup.grid.1D(N = 1000, L = 10)

pde1D <-function(t, C, parms)
{
  tran <- tran.1D(C = C, D = D,C.down = Cext, dx = Grid)$dC
list(tran - Q) # return value: rate of change
}
```

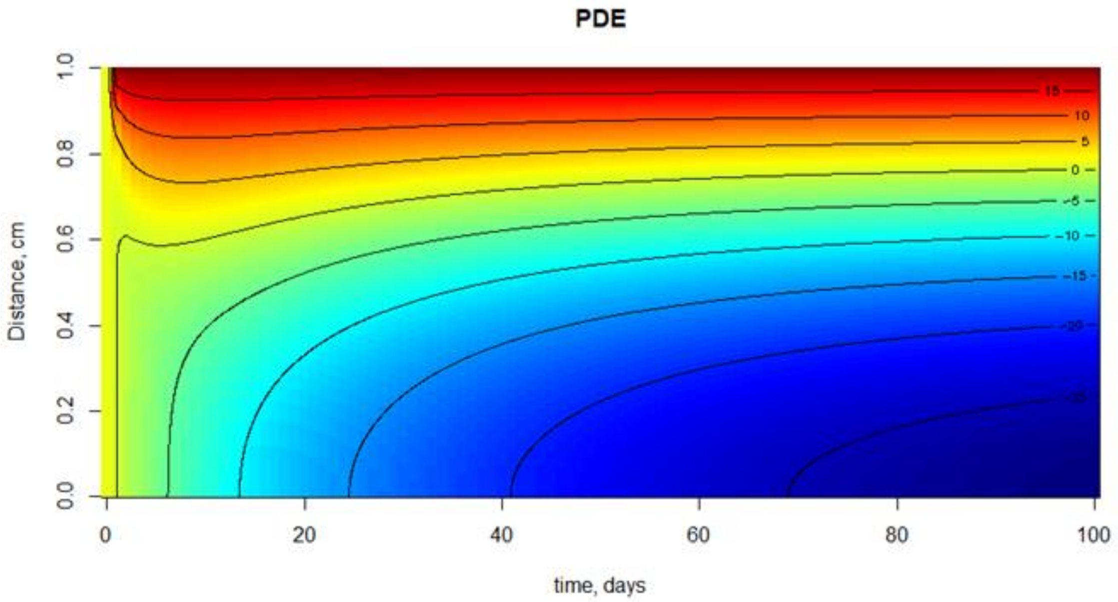
```r
# parameter initialization

D <- 1 # diffusion constant
Q <- 1 # uptake rate
Cext <- 20  # external concentration
```

```r
# solving 1-Dimensional PDE using "steady.1D"  and "ode.1D" functions

library(rootSolve)
print(system.time(std <- steady.1D(y = runif(Grid$N),func = pde1D, parms = NULL, nspec = 1)))
plot (Grid$x.mid, std$y, type = "l",lwd = 2, main = "steady-state PDE",xlab = "x", ylab = "C", col = "red")
```

```r
require(deSolve)
times <- seq(0, 100, by = 1)
system.time(out <- ode.1D(y = rep(1, Grid$N),times = times, func = pde1D, parms = NULL, nspec = 1))
tail(out[, 1:4], n = 3)

image(out, xlab = "time, days",ylab = "Distance, cm",main = "PDE", add.contour = TRUE)
```

1D-PDE solving using “ReacTran”





1D-PDE (Heat-equation) solving using **"MATLAB"**

The temperature $u(x,t)$ in a wall of unit length can be described by the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

The thickness of the wall is 1 m and the initial profile of the temperature in the wall at $t = 0$ sec is uniform at $T = 90^\circ$C. At time $t = 0$, the ambient temperature is suddenly changed to 15°C and

held there. If we assume that there is no convection resistance, the temperature of both sides of the wall is also held constant at 15°C. Determine the temperature distribution graphically within the wall from $t = 0$ to $t = 21{,}600$ sec. The wall property can be assumed as $\alpha = 4.8 \times 10^{-7}$ m/sec^2.

Solution:

*Use **"pdepe"** function available in Matlab-software*

1D-PDE solving using “pdepe”

*MATLAB (“**pdepe**”): valid for* ***parabolic & elliptical types of PDEs***

$$g\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^m f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + r\left(x,t,u,\frac{\partial u}{\partial x}\right)$$

where

$f(x,t,u,(\partial u/\partial x))$ is a flux term

$r(x,t,u,(\partial u/\partial x))$ is a source term

$g(x,t,u,(\partial u/\partial x))$ is a diagonal matrix

IC: $u(x,t_0) = u_0(x)$

BC: $p(x,t,u) + q(x,t) f\left(x,t,u,\frac{\partial u}{\partial x}\right) = 0$

```
sol = pdepe(m,@pdeTde,@pdeTic,@pdeTbc,x,t)
```

1D-PDE solving using “pdepe”

Creating/Defining a function

```
function [g,f,r] = pdeTde(x,t,u,DuDx)
alpha = 4.8e-7;
g = 1/alpha;
f = DuDx;
r = 0;
end
```

Assigning ICs:

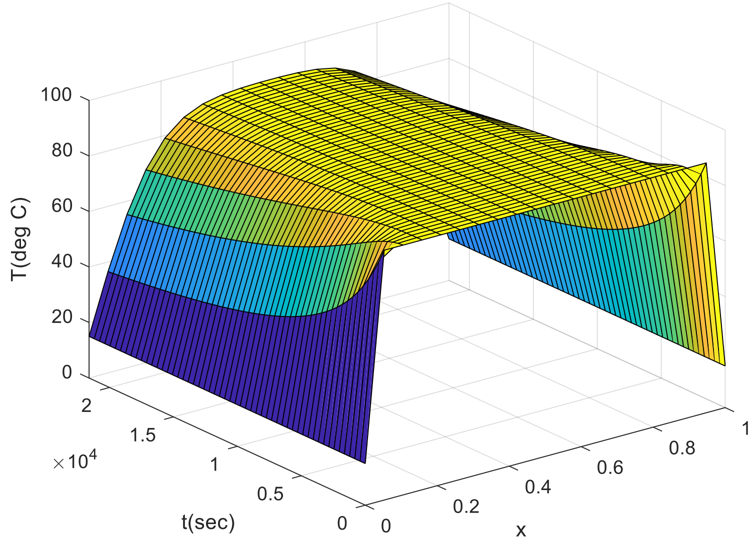
```
function u0 = pdeTic(x)
u0 = 90;
end
```

Assigning BCs:

```
function [pl,ql,pr,qr] = pdeTbc(xl,ul,xr,ur,t)
pl = ul-15;
ql = 0;
pr = ur-15;
qr = 0;
end
```

Solving PDE & result analysis:

```
m = 0;
x = linspace(0,1,20);
t = linspace(0,21600,54);
sol = pdepe(m,@pdeTde,@pdeTic,@pdeTbc,x,t);
T = sol(:,:,1); surf(x,t,T)
xlabel('x'), ylabel('t(sec)'), zlabel('T(deg C)')
```

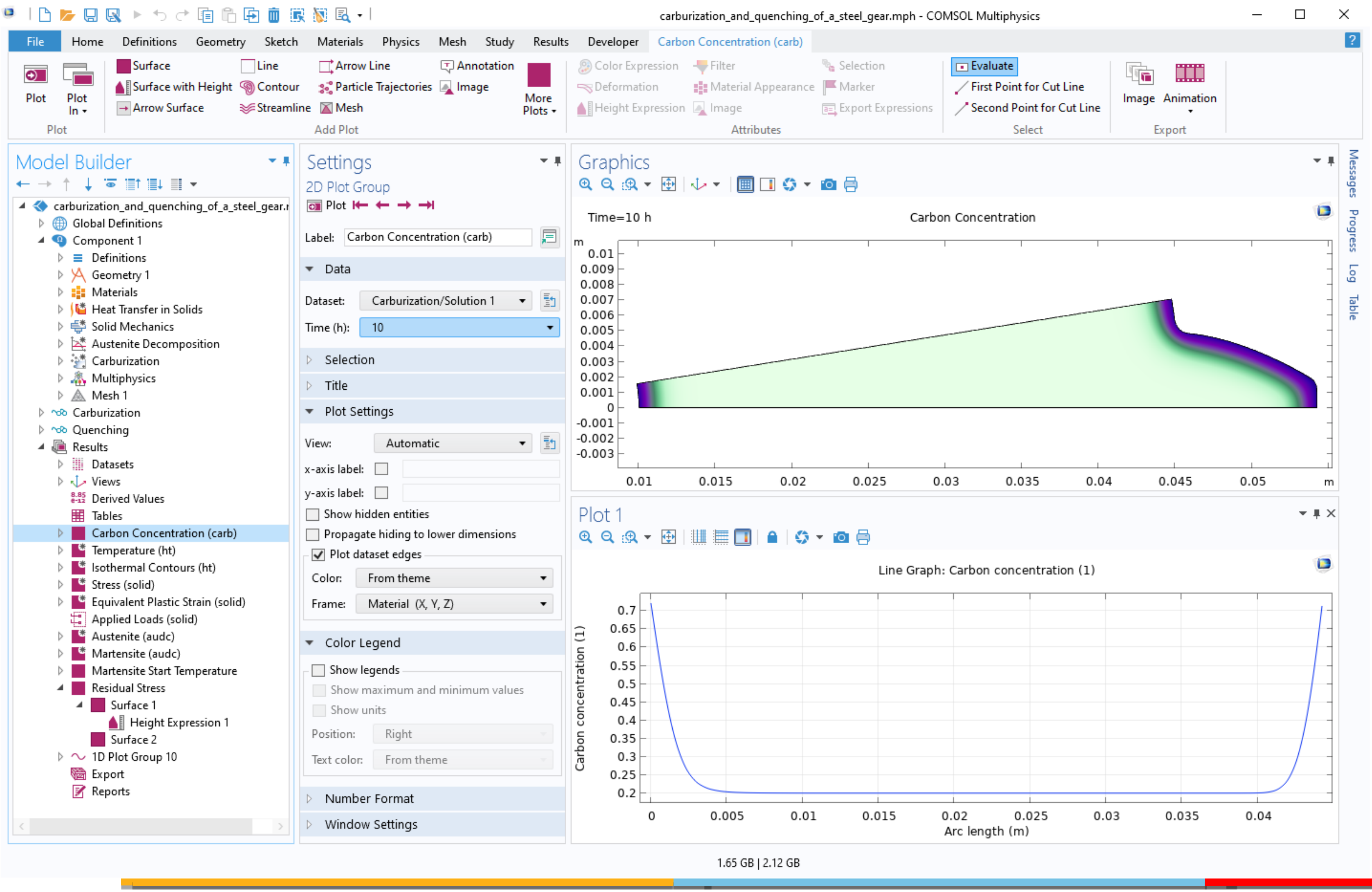


Module 8: Development & Validation of Model using COMSOL-Multiphysics

COMSOL-Multiphysics

(A CFD tool for solving 1 to 3-D distributed-parameter model: Steady-state & Transient Model)

Interface of COMSOL-Multiphysics

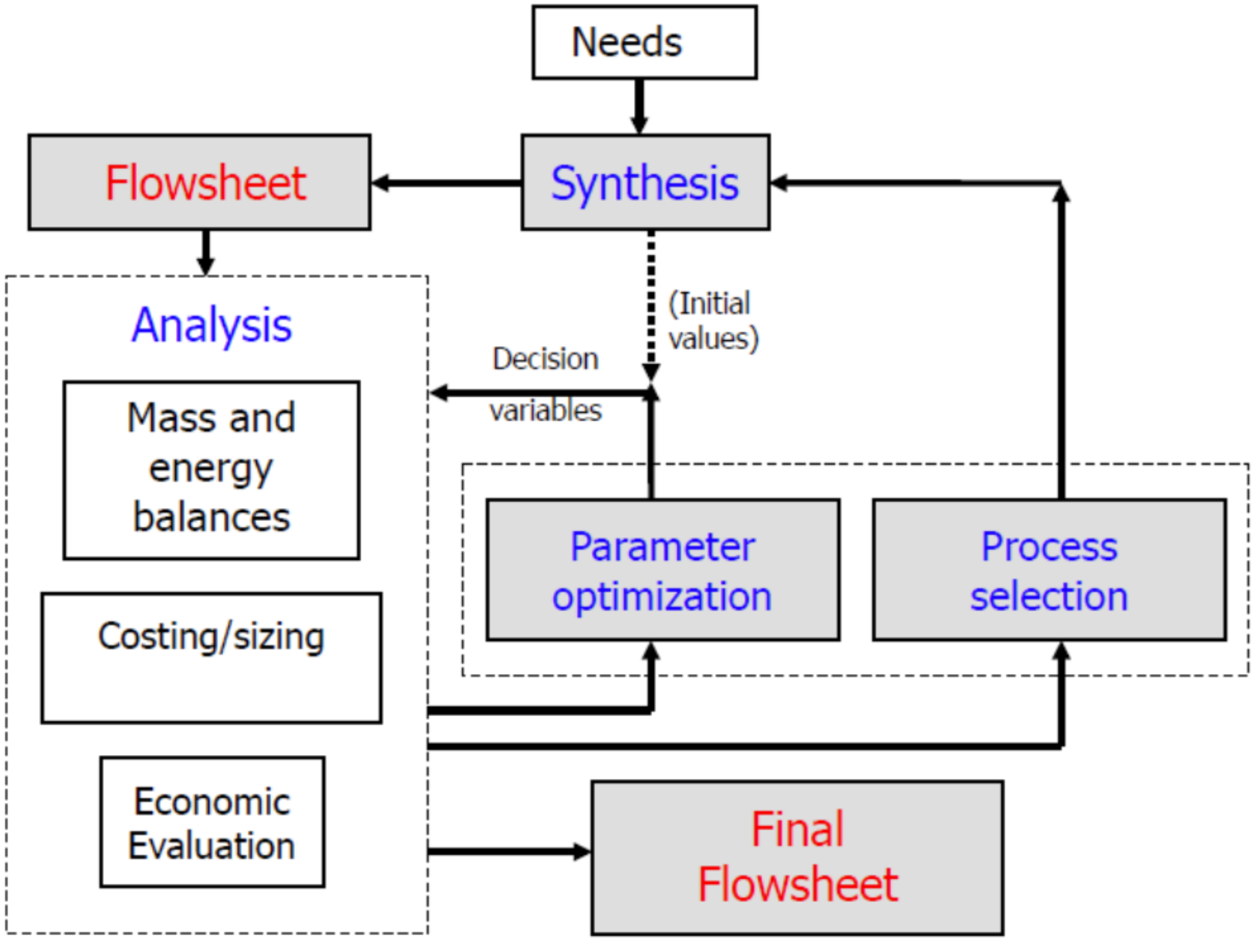


Steps Involved COMSOL-Multiphysics

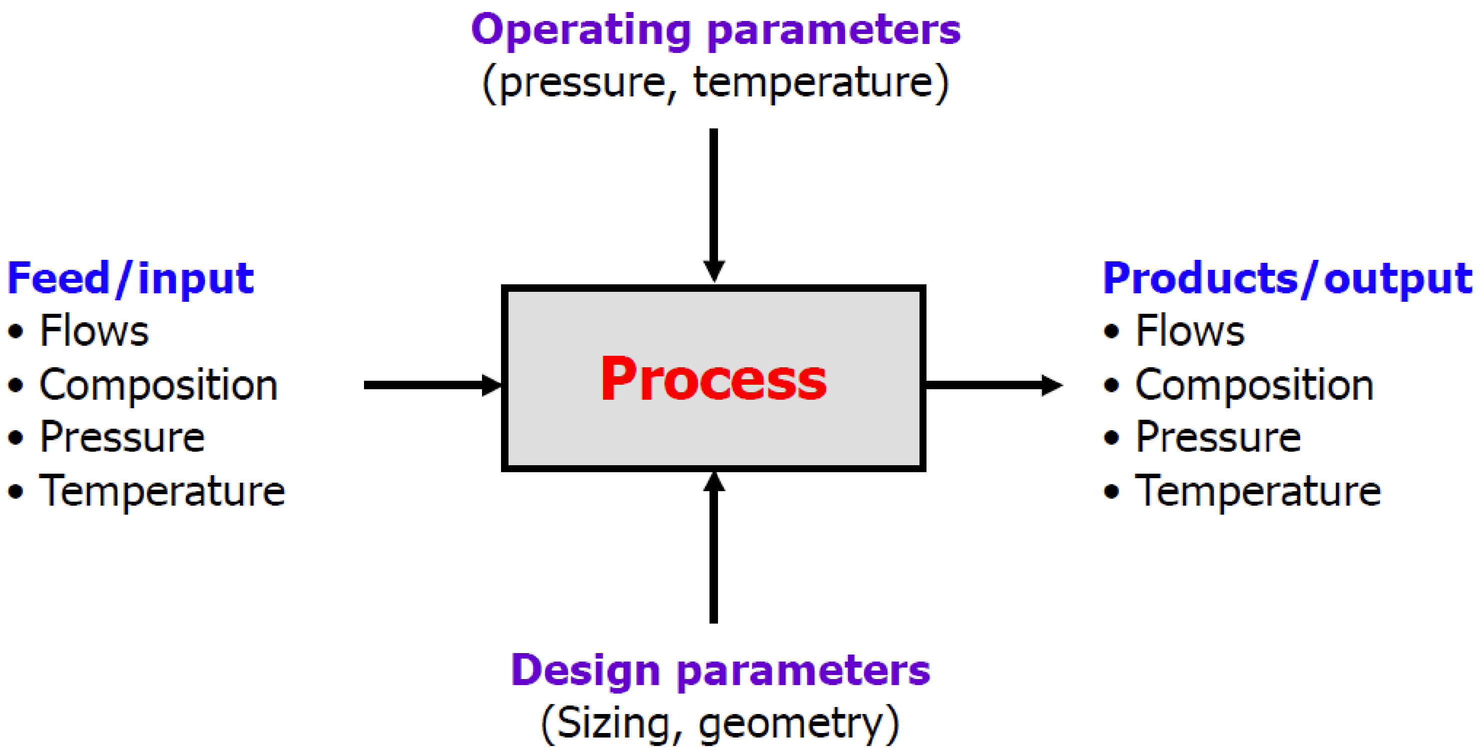
- Choosing the component (e.g., 1-D, 2-D or 3-D)
- Defining the type of study (i.e., stationary or dynamic)
- Creating the Geometry (i.e. control volume)
- Selecting the physics (e.g., fluid flow, heat-transfer, mass-transport, reaction engg)
- Initializing the variables and parameters
- Assigning the initial and boundary conditions
- Solving the physics
- Results-analysis & optimization

Module 9: Development & Validation of Model using ASPEN-Hysys

Flowsheet Modeling Concept (ASPEN)



Process (Flowsheet) Synthesis



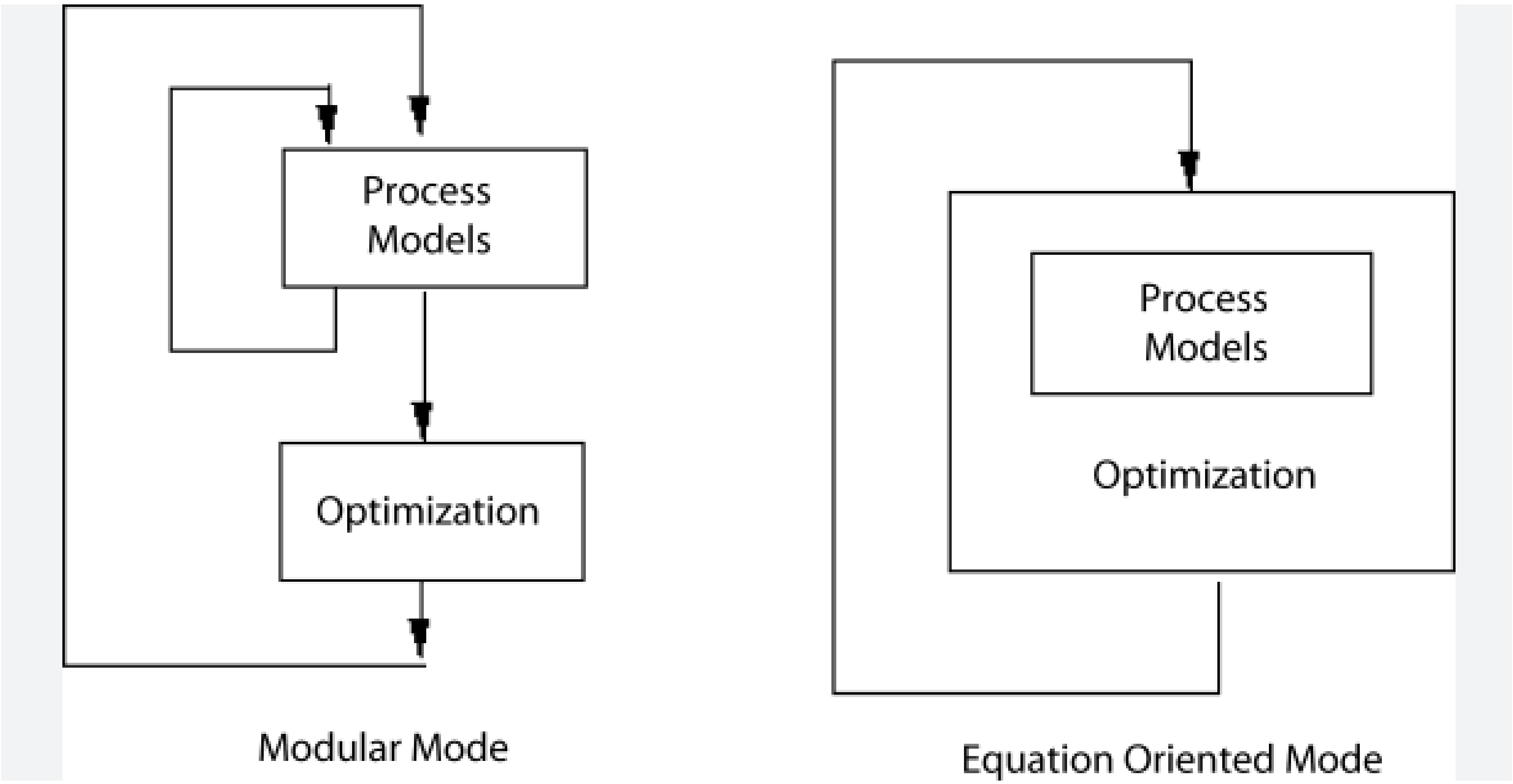
Steps involved,

- Flowsheet/process synthesis
- Flowsheet/process simulations
- Model validation & optimisation

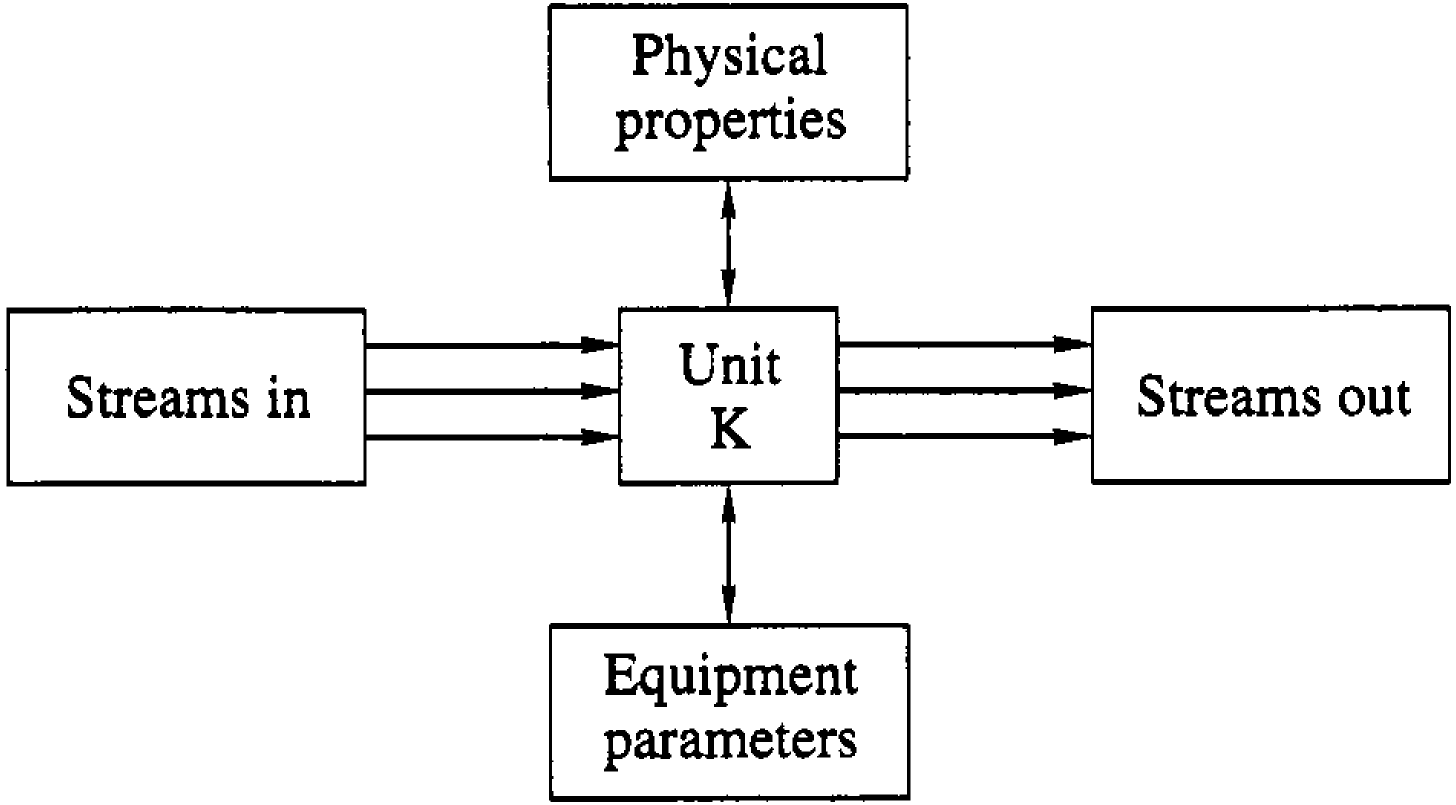
Flow-sheeting Technology

- Sequential modular (SM) approach
- Equation-oriented (EO) approach

Sequential-Modular (SM) vs Equation-Oriented (EO) Approach

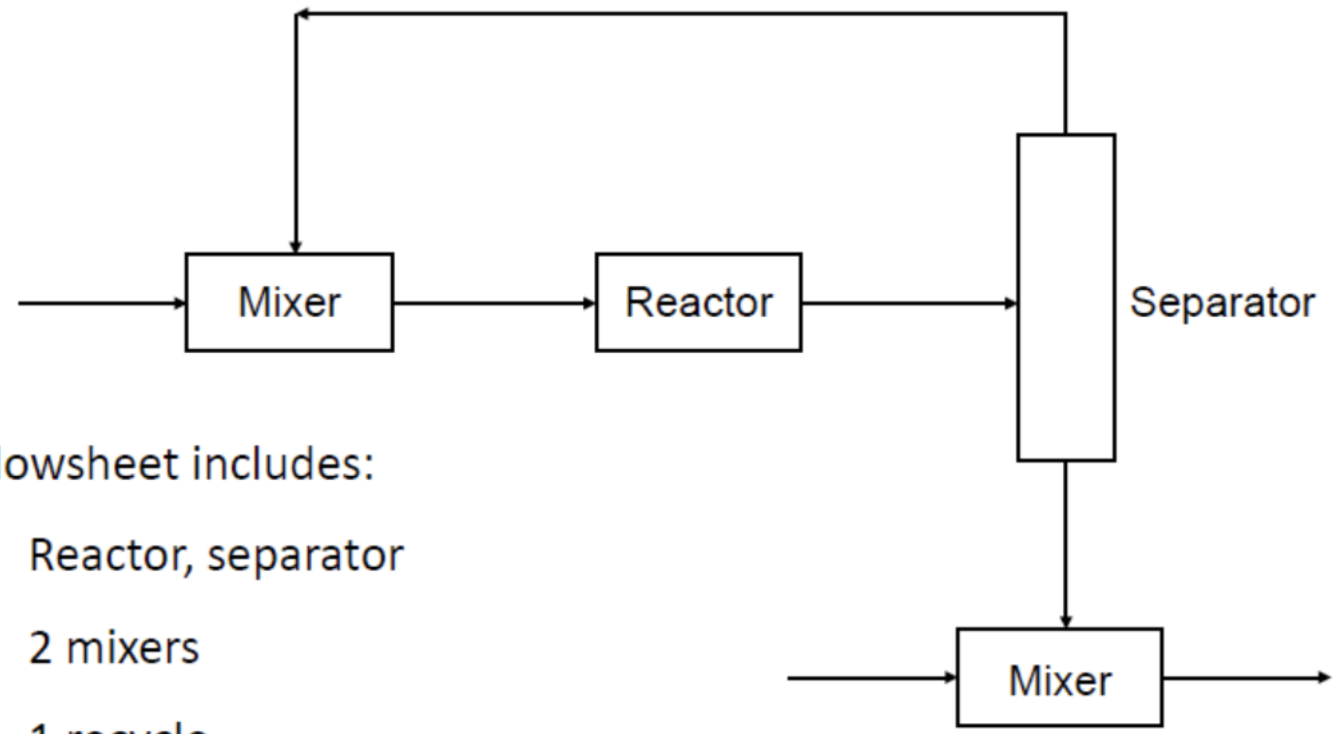


Sequential modular (SM) approach



Sequential Modular Approach

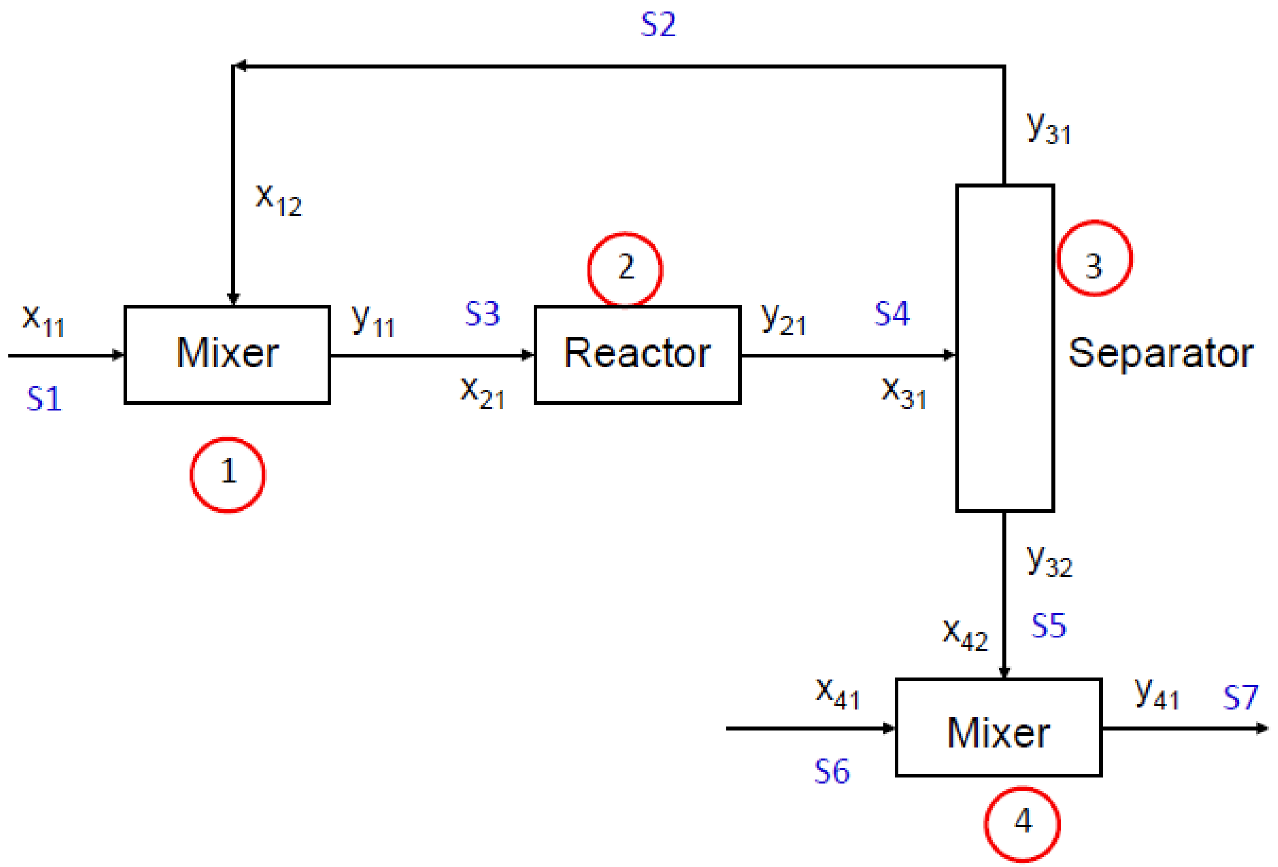
A simple flowsheet



Flowsheet includes:

- Reactor, separator
- 2 mixers
- 1 recycle

Sequential Modular Approach



Sequential Modular Approach

Simulation trade-offs and challenges:

- The "**sequential modular approach faces difficulties to converge in large problems with several recycle streams**". The simulation approach may have to iterate around distant (process unit) blocks

- The "**SM approach holds back on flowsheet calculations to ensure (robust) convergence for the individual blocks.**"

Basic idea

- Simultaneously converge all individual subsystems by linearizing (simplifying) around nominal operating points the I/Os of individual blocks

Commercial software

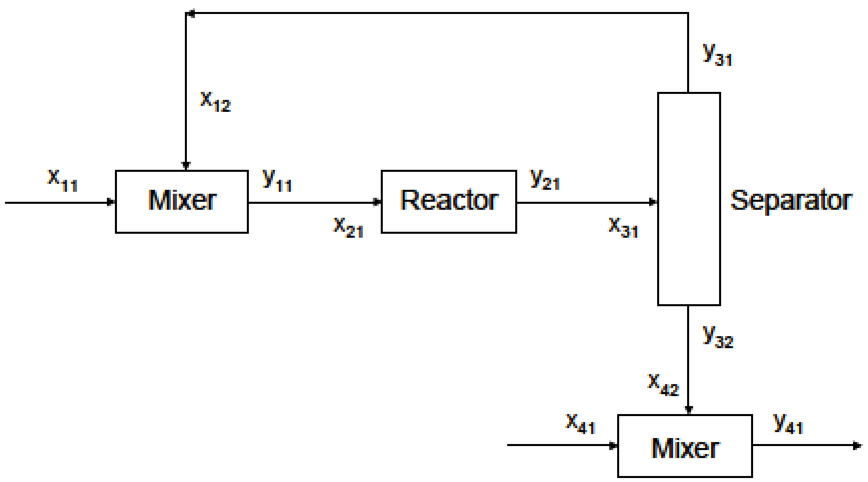
- Flowpack
- ASPEN, DWSIM
- Srsources: Rosen (1962) Umeda et al. (1972), Reklaitis (1979), Mahalec and Motard (1979), Biegler & Hughes (1982)

Mathematical representation and models

Sets of equations (constraints) for the flowsheet

- Constraints for each unit (balances: mass, energy etc; economics)

- mixer1: $f_1(x_{11},x_{12},y_{11})=0$
- reactor: $f2(x_{11},x_{12},y_{11})=0$
- seperator: $f_3(x_{11},x_{12},y_{11})=0$
- Mixer: $f4(x_{11},x_{12},y_{11})=0$



Generalization:

x_{ij} input j in unit i

y_{ij} output j from unit i

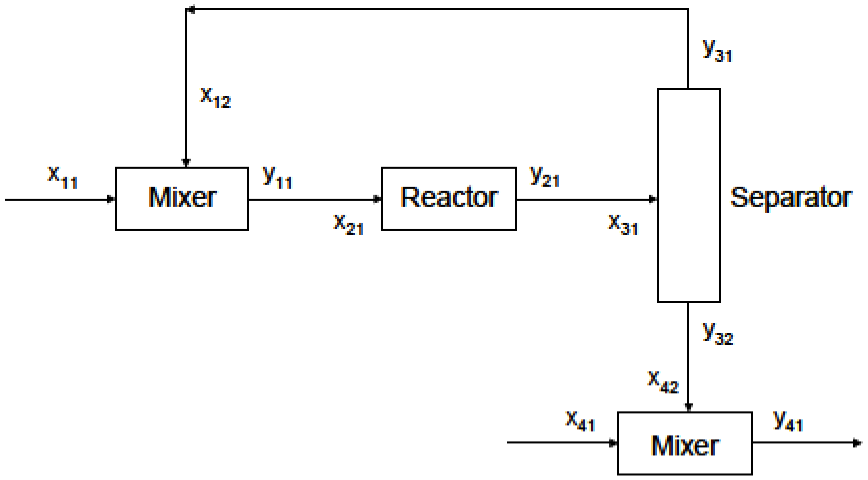
u_i parameter of unit i

Any other constraints;?

Mathematical Representation of Process

Connectivity constraints

- $X_{12}\text{-}y_{31} = 0$
- $X_{21}\text{-}y_{11} = 0$
- $X_{31}\text{-}y_{21} = 0$
- $X_{42} - y_{32} = 0$



Notes:

• unit constraints relate to mass and energy balances, constraints for physical properties, correlations, economics, upper/lower limits

• Unit parameters (design parameters) relate to specifications (e.g. temperature and pressure of a reactor) required to impose user preferences and/or make the balances a square set of equations and variables

Mathematical Representation of Process

Using such tearing, the sequence of calculations is

$$f_1(x_{11}, x_{12}, y_{11}) = 0 \Rightarrow y_{11} = g_{11}(x_{11}, x_{12})$$ (tear at x_{12}) $\longrightarrow$ convergence

$$f_2(x_{21}, x_{21}, \mathbf{u}_2) = 0 \Rightarrow y_{21} = g_{21}(x_{21}, \mathbf{u}_2)$$ (no tearing) $\longrightarrow$ convergence

$$f_3(x_{31}, y_{31}, y_{32}, \mathbf{u}_3) = 0 \Rightarrow y_{31} = g_{31}(x_{31}, \mathbf{u}_3)$$ (no tearing) $\longrightarrow$ convergence

$$\Rightarrow y_{32} = g_{32}(x_{32}, \mathbf{u}_3)$$ (no tearing) $\longrightarrow$ convergence

$$f_4(x_{41}, x_{42}, y_{41}) = 0 \Rightarrow y_{41} = g_{41}(x_{41}, x_{42})$$

Convergence in x_{12} ? If yes, stop. Otherwise, iterate

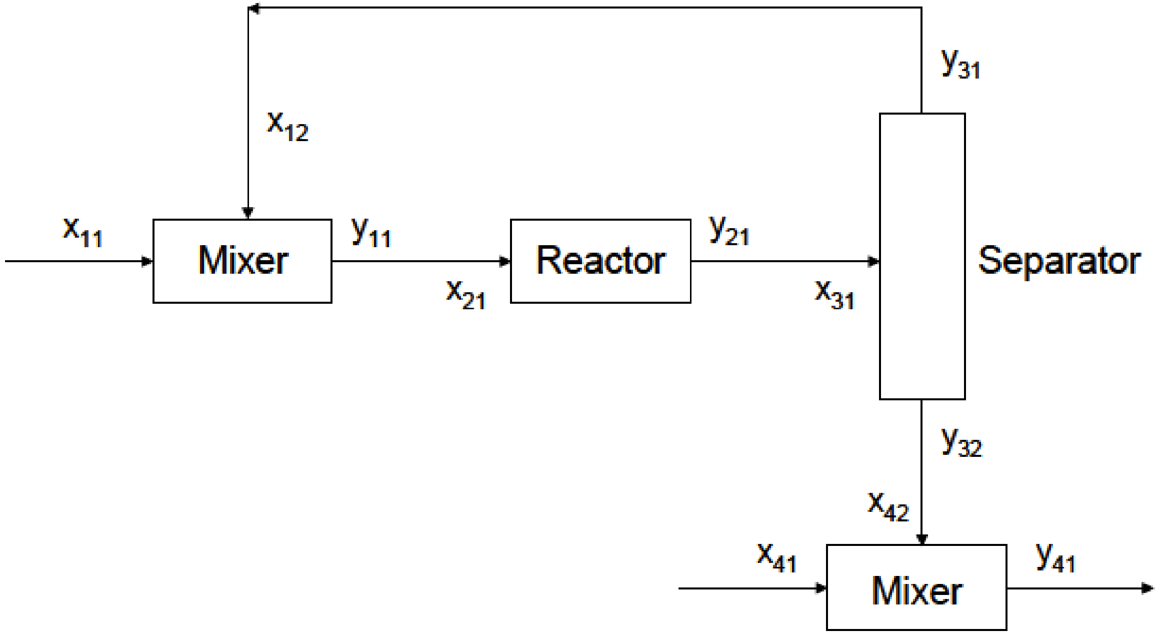
Tearing and its importance in convergence

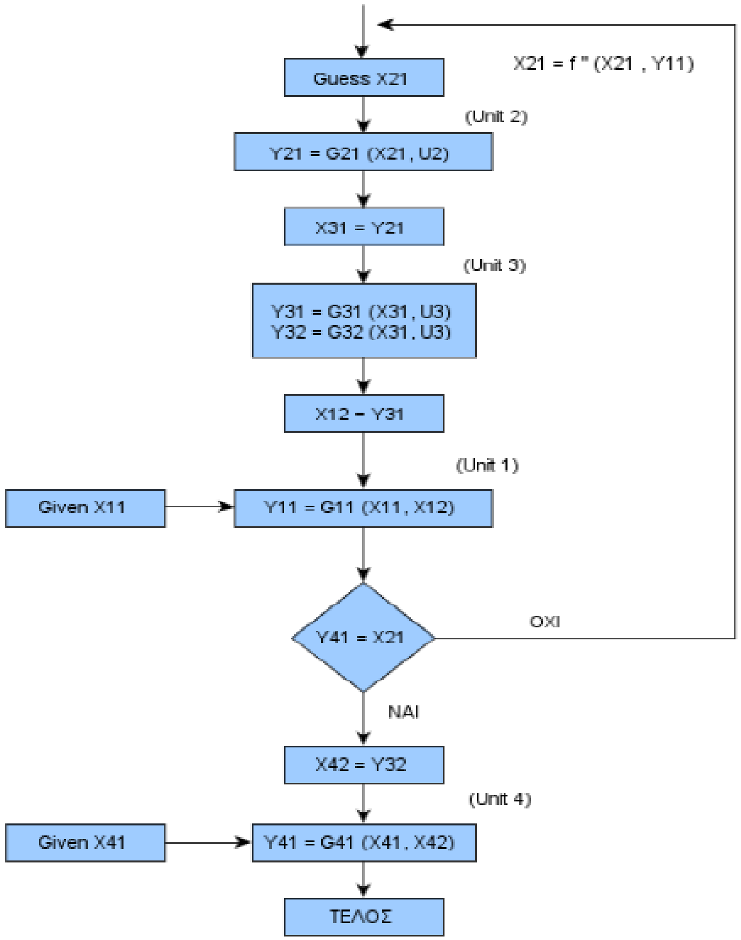
- In our case, the single tearing stream has been the recycle calculated as:

$$x_{12}^{k} = f'\left(x_{12}^{k-1}, y_{31}^{k-1}\right)$$

- There is no unique option for tearing. Indeed, there exist degrees of freedom around the tearing options and they can be exploited for better convergence
- Following natural flows in the flowsheet is not the best advice for the selection of tear streams
- Internally, the tearing is handled without any request by the user to define the tearing variables. However, the selection of tearing variables can be critical.
- Tearing may destabilize convergence. The case is pronounced when the number of recycles increase

Alternative Tearing Scenarios





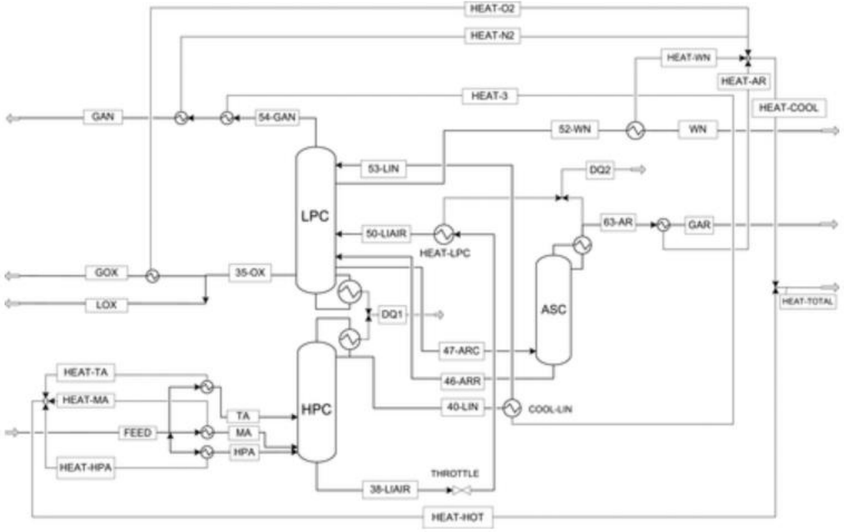
Decomposition of Networks

To make calculations sequential in a process plant with recycle and bypass streams, it is necessary to tear those streams, called “**tearing or decomposition of network”**

- ***Berkley & Motard (B & M) algorithm*** (SFG) basic tearing algorithm
- Reduced graph algorithm by **Murthy & Hussain (M & H) *algorithm*** (reduced graph algorithm)
- ***Kehat & Shacham (K & S) algorithm*** *for decomposition of networks*

- The criteria of tearing procedures (Husain 1986) are either a minimum number of variables associated with the tear streams or a minimum number of tear streams.
- This criterion suffers from the disadvantage that proper weighting factors are not readily known for all types of networks to be decomposed

EO Approach: Case Study



Flow diagram of the cryogenic air separation unit

$$L_{j-1}x_{j-1,i} + V_{j+1}y_{j+1,i} + F_j x_{Fi} = L_j x_{j,i} + V_j y_{j,i} \quad (1)$$

$$y_{j,i} = K_{j,i} x_{j,i} \quad (2)$$

$$\sum_{i=1}^{C} x_{j,i} = 1, \quad \sum_{i=1}^{C} y_{j,i} = 1 \quad (3)$$

$$L_{j-1}H_{L,j-1} + V_{j+1}H_{V,N+1} = L_j H_{L,j} + V_j H_{V,j} + Q_j \quad (4)$$

$$i \in \{N_2, Ar, O_2\}, \quad j \in \{1, ..., N\}$$

where “i” is the component index and “j” is the tray index. The **equilibrium constants Kj,i** and the enthalpy of streams in the liquid and vapor phases (**$H_{L,j}$ & $H_{V,j}$**) are obtained using the thermodynamic property method.

https://pubs.acs.org/doi/10.1021/acs.iecr.5b02768

EO Approach

	Liquid phase	Vapor phase
SM	see SM code below	see SM code below
EO	$f(ZL) = ZL^3 + a_1 ZL^2 + a_2 ZL + a_3 = 0$ $f'(ZL) = 3ZL^2 + 2a_1 ZL + a_2 \geq 0$ $f''(ZL) = 6ZL + 2a_1 \leq 0$	$f(ZV) = ZV^3 + a_1 ZV^2 + a_2 ZV + a_3 = 0$ $f'(ZV) = 3ZV^2 + 2a_1 ZV + a_2 \geq 0$ $f''(ZV) = 6ZV + 2a_1 \geq 0$

SM — Liquid phase

```
ZL=roots([1  a1  a2  a3]);
if isreal(ZL)
  ZL=min(ZL);
else
  for i=1:3
      if isreal(ZL(i))
          ZL=ZL(i);
          break;
      end
  end
end
```

SM — Vapor phase

```
ZV=roots([1  a1  a2  a3]);
if isreal(ZV)
  ZL=max(ZV);
else
  for i=1:3
      if isreal(ZV(i))
          ZV=ZV(i);
          break;
      end
  end
end
```