Modelling & Simulation of Chemical Engineering Systems

٥٠١ هعم : تمثيل الأنظمة الهندسية على الحاسب الآلى

Department of Chemical Engineering
King Saud University

LECTURE #5

Equations of Change

Total Mass balance

- **Mass in:**
- The mass entering in the x-direction at the cross sectional area ($\Delta y \Delta z$) is :

$$(\rho v_x)|_x \Delta y \Delta z \Delta t$$

- The mass entering in the y-direction at the cross sectional area ($\Delta x \Delta z$) is

$$(\rho \varpi_\psi)|_y \Delta x \Delta z \Delta t$$

- The mass entering in the z-direction at the cross sectional area ($\Delta x \Delta y$) is

$$(\rho v_z)|_z \Delta x \ \Delta y \ \Delta t$$

- **Mass out:**
- The mass exiting in the x-direction is:

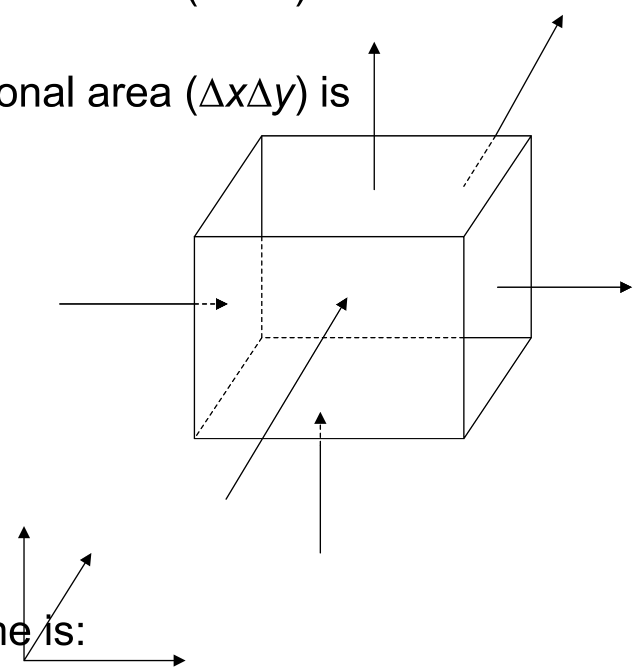
$$(\rho v_x)|_{x+\Delta X} \Delta y \Delta z \Delta t$$

- The mass exiting in the y-direction is:

$$(\rho \varpi_\psi)|_{y+\Delta y} \Delta x \Delta z \Delta t$$

- The mass exiting in the z-direction is:

$$(\rho v_z)|_{z+\Delta z} \Delta x \ \Delta y \ \Delta t$$



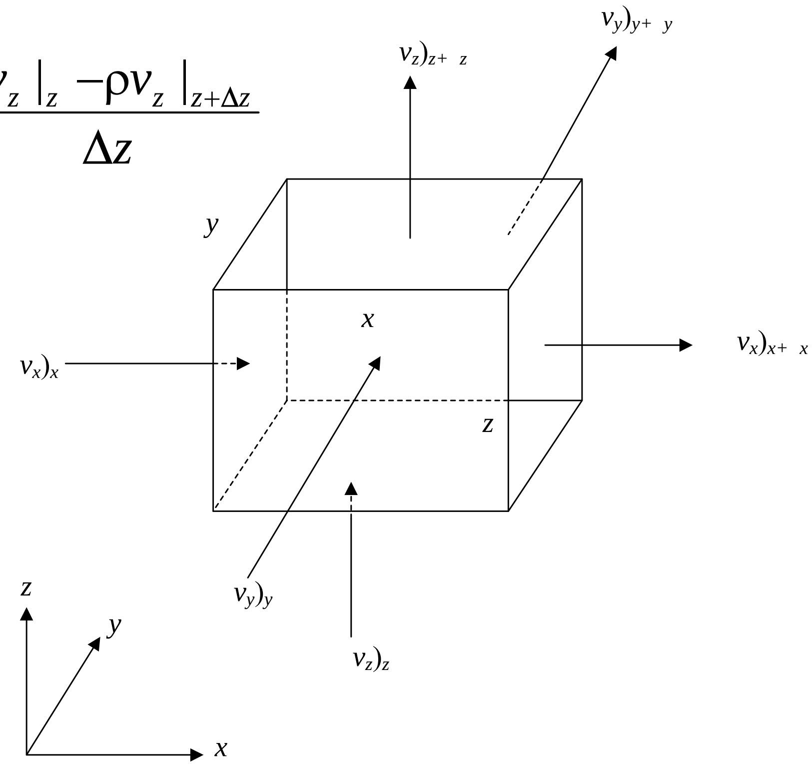
- **Rate of accumulation**:

The rate of accumulation of mass in the elementary volume is:

- $(\rho)|_{\tau+\Delta\tau} \Delta x \ \Delta y \ \Delta z - (\rho)|_t \Delta x \ \Delta y \ \Delta z$

Total Mass balance

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



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

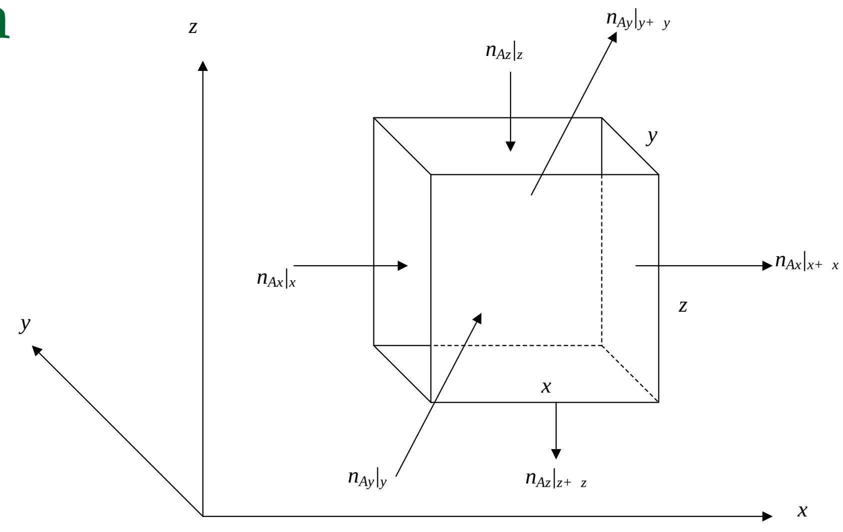
$$\frac{\partial \rho}{\partial t} + v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + v_z \frac{\partial \rho}{\partial z} = -\rho\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right)$$

Continuity equation

If the fluid is incompressible

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

Component Balance Equation



- $(\rho_A|_{t+\Delta t} - \rho_A|_t)\,\Delta x\,\Delta y\,\Delta z = (n_{Ax}|_{x+\Delta x} - n_{Ax}|_x)\Delta y \Delta z \Delta t + (n_{Ay}|_{y+\Delta y} - n_{Ay}|_y)\Delta x \Delta z \Delta t + (n_{Az}|_{z+\Delta z} - n_{Az}|_z)\Delta x \Delta y \Delta t + r_A \Delta x\,\Delta y\,\Delta z \Delta t$

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial n_{Ax}}{\partial t} + \frac{\partial n_{Ay}}{\partial t} + \frac{\partial n_{Az}}{\partial t} = r_A$$

$n_A = \rho_A v + j_A$

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

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

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

Component Balance Equation

- If the binary mixture is a dilute liquid and can be considered incompressible, then density ρ and diffusivity D_{AB} are constant

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

In molar units

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

Momentum Balance

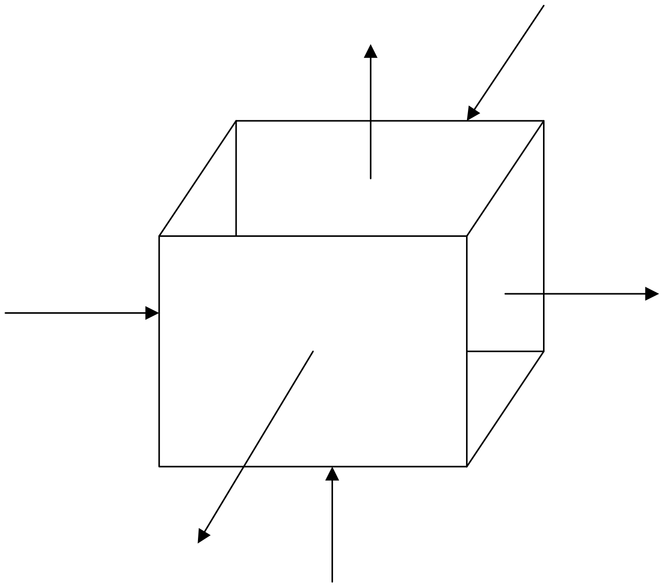
- Navier-Stock's equation (Newtonian, incompressible fluid)

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

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

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

Energy balance



$$\frac{\partial(\rho CpT)}{\partial t}+\frac{\partial(\rho CpTv_x)}{\partial x}+\frac{\partial(\rho CpTv_y)}{\partial y}+\frac{\partial(\rho CpTv_z)}{\partial z}+\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}=\Phi_H$$

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

$q_x \quad x$

for incompressible fluids $$\rho Cp\left(\frac{\partial T}{\partial t}+v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z}\right)+\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}=\Phi_H$$

$$q_u=-k\frac{dT}{du}$$

$$\underbrace{\rho Cp\frac{\partial T}{\partial t}}_{accumulation}+\underbrace{\rho Cp\left(v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z}\right)}_{\text{Transport by bulk flow}}=\underbrace{k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)}_{\text{Transport by thermal diffusion}}+\underbrace{\Phi_H}_{generation}$$

- For solids, the density is constant and with no velocity, i.e. *v* = 0, the equation is reduced to:

$$\underbrace{\rho Cp\frac{\partial T}{\partial t}}_{accumulation} = \underbrace{k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)}_{\text{Transport by thermal diffusion}} + \underbrace{\Phi_H}_{generation}$$

Balance Equations in Cartesian Coordinates

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

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

$$\rho Cp\frac{\partial T}{\partial t}+\rho Cp(v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z})=k(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2})+\Phi_H$$

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

$$\rho\frac{\partial v_y}{\partial t}+\rho(v_x\frac{\partial v_y}{\partial x}+v_y\frac{\partial v_y}{\partial y}+v_z\frac{\partial v_y}{\partial z})=\mu(\frac{\partial^2 v_y}{\partial x^2}+\frac{\partial^2 v_y}{\partial y^2}+\frac{\partial^2 v_y}{\partial z^2})-\frac{\partial P}{\partial y}+\rho g_y$$

$$\rho\frac{\partial v_z}{\partial t}+\rho(v_x\frac{\partial v_z}{\partial x}+v_y\frac{\partial v_z}{\partial y}+v_z\frac{\partial v_z}{\partial z})=\mu(\frac{\partial^2 v_z}{\partial x^2}+\frac{\partial^2 v_z}{\partial y^2}+\frac{\partial^2 v_z}{\partial z^2})-\frac{\partial P}{\partial z}+\rho g_z$$

Balance Equations in Cylindrical Coordinates

$x = r\cos(\theta), \quad y = r\sin(\theta), \quad z = z$

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

$$\frac{\partial C_A}{\partial t} + \left(v_r \frac{\partial C_A}{\partial r} + v_\theta \frac{1}{r}\frac{\partial C_A}{\partial \theta} + v_z \frac{\partial C_A}{\partial z}\right) = D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2} + \frac{\partial^2 C_A}{\partial z^2}\right) + R_A$$

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

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

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

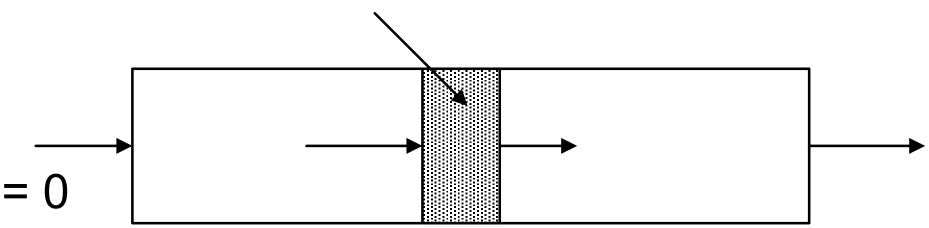
$$\rho\frac{\partial v_z}{\partial t} + \rho\left(v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z}\right) = \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2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

Examples of Application of Equations of change

1. Liquid flow in a Pipe

- One dimensional flow through the pipe of an incompressible fluid
- Cylindrical coordinate, Continuity Equation

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



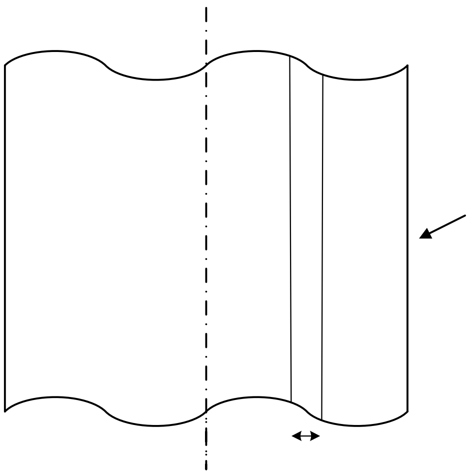
The plug flow assumptions imply that $v_r = v_\theta = 0$

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

Examples of Application of Equations of change

2 Diffusion with Chemical Reaction in a Slab Catalyst

- To model the steady state diffusion with chemical reaction of species *A* in a slab catalyst, we use the component balance equation of change .
- The fluid properties are assumed constant
- One dimensional, Cartesian coordinate



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

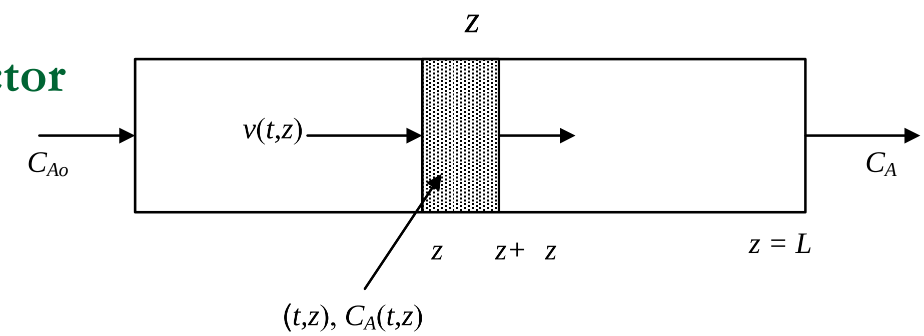
Steady State $\frac{\partial C_A}{\partial t} = 0$

No bulk flow: $v_x = v_y = v_z = 0$

One dimension, z

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

Examples of Application of Equations of change- Plug Flow Reactor



- The isothermal plug flow reactor can be modeled using the component balance equation

$$\frac{\partial C_A}{\partial t} + \left(v_r \frac{\partial C_A}{\partial r} + v_\theta \frac{1}{r}\frac{\partial C_A}{\partial \theta} + v_z \frac{\partial C_A}{\partial z} \right) = D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial C_A}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2} + \frac{\partial^2 C_A}{\partial z^2}) \right) + R_A$$

- The one dimensional assumption and plug flow conditions imply that $vr = v_\theta = 0$ and

. :

$$\frac{\partial C_A}{\partial t} = -v_z \frac{\partial C_A}{\partial z} + D_{AB}\frac{\partial^2 C_A}{\partial z^2} - R_A$$

Non-isothermal PFR

- For fluid with constant properties and at constant pressure, we have:

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

Using the plug-flow assumptions, $v_r = v_\theta = 0$ and , and neglecting the viscous forces, the term Φ_H includes the heat generation by reaction rate R_A and heat exchanged with the cooling jacket, $h_t A(T - Tw)$. :

$$\rho Cp\frac{\partial T}{\partial t}=-\rho Cpv\frac{\partial T}{\partial z}+k\frac{\partial^2 T}{\partial z^2}-\Delta H_r k_o e^{-E/RT}C_A-h_t\frac{\pi D}{A}(T-T_w)$$