I.C. $T(t=0) = T_0$

$[X_i](t=0) = [X_i]_0$

$$\frac{dT}{dt} = \frac{\dot{Q}/V - \sum_i \bar{h}_i \dot{\omega}_i}{\sum_i ([X_i]\bar{c}_{p,i})}$$

const P, fixed mass

$$\frac{d[X_i]}{dt} = \dot{\omega}_i - [X_i]\left(\frac{\sum_i \dot{\omega}_i}{\sum_j [X_j]} + \frac{1}{T}\frac{dT}{dt}\right)$$

V = const.
m = const

$$m\frac{dU}{dt} = \dot{Q}_{in} - \dot{W}_{out} + \dot{E}_{in} - \dot{E}_{out}$$

$$\frac{du}{dt} = \dot{Q}/m$$

$$\Rightarrow \frac{dT}{dt} = \frac{(\dot{Q}/V) - \sum_i (\bar{u}_i \dot{\omega}_i)}{\sum_i ([X_i]\bar{c}_{v,i})}$$

$\bar{u}_i = \bar{h}_i - R_u T \qquad \bar{c}_{v,i} = \bar{c}_{p,i} - R_u$

$$\boxed{\frac{dT}{dt} = \frac{(\dot{Q}/V) + R_u T \sum_i \dot{\omega}_i - \sum_i (\bar{h}_i \dot{\omega}_i)}{\sum_i ([X_i](\bar{c}_{p,i} - R_u))}}$$

need $\frac{dP}{dt}$ for const. V

$$VP = \sum_i N_i R_u T$$

$$P = \sum_i [X_i] R_u T$$

$$\frac{dP}{dt} = R_u T \sum_i \frac{d[X_i]}{dt} + R_u \sum_i [X_i] \frac{dT}{dt}$$

$$\dot{\omega}_i = \frac{d[X_i]}{dt} + \frac{[X_i]}{V}\frac{dV}{dt} = \frac{d[X_i]}{dt}$$

$$\frac{dP}{dt} = R_u T \sum_i \dot{\omega}_i + R_u \sum_i [X_i] \frac{dT}{dt}$$

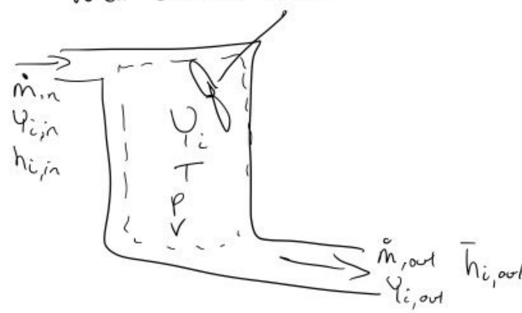
$$\frac{dT}{dt} = f([X_i], T)$$

$$\frac{d[X_i]}{dt} = \dot{\omega}_i = f([X_i], T)$$

$T(t=0) = T_0$

$[X_i](t=0) = [X_i]_0$

Well-Stirred Reactor



mass:

$$\frac{dm_{i,cv}}{dt} = \dot{m}_{i,in} - \dot{m}_{i,out} + \dot{m}_i''' V$$

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

$$\dot{m}_i''' = \dot{\omega}_i MW_i$$

$\dot{m}_i = \dot{m} Y_i$ (no diffusion)

S.S.

$$0 = \dot{\omega}_i MW_i V + \dot{m}(Y_{i,in} - Y_{i,out})$$

$$Y_i = \frac{[X_i] MW_i}{\sum_i [X_i] MW_i}$$

energy:

$$\frac{dU}{dt} = E_{in} - E_{out} + \dot{Q} - \dot{W}$$

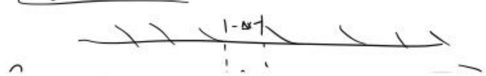
($\frac{dU}{dt} \to 0$, $E_{in} \to \dot{m} h_{in}$, $E_{out} \to \dot{m} h_{out}$, $\dot{W} \to 0$)

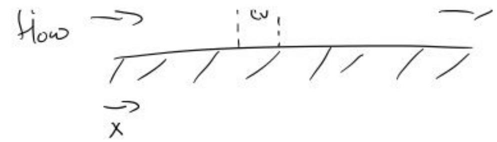
$$\dot{Q} = \dot{m}(h_{out} - h_{in})$$

residence time:

$$t_R = \frac{\rho V}{\dot{m}} \frac{[kg]}{[kg/s]} = [time]$$

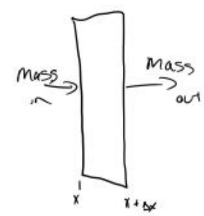
Plug Flow Rxt





1) SS.
2) no axial mixing
3) 1-D flow (uniform properties perpendicular to flow)
4) ideal frictionless flow
5) ideal gas

Mass balance:



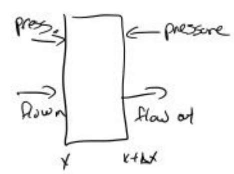
$$\dot{m} = \rho \frac{V}{s} = \rho V_x A$$

$$(\rho V_x A)_x - (\rho V_x A)_{x+\Delta x} = 0$$

$$\Delta x \to 0$$

$$\frac{d}{dx}(\rho V_x A) = 0$$

X-momentum

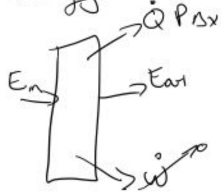


acc. mom = mom. flow in-out + mom. forces

e.g. $(PA)_x$

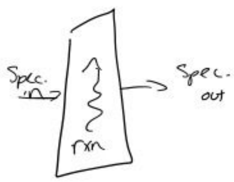
$$(PA)_{x+\Delta x} = (PA)_x + \frac{d}{dx}(PA)\,dx$$

energy:



$ke + \bar{h}$

Species



$\dot{m} Y_i$

$$\frac{dm_i}{dt} = \dot{m}_{i,in} - \dot{m}_{i,out} + \dot{m}_{gen}$$

$$\dot{m}_{i,gen} = \dot{m}_i''' A\,dx = \dot{\omega} MW_i A\,dx$$

mass: $$\frac{d(\rho v_x A)}{dt} = 0$$

momentum: $$\frac{dP}{dx} + \rho v_x \frac{dv_x}{dx} = 0$$

energy: $$\frac{d\left(h + v_x^2/2\right)}{dx} + \frac{\dot{Q}'' \, Perim}{\dot{m}} = 0$$

species: $$\frac{dY_i}{dx} - \frac{\dot{\omega}_i MW_i}{\rho v_x} = 0$$