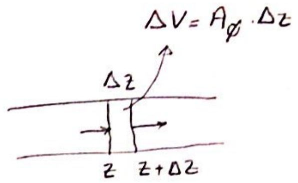
① Chemical rxn with Dispersion



- MBE
  - → for a tubular flow reactor with axial dispersion, for reactant A
  - →
$$-\left[(uC_A)_{z+\Delta z} - (uC_A)_z\right] + \left[D_L \frac{dC_A}{dz}\bigg|_{z+\Delta z} - D_L \frac{dC_A}{dz}\bigg|_z\right] = -r_A \cdot \Delta z$$
  - $\div \Delta z$, $\Delta z \to 0$
$$-\frac{d}{dz}(uC_A) + \frac{d}{dz}\left(D_L \frac{dC_A}{dz}\right) = -r_A \qquad (1)$$
  - → Hard to solve analytically if u and D_L are functions of z.
  - → Eq. (1) is a fairly general form for a 1D model.
  - → Assumption
    - → D_L is constant (usually)
    - → u " " (for a constant density system).
  - → Hence, the governing eq. becomes: $D_L \dfrac{d^2C_A}{dz^2} - u\dfrac{dC_A}{dz} = -r_A$
  - → Dimensionless variables: $C_A^* = \dfrac{C_A}{C_{A0}}$, $z^* = \dfrac{z}{L}$, $\tau = \dfrac{V}{v_0} = \dfrac{L}{u_0} = \dfrac{L}{u}$ (for a constant density system)

$$\Rightarrow \left(\frac{D_L}{uL}\right)\cdot\frac{d^2C_A^*}{dz^{*2}} - \frac{dC_A^*}{dz} - \frac{\tau}{C_{A0}}(-r_A) = 0 \qquad (2)$$

B.C.s
- → #1: @ $z^* = 1$: $\dfrac{dC_A^*}{dz^*} = 0$
- → #2: @ $z^* = 0$: $C_A^* - \dfrac{D_L}{uL}\cdot\dfrac{dC_A^*}{dz^*} = 1$

→ no axial dispersion in feed line, → $-D\dfrac{dC}{dz} + uC = uC_0$

- → for 1st order rxns ($-r_A = kC_A$), analytical solution gives:

$$C_A^*\Big|_L = \frac{C_{AE}}{C_{A0}} = \frac{4\alpha \cdot \exp\left(\frac{1}{2}\cdot\frac{uL}{D_L}\right)}{(1+\alpha)^2 \exp\left(\frac{\alpha}{2}\cdot\frac{uL}{D_L}\right) - (1-\alpha)^2 \exp\left(-\frac{\alpha}{2}\cdot\frac{uL}{D_L}\right)}$$

, which $\alpha = \sqrt{1 + 4k\tau\left(\dfrac{D_L}{uL}\right)}$

- limiting cases: $\dfrac{D_L}{uL} = 0 \Rightarrow$ PFR , $\dfrac{D_L}{uL} = \infty \Rightarrow$ CSTR
- for small durations from plug flow ($\dfrac{D_L}{uL}$ ≡ small), we have: $\dfrac{C_A}{C_{A0}} = \exp\left[-k\tau + (k\tau)^2 \cdot \dfrac{D_L}{uL}\right]$
- Performance of a real reactor compared with an ideal one is given by
  - → $\dfrac{L}{L_p} = \dfrac{V}{V_p} = 1 + k\tau\dfrac{D_L}{uL}$, for the same $C_{A,out}$
  - → $\dfrac{C_A}{C_{A,p}} = 1 + (k\tau)^2\dfrac{D_L}{uL}$, for " " V
  - → performance charts and treatment for n^{th} order kinetics are given in Levenspiel.

② Laminar flow Reactor

- Velocity in axial direction is parabolic, and velocity profile is: $u(r) = \dfrac{2Q}{\pi r_0^2}\left[1 - \left(\dfrac{r}{r_0}\right)^2\right]$ 1

  radial position; $Q \triangleq$ volumetric flowrate; → tube radius

- Residence time, t, at any r is: $t = \dfrac{L}{u} = \dfrac{\pi r_0^2}{2Q}\cdot\dfrac{L}{\left[1 - \left(\frac{r}{r_0}\right)^2\right]}$ 2 $\xrightarrow[V = L\pi r_0^2]{}$ $t = \dfrac{V/Q}{2\left[1 - \left(\frac{r}{r_0}\right)^2\right]} = \dfrac{t_m}{2\left[1 - \left(\frac{r}{r_0}\right)^2\right]}$ 3

- Fraction of the effluent with a radius between r and $r+dr$ = $dF(r) = \dfrac{u(r)\cdot 2\pi r\,dr}{Q} = dF(t)$ = Fraction of the effluent with residence time between t and $t + \Delta t$

$$\xrightarrow{①} dF(t) = \frac{4}{r_0^2}\left[1 - \left(\frac{r}{r_0}\right)^2\right] r\,dr \qquad 4$$

③ → $t = \dfrac{t_m}{2\left[1-\left(\frac{r}{r_0}\right)^2\right]} \Longrightarrow \dfrac{dt}{dr} = \dfrac{t_m}{2}\cdot\dfrac{2\,{}^{r}/_{r_0^2}}{\left[1-\left(\frac{r}{r_0}\right)^2\right]^2} = \dfrac{t_m}{r_0^2}\cdot\dfrac{r}{\left[1-\left(\frac{r}{r_0}\right)^2\right]^2} \Longrightarrow r\,dr = \left[1-\left(\frac{r}{r_0}\right)^2\right]^2 \dfrac{r_0^2}{t_m}\,dt$ $\underline{5}$

$\overset{③}{\Longrightarrow} r\,dr = \left(\dfrac{t_m}{2t}\right)^2 \dfrac{r_0^2}{t_m}\,dt = \dfrac{t_m r_0^2}{4t^2}\,dt$

④ $\Longrightarrow dF(t) = \dfrac{4}{r_0^2}\cdot\dfrac{t_m}{2t}\cdot\dfrac{t_m r_0^2}{4t^2}\,dt = \dfrac{t_m^2}{2t^3}\,dt$ $\underline{6}$ $\Longrightarrow \boxed{E(t) = \dfrac{dF(t)}{dt} = \dfrac{1}{2}\cdot\dfrac{t_m^2}{t^3}}$

- In integration of eq. $\underline{06}$ we should note that the ~~max~~ min residence time is not zero, but corresponds to the max velocity at the center of the tube. Which is twice the average velocity. ($t_{min} = \frac{1}{2} t_m$)

- hence: $F(t) = \displaystyle\int_{t_m}^{t} \frac{1}{2}\cdot\frac{t_m^2}{t^3}\,dt = \frac{t_m^2}{2}\int_{t_m}^{t}\frac{dt}{t^3} \Longrightarrow F(t) = \begin{cases} 1 - \frac{1}{4}\left(\frac{t}{t_m}\right)^{-2} & , \text{for } t \geq t_m/2 \\ 0 & , \text{for } t \leq t_m/2 \end{cases}$