

February 28, 2013

PERTINENT NOTES ON TUBULAR REACTORS

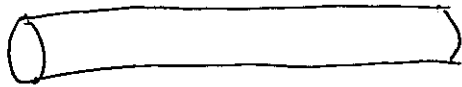
This is scan of handwritten notes taken by S. Nayak my past student, after my type-written notes taken by some students to proofread them mysteriously disappeared. Unfortunately, the electronic version got lost too due to a corrupt disk. The notes contain the following material:

1. Brief discussion of the laminar flow reactor in empty tubes and possible approaches. Comparison of Axial dispersion model (ADM) and segregated flow model. Issues of scale up.
2. Modeling of packed beds (inert packing). ADM and cross flow model. Development of cross flow model equations and their use.
3. Development of the wave model for tubular reactors and packed beds. Westerterp's papers for use of the wave model.
4. Distinction between convection and diffusion dominated systems. Scale up issues.

PERTINENT NOTES ON TUBULAR REACTION, PACKED BEDS, CROSS-FLOW S. NAYAK

04/01/04

Laminar Flow



Segregated Flow model works for set Pe_1, Pe_2
Axial dispersion

$$\frac{dC}{dt} = D_{app} \frac{\partial^2 C}{\partial z^2} - \bar{u} \frac{dC}{dz} - R$$

$$Pe_{app} = \frac{\bar{u}^2 R^2}{4gD}$$

$$\frac{1}{Pe_{app}} \frac{\partial^2 C}{\partial \xi^2} - \frac{\partial C}{\partial \xi} - Pe_{ax} C^n = \frac{\partial C}{\partial \theta}$$

$$\theta = \frac{t}{\bar{\tau}} \quad \bar{\tau} = \frac{L}{\bar{u}} \quad \xi = \frac{z}{L}$$

$$Da = k C_{in}^{n-1} \bar{\tau}$$

$$C = \frac{C_{in}}{C_{in0}}$$

$$\xi = 0 \quad C|_0 - \frac{1}{Pe_{app}} \frac{dC}{d\xi} \Big|_0 = C_0(\theta) \quad (\stackrel{\text{steady}}{=} 1)$$

$$\xi = 1 \quad \frac{dC}{d\xi} = 0$$

$$Pe_{app} = \frac{\bar{u}L}{D_{app}} = \frac{\bar{u}dt}{D_{app}} \left(\frac{L}{dt} \right)$$

Laminar flow

$$P_{app} = P_T = \frac{\bar{u}^2 R^2}{48D} + 0$$

Turbulent flow
 $E_z \propto dt \bar{u}^x$

$$u^x = \sqrt{\frac{f}{2}} \bar{u}$$

$$E_z = K \bar{u} dt \sqrt{f} \quad f = 0.0791 Re^{-0.25}$$

$$K = 3.57 \quad (\text{Taylor})$$

Correlation

$$\frac{E_z}{\bar{u} dt} = \frac{3 \times 10^7}{Re^{2.1}} + \frac{1.35}{Re^{1.8}}$$

* Use Axial dispersion model for $Pe_{app} > 5$
 For $Pe_{app} < 1$ don't use axial dispersion models

Generalization of Tank in series

$$E_0(\theta) = \frac{N^N \theta^{N-1} e^{-N\theta}}{(N-1)!} \quad \sigma_D^2 = \frac{1}{N}$$

* Dispersion as Dominant in spreading material

$$E \approx \frac{1}{2 \sqrt{\pi \frac{DL}{\bar{u}^3}}} e^{-\frac{(t-\bar{t})^2}{4 \frac{DL}{\bar{u}^3}}} \quad \left. \begin{array}{l} \sigma^2 \propto L \\ \sigma \propto \sqrt{L} \end{array} \right\}$$

$$\sigma^2 = \frac{2 P_{app}}{\bar{u} L} \times \left(\frac{L}{\bar{u}}\right)^2 = 2 \frac{P_{app} L}{\bar{u}^3}$$

But at sufficiently large Re

$$\frac{E_z}{\bar{u} d_t} = \text{constant} \quad b=0$$

$$\frac{d_{tLS}}{d_{tPP}} = S^{1/3} = \frac{L_{LS}}{L_{PP}} \Rightarrow \text{geometric similarity holds} \parallel$$

$$\Delta P_{LS} = S^{1/2} \Delta P_{PP}$$

Laminar Flow

$$\Delta P = 32 (\rho \bar{u}^2) \left(\frac{L}{d_t} \right) Re^{-1}$$

Eqs (1) and (2) must hold $E_z = Dax$

$$\frac{\bar{u} L}{Dax} = \left(\frac{L}{d_t} \right) \left(\frac{192 D}{\bar{u} d_t} \right) \Rightarrow \text{scale up } d_{tLS} = d_{tPP}$$
$$Re_{LS} = S Re_{PP}$$

$$|\Delta P_{LS} = S^2 \Delta P_{PP}|$$

Packed beds \rightarrow Plug flow with superimposed dispersion

(A.D.M) Axial Dispersion model most frequently used

A D M
 $\left(\frac{u d_p}{E_z}\right)$ from σ_D^2

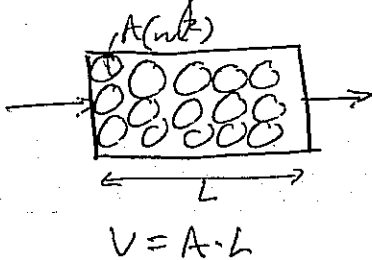
- Several problem
- 1] No trace present in upstream of injection point - contrary to model
 - 2] Does not scale right with L
 - 3] Speed of propagation from not infinite as predicted by model.

Instead people suggested

- \rightarrow Tank in series
- Cell model
- Cross flow model

|| Krishna, Jackson and Sundareshan ||
 AICHE (1980) Vol 26, 274.

Cross flow model



- 1] Fluid that actively flow through
- 2] Fluid trapped behind particles forming wakes, recirculating cells, stagnant zones and exchange betⁿ two fluid

	x	$x + \Delta x$
$E_A A \rightarrow$ flowing fluid	$\uparrow G$	
$E_B A \rightarrow$ Stagnant fluid	$\downarrow G_2$	
Packed bed		

$(E_A + E_B) A = EA$
 \uparrow
 Voidage

* Solid is non porous non catalytic

$$\bar{u} = \frac{Q}{A}$$

$$\bar{u}_a = \frac{Q}{E_a A}$$

$$\bar{F} = \frac{E A L}{Q} = \frac{E V}{Q} = \frac{E L}{E_a \bar{u}_a} = E \frac{L}{\bar{u}}$$

* Balance for flowing zone

$$u_a E_a A C_1 \Big|_x - u_a E_a A C_1 \Big|_{x+\Delta x} - \int A \Delta x (C_1 - K C_2) + R_1 E_a A \Delta x = E_a A \Delta x \frac{dC_1}{dt} \quad \text{--- (1)}$$

$\int \left(\frac{m^3}{m^3 \cdot s} \right) =$ exchange flow rate between flowing and stagnant liquid per unit volume of bed

* Balance for stagnant zone

$$\int A \Delta x (C_1 - K C_2) + R_2 E_b A \Delta x = E_b A \Delta x \frac{dC_2}{dt} \quad \text{--- (2)}$$

$R_2 \frac{\text{mol}}{m^3 \cdot \text{sec}}$ = rate of formation of our species in zone per unit vol fluid

$$K = \left(\frac{C_2}{C_1} \right)_{\text{eq}} = 1$$

For eq (1)

$$-u_a \epsilon_a \frac{dC_1}{dx} - f(C_1 - C_2) + R \frac{\epsilon_a}{\epsilon} = \epsilon_a \frac{dC_1}{dt} \quad \text{--- (3)}$$

For eq (2)

$$f(C_1 - C_2) + R \frac{\epsilon_b}{\epsilon} = \epsilon_b \frac{dC_2}{dt} \quad \text{--- (4)}$$

$$t=0 \quad C_1 = C_2 = 0$$

$$x=0 \quad C_1 = C_0$$

Define

$$Y_1 = \frac{C_1}{C_0}$$

$$Y_2 = \frac{C_2}{C_0}$$

$$\tau = \frac{\bar{u} t}{d_p \epsilon} \quad s = \frac{\epsilon_b}{\epsilon}$$

$$y = \frac{x}{d_p}$$

$$\bar{R} = \frac{d_p R}{\epsilon C_0}$$

$$F = \frac{f d_p}{\bar{u}}$$

So eq (3)

$$-\frac{\partial Y_1}{\partial y} - F(Y_1 - Y_2) + (1-s)\bar{R} = (1-s) \frac{\partial Y_1}{\partial \tau} \quad \text{--- (5)}$$

So eq (4)

$$F(Y_1 - Y_2) + s\bar{R} = s \frac{\partial Y_2}{\partial \tau} \quad \text{--- (6)}$$

$$\tau=0 \quad Y_1 = Y_2 = 0 \quad y=0$$

$$Y_{10} = Y_{10}(\tau)$$

$$Y_1\left(\tau, \frac{y}{d_p}\right)$$

Ergebn Equation

$$-\frac{dP}{dz} = \underbrace{150 \mu (1-\epsilon)^2 \bar{u}}_{\text{Drag}} + \underbrace{1.75 \left(\frac{1-\epsilon}{\epsilon^3}\right) \rho \bar{u}^2}_{\text{Turbulence}} \frac{d\eta}{d\eta}$$

Hypothesis

$$-\epsilon a \left(\frac{dP}{dz}\right)' = \int \rho \frac{\bar{u}^2}{\epsilon a}$$

$$\left(\frac{dP}{dz}\right)' = \int \frac{\rho \bar{u}^2}{\epsilon a^2} = 1.75 \left(\frac{1-\epsilon}{\epsilon^3}\right) \frac{\rho \bar{u}^2}{d\eta}$$

$$F = \int \frac{d\eta}{\bar{u}} = 1.75 \left(\frac{1-\epsilon}{\epsilon}\right) (1-s)^2 \quad (*) \quad \left\{ \begin{array}{l} 1-s = \frac{\epsilon a}{E} \end{array} \right.$$

$$\bar{Y}_1 = \mathcal{L}\{Y_1\} \quad \bar{Y}_2 = \mathcal{L}\{Y_2\} \quad \left\{ \begin{array}{l} \mathcal{L}\left(\frac{\partial Y_1}{\partial z}\right) = s \bar{Y}_1 - \frac{Y_1(z=0)}{c} \end{array} \right.$$

$$\frac{d\bar{Y}_1}{dy} = -F(\bar{Y}_1 - \bar{Y}_2) - (1-s)s\bar{Y}_1 \quad (7)$$

$$F(\bar{Y}_1 - \bar{Y}_2) = s s \bar{Y}_2 \quad (8)$$

Solve for \bar{Y}_2

$$\frac{d\bar{Y}_1}{dy} = - \left[\frac{F s s}{F + s s} + (1-s)s \right] \bar{Y}_1; \quad y=0 \quad \bar{Y}_1 = 1$$

$$\bar{Y}_1 = e^{-\left[\frac{FSs}{F+Ss} + (1-s)s \right] y}$$

$$\bar{Y}_{1 \text{ exit}} = \bar{Y}_1 \left(s, y = \frac{L}{dp} \right) = e^{-\frac{L}{dp} \left[\frac{FSs}{F+Ss} + (1-s)s \right]} \quad (*)$$

$$\bar{Y}_{1 \text{ exit}} = e^{-\frac{L}{dp} \left[F - \frac{F}{1 + \frac{S}{F}s} + (1-s)s \right]}$$

by binomial

$$= e^{-\frac{L}{dp} \left[s - \frac{S^2}{F}s + \frac{S^3}{F^2} - \dots \right]}$$

$$= 1 - \frac{L}{dp} s + \left[\frac{S^2}{F} \frac{L}{dp} + \frac{1}{2} \left(\frac{L}{dp} \right)^2 \right] s^2 - O(s^3)$$

compare with

$$\bar{Y}_{1 \text{ exit}} = \mu_0 - \mu_1 s + \frac{\mu_2}{2} s^2 - \frac{\mu_3}{6} s^3$$

$$\mu_0 = 1$$

$$\mu_1 = \frac{L}{dp}$$

$$\mu_2 = 2 \left[\frac{S^2}{F} \frac{L}{dp} + \frac{1}{2} \left(\frac{L}{dp} \right)^2 \right]$$

$$\frac{s^2}{F} \frac{dp}{L} = \frac{1}{B_0} \frac{dp}{L}$$

$$\frac{s^2}{F} = \frac{1}{B_0} \quad \text{--- } (**)$$

$$F = \int \frac{dp}{u} = 1.75 \left(\frac{1-\epsilon}{\epsilon} \right) (1-s)^2 (***)$$

From (**) (***)

$$s = \frac{\sqrt{\frac{1.75}{B_0} \left(\frac{1-\epsilon}{\epsilon} \right)}}{1 + \sqrt{\frac{1.75}{B_0} \left(\frac{1-\epsilon}{\epsilon} \right)}}$$

$$F = \frac{1.75 \left(\frac{1-\epsilon}{\epsilon} \right)}{\left[1 + \sqrt{\frac{1.75}{B_0} \left(\frac{1-\epsilon}{\epsilon} \right)} \right]^2}$$

Steady State reactor model ^{1st order}
 Rate of formation

$$\frac{dY_1}{dy} = -F(Y_1 - Y_2) + (1-s) \bar{R}_{Y_1} \quad (1)$$

$$F(Y_1 - Y_2) + s \bar{R}_{Y_2} = 0 \quad (2)$$

↑ Rate of formation

$$y = 0 \quad Y = 1$$

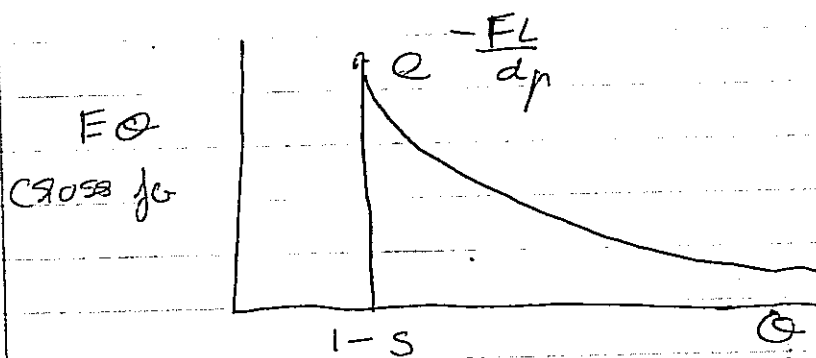
$$R = Da Y^n$$

$$E_{\theta}(\theta) = \left(\frac{L}{d_p} \right) Y_{1, \text{exit}}(\tau)$$

$$\theta = \frac{\bar{u}}{EL} t = \left(\frac{d_p}{L} \right) \tau$$

$$E_{\theta}(\theta) = e^{-L F / d_p} e^{-F H / d_p s (\theta - (1-s))} \left\{ \frac{L}{d_p} s (\theta - (1-s)) \right\}$$

$$+ \frac{F L / d_p}{\sqrt{s / \theta - (1-s)}} I_1 \left(2 F \frac{L}{d_p} \sqrt{\frac{\theta - (1-s)}{s}} \right) H(\theta - (1-s))$$



Packed bed model must match t and variance. Always match various physical meaning

$$\frac{dc}{dz} = -Da f(c) \quad \text{PFR}$$

$$z=0 \quad c=1$$

ADM

Cells in series

Recycle model

Cross flow mode

$$\sigma_D^2 = \frac{2}{Peax} - \frac{2}{Peax} (1 - e^{-Peax})$$

y_N

$R/(1+R)$

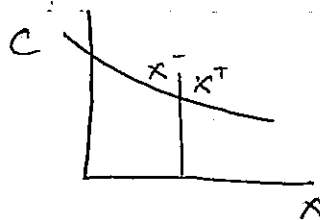
$$\frac{2}{F}$$

Micro flow Howard Benner

Macro Transport processes. Finans book

Fickes 1st Law

$$J_x = -D \frac{dc}{dx}$$



$$J_x(x, t+\tau) = -D \frac{dc}{dx}(x, t)$$

$$J_x(x, t+\tau) = J_x(x, t) + \frac{dJ}{dt}(x, t)(\tau - t)$$

$$j + \tau \frac{dj}{dt} = -D \frac{dc}{dx}$$

$$\tau = \frac{L}{U}$$

$$D \propto LU$$

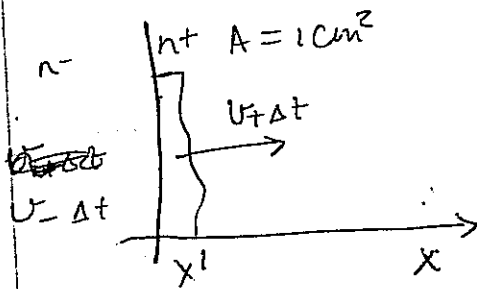
$$\frac{SDa}{20}$$

Ref: ^{Richard} Robert P. Feynman, Robert B Leighton,
^{Matthew} Sands

The Feynman lectures of Physics I and II
 Addison - Wesley, Cal Tech, 1963

02/10/05

Random walk \rightarrow diffusion



$$j_x = \frac{n_- v_{\Delta t} - n_+ v_{\Delta t}}{\Delta t} = (n_- - n_+) v \quad (1)$$

$$n_+ - n_- = \frac{dc}{dx} = \alpha l \frac{dc}{dx} \quad (2)$$

$$j_x = -\alpha l v \frac{dc}{dx} = -D \frac{dc}{dx} \quad (3)$$

$$D = \frac{1}{3} v l \quad (4a)$$

$$l = \lambda v \quad (5)$$

$$\text{mean free path} = \left(\begin{array}{l} \text{mean} \\ \text{time} \\ \text{bet}^n \\ \text{collision} \end{array} \right) \times \left(\begin{array}{l} \text{mean} \\ \text{molecular} \\ \text{velocity} \end{array} \right)$$

O₂ at 25°C, 1 atm

$$v = \left(\frac{8RT}{\pi M} \right)^{1/2} = 444 \text{ m/sec}$$

$$l = \frac{l}{\sqrt{2} \pi \left(\frac{N}{V} \right) d^2} = 2.28 \times 10^{-7} \text{ m}$$

$$\tau = \frac{l}{v} = 5 \times 10^{-10} \text{ (s)} \quad \text{Mean free path } l = \lambda$$

$$J_x(t + \tau) = -D \frac{\partial C(t)}{\partial x} \quad (9)$$

$$J_x(t + \tau) = J_x(t) + \tau \frac{\partial J_x}{\partial t} = -D \frac{\partial C}{\partial x} \quad (10)$$

If we make an unsteady state balance
if we use eq (3)

$$\frac{\partial C}{\partial t} = D \nabla^2 C \rightarrow \text{or in 1D} \quad \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Count particles that reach position x at time t which has their last collision at time $(t - \eta)$ at the point $(x - \eta v_t)$ ($\eta > 0$) and obtained velocity v_t in the positive x direction moved during time η without further collision and without disappearing by reaction.

The total number of collision at point $x - \eta v_+$ and at time $t - \eta$, in terms of continuous function $C(x, t)$ is equal to

$$\frac{C(x - \eta v_+, t - \eta)}{\tau} \quad \text{where, } \tau \text{ is mean time bet}^n \text{ collision}$$

The flux of particle at x, t from left to right.

$$J_+(x, t) = \frac{p_+ v_+}{\tau} \int_0^{\infty} G(\eta) H(\eta) C(x - \eta v_+, t - \eta) d\eta \quad \text{--- (11)}$$

$G(\eta) =$ Probability that particle survives time η without colliding

$H(\eta) =$ Probability without reacting

$$H(\eta) = e^{-k\eta} \quad \text{--- (14)}$$

$$G(\eta) = e^{-\eta/\tau} \quad \text{--- (13)}$$

$$J_-(x, t) = \frac{p_- v_-}{\tau} \int_0^{\infty} G(\eta) H(\eta) C(x + \eta v_-, t - \eta) d\eta \quad \text{--- (12)}$$

$$P_+ v_+ = P_- v_- \quad (13a)$$

Concentration Definition

$$c = \frac{j_+}{v_+} + \frac{j_-}{v_-} \quad (13b)$$

Net Flux

$$j = j_+ - j_- \quad (13c)$$

Probability

$$P_+ + P_- = 1 \quad (13d)$$

For j_+
Consider eq (11) drop subscript for now.

$$j = \frac{P_+ v_+}{2} \int_0^{\infty} e^{-a\eta} c(x - \eta v_+, t - \eta) d\eta \quad (16)$$

where

$$a = \left(k + \frac{1}{\tau} \right)$$

Integrate by parts

$$u = c(x - \eta v_+, t - \eta) \quad du = -v_+ \frac{dc}{dx}$$

$$du = \frac{dc}{dw} + \frac{dw}{d\eta} + \frac{\partial c}{\partial \theta} \cdot \frac{\partial \theta}{\partial \eta} = -v_+ \frac{dc}{dx} - \frac{dc}{dt}$$

$$dv = e^{-a\eta} d\eta \quad v = -\frac{1}{a} e^{-a\eta}$$

$$j = \frac{\rho v}{\epsilon} \left\{ \left[-\frac{1}{a} e^{-a\eta} c(x-\eta v, t-\eta) \right]_0^{\infty} - \frac{1}{a} \int_0^{\infty} e^{-a\eta} \left(v \frac{dc}{dx} + \frac{dc}{dt} \right) d\eta \right\}$$

$$a j^{\circ} = \frac{\rho v}{\epsilon} c(x, t) - \frac{\rho v}{\epsilon} v \int_0^{\infty} e^{-a\eta} \frac{dc}{dx} (x-\eta v, t-\eta) d\eta - \frac{\rho v}{\epsilon} \int_0^{\infty} e^{-a\eta} \frac{dc}{dt} d\eta$$

But

$$\frac{dj^{\circ}}{dc} = \frac{\rho v}{\epsilon} \int_0^{\infty} e^{-a\eta} \frac{dc}{dx} d\eta$$

$$\frac{dj^{\circ}}{dt} = \frac{\rho v}{\epsilon} \int_0^{\infty} e^{-a\eta} \frac{dc}{dt} d\eta$$

Put $j = j^+$

$$a j^{\circ} = \frac{\rho v}{\epsilon} c - v \frac{dj^{\circ}}{dx} - \frac{dj^{\circ}}{dt} \quad (17a)$$

For $j = j^-$

$$a j^{\circ} = \frac{\rho - v}{\epsilon} c + v \frac{dj^{\circ}}{dx} - \frac{dj^{\circ}}{dt} \quad (17b)$$

$$\left(k + \frac{1}{z}\right) j_+ = \frac{p_+ u_+}{z} C - u_+ \frac{dj_+}{dx} - \frac{dj_+}{dt} \quad (18a)$$

$$\left(k + \frac{1}{z}\right) j_- = \frac{p_- u_-}{z} C + u_- \frac{dj_-}{dx} - \frac{dj_-}{dt} \quad (18b)$$

Divide 18a by u_+ and 18b by u_- and adding 18a and 18b

$$\begin{aligned} \left(k + \frac{1}{z}\right) \left(\frac{j_+}{u_+} + \frac{j_-}{u_-}\right) &= \left(\frac{p_+}{z} + \frac{p_-}{z}\right) C - \left[\frac{1}{u_+} \frac{dj_+}{dt} + \frac{1}{u_-} \frac{dj_-}{dt}\right] \\ \text{Sub to (15b)} \quad C & - \underbrace{\left(\frac{dj_+}{dx} - \frac{dj_-}{dx}\right)}_{(15c) \frac{dj}{dx}} \quad \underbrace{\left(\frac{1}{u_+} \frac{dj_+}{dt} + \frac{1}{u_-} \frac{dj_-}{dt}\right)}_{(15d) \frac{dC}{dt}} \end{aligned}$$

$$\frac{dC}{dt} + \frac{dj}{dx} + kC = 0 \quad (19a)$$

Subtract 18b from 18a

$$\begin{aligned} \left(k + \frac{1}{z}\right) (j_+ - j_-) &= \left(\frac{p_+ u_+}{z} - \frac{p_- u_-}{z}\right) C - \frac{d}{dt} (j_+ - j_-) \\ & - u_+ \frac{dj_+}{dx} - u_- \frac{dj_-}{dx} \end{aligned}$$

$$\left(k + \frac{1}{z}\right) j = - \frac{dj}{dt} - u_+ \frac{dj_+}{dx} - u_- \frac{dj_-}{dx} \quad (*)$$

Adding and subtracting eq X

$$\left(k + \frac{1}{\tau}\right) j^{\circ} = -\frac{dj^{\circ}}{dt} \left(-u_+ \frac{dj^{\circ}}{dx} \right) - \left[u_- \frac{dj^{\circ}}{dx} \right] \\ + u_+ \frac{dj^{\circ}}{dx} - u_- \frac{dj^{\circ}}{dx} - \left[+u_+ \frac{dj^{\circ}}{dx} \right] - u_- \frac{dj^{\circ}}{dx}$$

$$\left(k + \frac{1}{\tau}\right) j^{\circ} = -\frac{dj^{\circ}}{dt} - u_+ \frac{dj^{\circ}}{dx} + u_- \frac{dj^{\circ}}{dx} - u_- \frac{dj^{\circ}}{dx} \\ - u_+ \frac{dj^{\circ}}{dx} \\ \text{From (13 b)} \\ -u_+ u_- \frac{dc}{dx}$$

$$\left(k\tau + 1\right) j^{\circ} + \tau \frac{dj^{\circ}}{dt} + (u_+ - u_-) \tau \frac{dj^{\circ}}{dx} + u_+ u_- \tau \frac{dc}{dx} = 0$$

Hyperbolic equation with finite speed of propagation define the "diffusion Phenomena" (19b)

(19a) and (19b)

Solved for C and j subject to I.C and B.C
No 1st order reaction $k=0$

Ref: Westerberg, K.R., Delman V.V., Kronberg, A.E

Wave model for longitudinal dispersion: I Development of the model.

AIChE J. 41 (9), 2013 - 2029 (1995)

Part II : Analysis and Application
 AIChE J 4(9), 2029-2039 (1995)

ADM replaced by

$$\frac{d\bar{C}}{dt} + \bar{u} \frac{d\bar{C}}{dx} + \frac{d_j}{dx} = 0$$

$$j + \frac{1}{15} \frac{a^2}{D} \left(\frac{d_j}{dt} + \frac{5\bar{u}}{4} \frac{d_j}{dx} \right) = -De \frac{d\bar{C}}{dx} \quad \therefore De = \frac{a^2 \bar{u}^2}{48D}$$

Handbook

61, 62, 63, 64, 66, 68

1 H.W 2

2) Axial Dispersion model

a) Perturbation technique. Plug flow than
 the accurate

c) Assume Segregated flow & generalise
 tank of series model.

Cross flow model

$$-\frac{dy_1}{dz} - F(y_1 - y_2) - (1-s) Da_1 y_1^2 = 0$$

$$F(y_1 - y_2) - s Da_1 y_2^2 = 0$$

$$(\xi, \tau) \rightarrow (y, \theta)$$

$$\frac{\partial}{\partial \xi} = \frac{\partial}{\partial y} \frac{\partial y}{\partial \theta} + \frac{\partial}{\partial \theta} \frac{\partial \theta}{\partial \xi}$$

Convection Dominates

$$E \approx \frac{L}{\sqrt{2\pi}\sigma^2} e^{-\frac{(t-\bar{t})^2}{2\sigma^2}}$$

$$\bar{t} = \text{constant}$$

$$\sigma^2 \propto \left(\frac{L}{\bar{v}}\right)^2$$

$$\sigma \propto L$$

Ref: Levenspiel and Fitzgerald

"A Warning on the Miss use of the Dispersion Model" CES 38 # 3, 489-491, 1982
Chem Engg Sci

Scale up of Tubular Reactors with Premixed Feed

$$\text{Scale up ratio} = S = \frac{Q_{\text{Full Scale}}}{Q_{\text{Pilot Plant}}} = \frac{Q_{FS}}{Q_{PP}}$$

Scale up by multiplication use S tubes of same d_t , L and Q_{PP} as used in single tube in the pilot

$$P.P : L, \bar{u}, d_t \rightarrow R_{PP} X_A$$

$$Q_{PP} = \frac{d_{t,PP}^2}{4} \pi \bar{u}$$

$$V_{PP} = \frac{d_{t,PP}^2}{4} \pi L$$

$$\bar{t} = \frac{L}{\bar{u}}$$

For scale up

1] Mean must be constant

2] Variance must be constant.

02/03/05

Scaleup of Tubular Reactors

- By multiplication

$$S = \frac{Q_{LS}}{Q_{PP}}$$

and satisfactory performance was obtained in PP in a tube of d_t , L use S much larger in plant

Empty Tubes

Turbulent \odot

$$Re > 2,100$$

$$\bar{t} = \text{constant} = \left(\frac{L}{\bar{u}}\right)_{PP} = \left(\frac{L}{\bar{u}}\right)_{LS}$$

$$\sigma_D^2 = \text{const} = \left(\frac{\bar{u}L}{E_z}\right)_{PP} = \left(\frac{\bar{u}L}{E_z}\right)_{LS}$$

$$\frac{E_z}{\bar{u} d_t} = a Re^{-b} \quad Re = \frac{\bar{u} d_t}{\nu}$$

$$E_z = a \nu^b d_t^{1-b} \bar{u}^{1-b}$$

$$\frac{d_{tLS}}{d_{tPP}} = S^{\frac{1+b}{3+b}} (*) \quad \frac{L_{LS}}{L_{PP}} = \frac{\bar{u}_{LS}}{\bar{u}_{PP}} = S \quad (1-b)/3+b \quad (**)$$

$$\Delta P_{LS} = S^{\frac{3-8b}{2(3+b)}} \Delta P_{PP} \quad \text{Typically } b = \frac{1}{8}$$