CBE 40445
10/9/20

CHAPTER 8: NON IDEAL FLOW IN REACTORS

THE OVERARCHING ISSUE IS TO MAKE SURE THAT YOU KNOW "WHERE" THE (SUPPOSEDLY) MOVING FLUIDS ARE IN YOUR REACTOR OR ANY PROCESS DEVICE ... BLOOD/FLUID FLOW IN PHYSIOLOGICAL SITUATION

AND "WHEN" THE FLUID HAS BEEN THERE ... HOW LONG HAS FLUID BE IN DEVICE

OUTLINE

REVIEW OF

1) EFFECT OF NON UNIFORM VELOCITY PROFILE

2) RESIDENCE TIME DISTRIBUTION FUNCTION

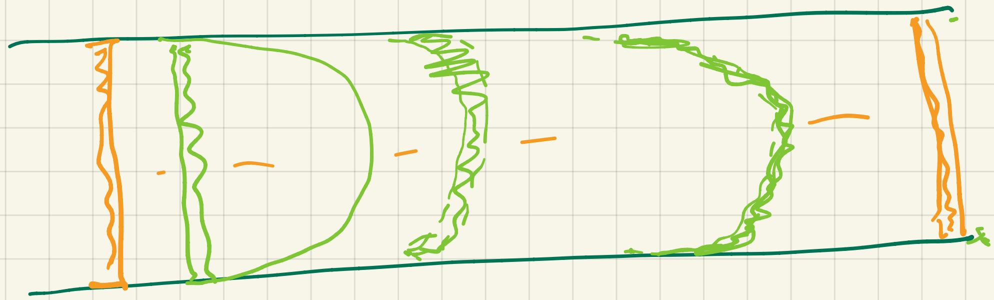
3) CONVERSION IN CSTR FROM RTD

4) TRAVELING DISTURBANCE AND DISPERSION IN TUBULAR REACTOR

5) DISPERSION W/ REACTION

A SIMPLE CASE THAT CAN BE QUANTIFIED

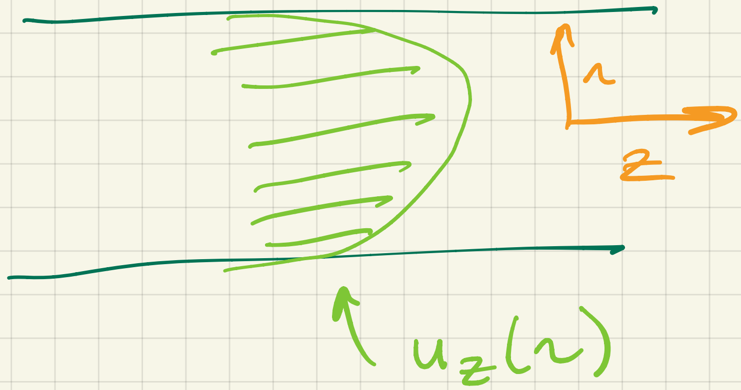
OPEN PIPE REACTOR



IF "PLUG FLOW" THEN

IF LAMINAR FLOW, CENTER OF PIPE WOULD EXIT FIRST

HOW DOES THIS AFFECT THE CONCENTRATION OF OUR FAVORITE $A \rightarrow M$ REACTION



REACTION AND DIFFUSION IN A FLOWING SYSTEM

$$u_z \frac{dC_A}{dz} = -k C_A$$

BUT MORE GENERALLY:

$$\frac{\partial C_A}{dt} + \vec{u} \cdot \vec{\nabla} C = D_A \nabla^2 C_A + \sum \nu_i r_i$$

FOR OUR FLOW SITUATION

LAMINAR FLOW IN A TUBE

$$\bar{u}(\bar{r}) = 2u\left(1 - \left(\frac{r}{r_t}\right)^2\right)$$

AVERAGE VELOCITY

$$\bar{u}(\bar{r})\frac{dC_A}{dz} = -kC_A$$

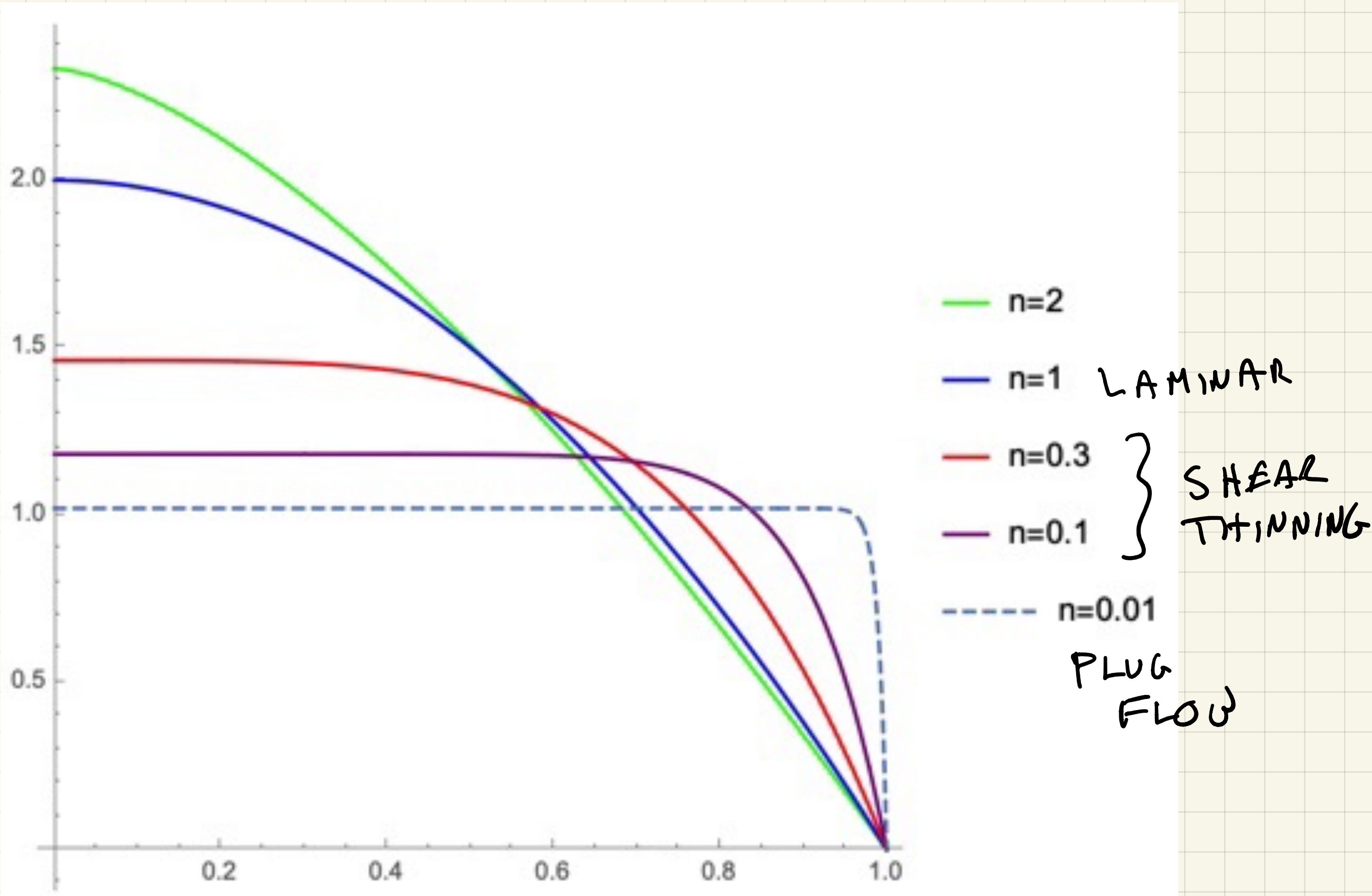
INTEGRATE IN Z:

$$C_A(\bar{r}) = C_A^0 \exp\left[-\frac{kz}{\bar{u}(\bar{r})}\right]$$

INTEGRATE ACROSS PIPE TO GET AVERAGE CONCENTRATION!

$$\overline{C_A} = \frac{\int_0^{\bar{r}_t} C_A(\bar{r})\,\bar{u}(\bar{r})\,2\pi\bar{r}\,d\bar{r}}{\int_0^{\bar{r}_t} \bar{u}(\bar{r})\,2\pi\bar{r}\,d\bar{r}}$$

POWER-LAW VELOCITY PROFILES



$$u(r) = \frac{2^{-1/n}\, n \left(\frac{\text{dpdz}}{K}\right)^{1/n} \left(R^{\frac{n+1}{n}} - r^{\frac{n+1}{n}}\right)}{n+1}$$

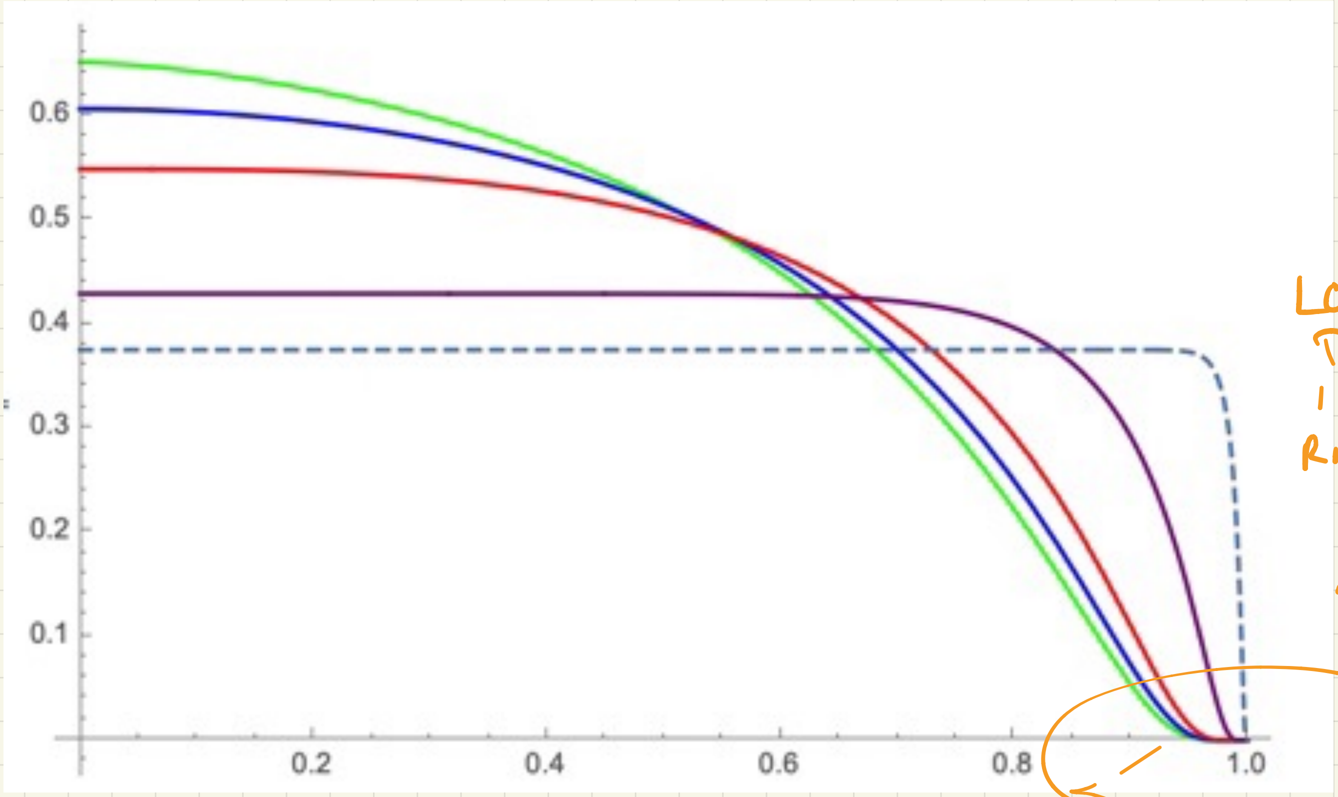
$$\bar{u} = \frac{2^{-1/n}\, n \left(R^{\frac{1}{n}+2} - \frac{n\, R^{\frac{1}{n}+2}}{2\,n+1}\right) \left(\frac{\text{dpdz}}{K}\right)^{1/n}}{n+1}$$

FOR $\tau = 1$, $k = 1$,

$\exp(-k\tau) = .368$

FOR FLOW REACTOR

n	$\bar{C}_A^{EXIT}$
2	.453
1	.443
.5	.429
.3	.416
.1	.392
.01	.371



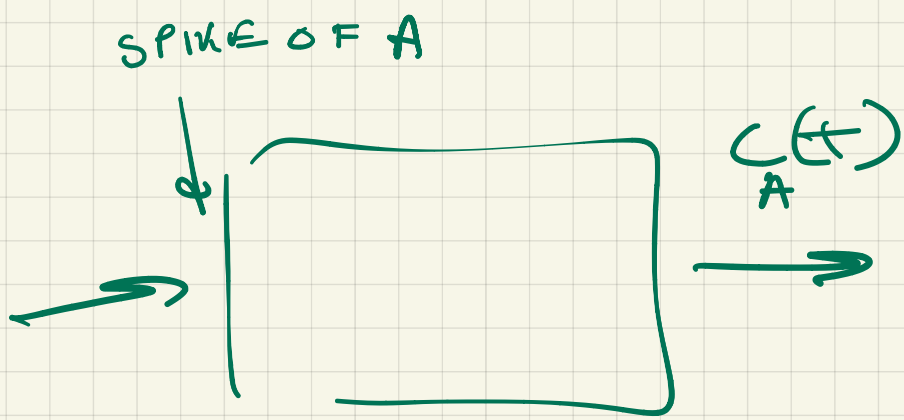
LONG TIME IN REACTOR

HOW TO QUANTIFY "IDEALITY"

RESISIDENCE TIME DISTRIBUTION

$E(t) \longrightarrow$ EXIT TIMES OF TRACER SPECIES

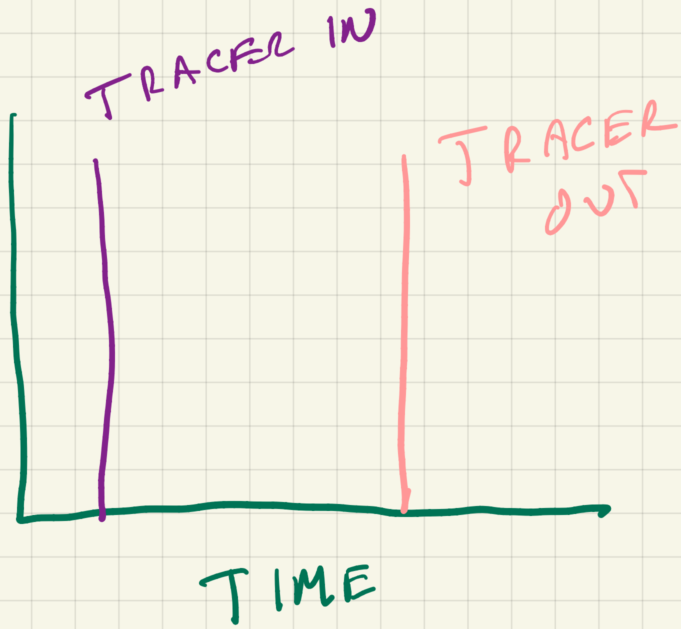
(= NOMINAL FLUID ELEMENTS)



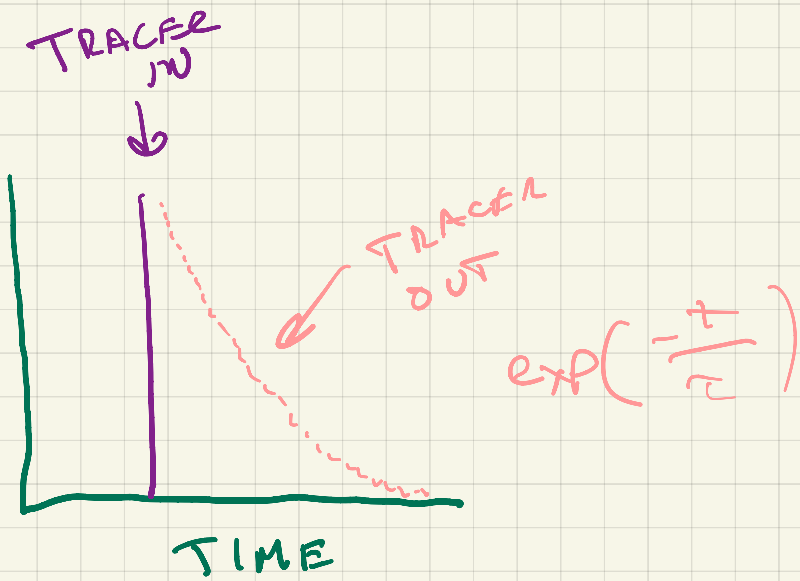
$$E(t) = \frac{C_A(t)}{\int_0^{\infty} C_A(\bar{t})\,d\bar{t}}$$

$$\int_0^{\infty} E(\bar{t})\,d\bar{t} = 1$$

PFR



CSTR



WE WILL USE LATER

CAN SHOW (pp 264–265) THAT

FOR PERFECT MIXING

$$E(t) = \frac{\exp\left(-\frac{t}{\tau}\right)}{\tau}$$

τ = MEAN RESIDENCE TIME

BUILT INTO STANDARD CSTR ANALYSIS

$$V \frac{dC_A}{dt} = q\left(C_{Af} - C_A\right)$$

$@\ t = 0 \quad C_A^0 \rightarrow 0 \quad \uparrow C_{Af}$

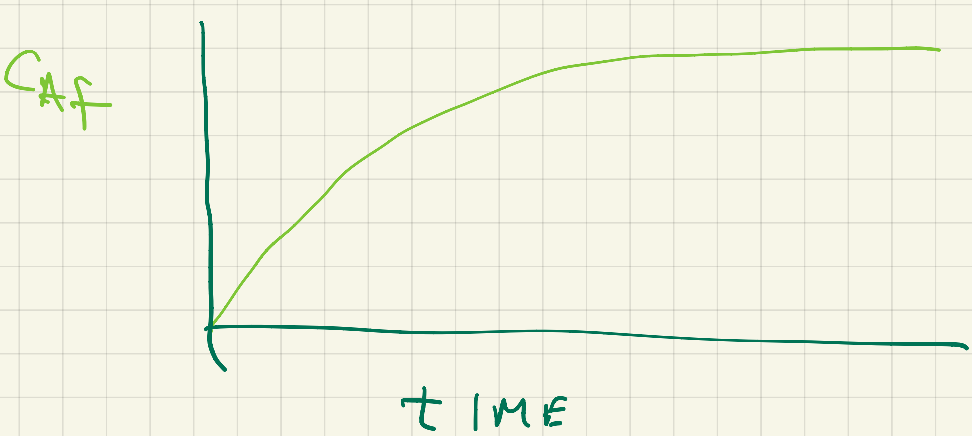
$$\frac{dC_A}{\left(C_A - C_{Af}\right)} = -\frac{q}{V}\,dt$$

$$\ln \frac{C_A - C_{Af}}{C_A^0 - C_{Af}}$$

$C_A^0 = 0$

$$-\frac{C_A - C_{Af}}{C_{Af}} = \exp\left(-\frac{q}{V}t\right)$$

$$C_A = C_{Af}\left(1 - \exp\left(-\frac{q}{V}t\right)\right)$$



MORE LIKELY

NONIDEAL

$$\int_0^{t_1} E(t)\,dt$$

HOW DOES AN RTD DISTRIBUTION ACTALLY AFFECT CONVERSION?

[MEAN CONCENTRATION OF REACTANT AT REACTOR OUTLET] =

Σ [CONCENTRATION OF REACTANT REMAINING IN A FLUID ELEMENT OF AGE BETWEEN t AND t+dt] [FRACTION OF EXIT STREAM THAT CONSISTS OF FLUID ELEMENTS OF AGE BETWEEN t + t+Δt]

$$\langle C_A \rangle = \int_0^\infty C_A(\bar{t})\, E(\bar{t})\, d\bar{t}$$

PICK 1ST ORDER (FOR AN IDEALIZED FLUID ELEMENT)

$$\frac{dC_A}{dt} = -k C_A \quad , \quad C_A(0) = C_A^\circ$$

$$C_A = C_A^\circ \exp[-kt]$$

$$\langle C_A \rangle = \int_0^\infty C_A^0 \exp(-kt)\, E(t)\, dt$$

INSERT EXPRESSION FOR $E(t)$

$$\langle C_A \rangle = \frac{C_A^0}{\tau} \int_0^\infty \exp(-k\bar{t}) \exp\left(-\frac{\bar{t}}{\tau}\right) d\bar{t}$$

$$\frac{\langle C_A \rangle}{C_A^0} = \frac{1}{\tau} \int_0^\infty \exp\left[-\left(k+\frac{1}{\tau}\right)\bar{t}\right] d\bar{t}$$

WE INTEGRATE:

$$\frac{\langle C_A \rangle}{C_A^0} = \frac{1}{\tau} \left[-\frac{1}{\left(k+\frac{1}{\tau}\right)} \exp\left[-\left(k+\frac{1}{\tau}\right)\bar{t}\right] \right]_0^\infty$$

$$\frac{\langle C_A \rangle}{C_A^0} = \frac{1}{1+k\tau} \quad !!$$

THIS DOESN'T WORK FOR
A 2ND ORDER REACTION

BATCH 2ND ORDER REACTION

$$\frac{dC_A}{dt} = -k C_A^2 \quad , \quad C_A(0) = C_{A0}$$

$$\frac{C_A}{C_{A0}} = \frac{1}{1 + C_{A0} k t}$$

A 2ND ORDER CSTR

$$0 = q\left(C_A^0 - C_A\right) - k C_A^2 V$$

$$C_A = \frac{-1 + \sqrt{1 + 4 C_A^0 k \tau}}{2 k \tau}$$

TRY THE INTEGRAL

$$\frac{1}{\tau}\int_0^{\infty}\left(\frac{1}{1 + C_A^0 k t}\right)\exp\left(-\frac{t}{\tau}\right)dt$$

$$= -\frac{1}{\tau} \frac{\exp\left(\frac{1}{C_{A0} k \tau}\right) \int_{C_{A0} k \tau}^{\infty} \exp(-t)/t \, dt}{C_{A0} k}$$

EXPONENTIAL INTEGRAL

$$-\frac{e^{\frac{1}{\text{ca0}\, k\, \tau}}\, \text{Ei}\left(-\frac{1}{\text{ca0}\, k\, \tau}\right)}{\text{ca0}\, k\, \tau}\Bigg|$$

PICK $k = 1$, $\tau = 1$, $C_{A0} = 1$

$$\frac{C_A}{C_{A0}} = .596 \quad \left(= .201 \text{ IF } k = 10 \right)$$

FOR ACTUAL 2ND ORDER CSTR:

$$\frac{C_A}{C_{A0}} = .618 \quad \left(= .27 \text{ IF } k = 10 \right)$$

FOR A FIRST ORDER PROCESS A FLUID ELEMENT "DEPENDS" ONLY ON ITSELF

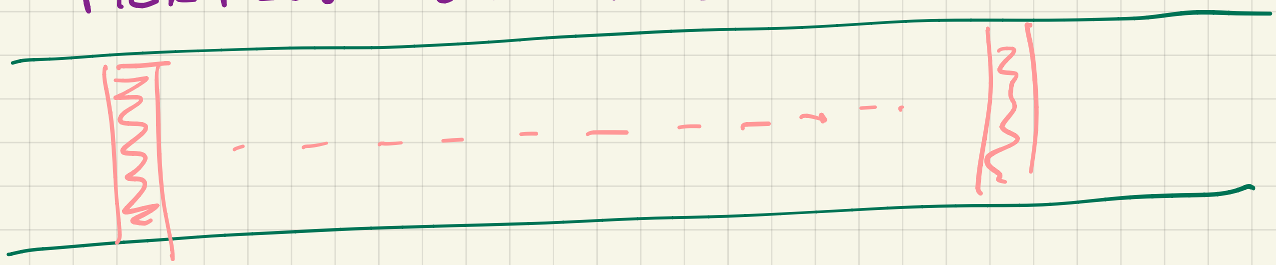
SO ONLY REACTION TIME IS NEEDED TO GET FINAL CONCENTRATION

FOR 2ND ORDER, CONCENTRATION AROUND IT MATTERS

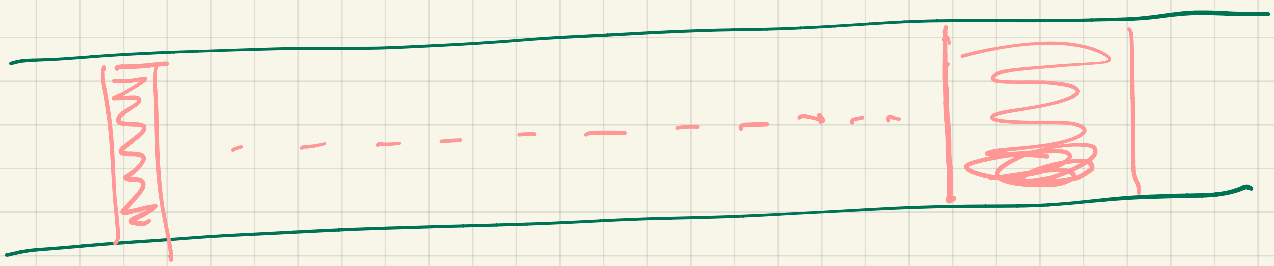
SO LOCATION INSIDE REACTOR AS WELL AS TIME MATTERS

LET'S LOOK AT WHAT ELSE REALLY COULD HAPPEN IN A FLOWING TUBULAR REACTOR

PICK PLUG FLOW FOR NOW

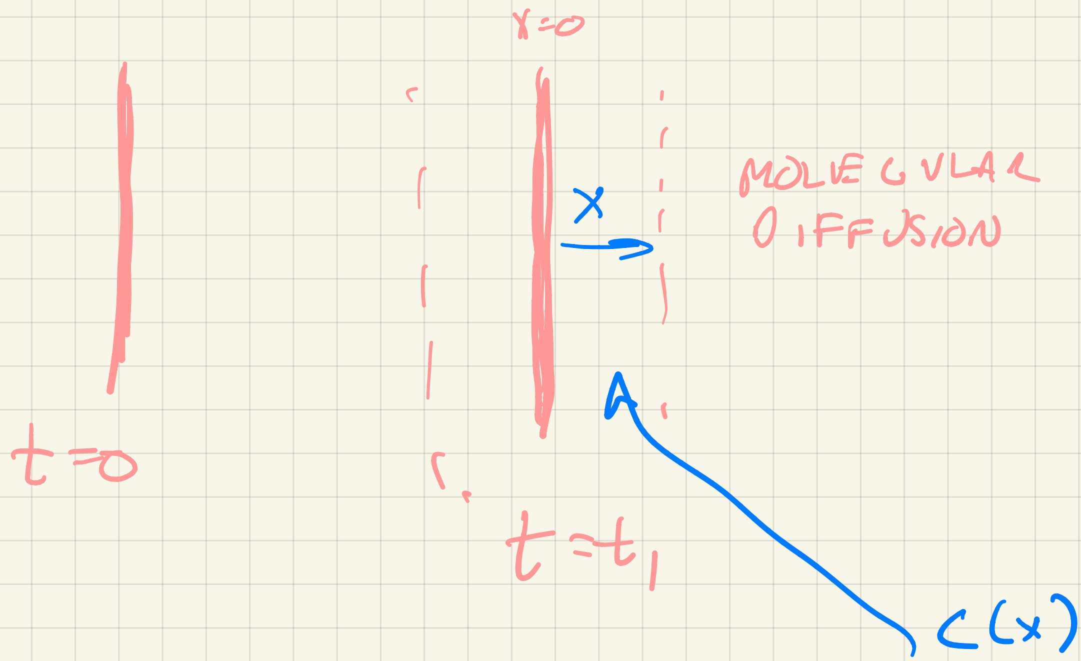


- A TRACER SIMPLY TRAVERSES BED OR PARTICLES



- MORE LIKELY SIGNIFICANT DISPERSION WILL OCCUR

IF WE FOLLOW THE SPIKE DOWN THE BED WE WOULD SEE THE SPREAD AS A CHANGE IN TIME



THE APPARENT GOVERNING EQUATION FOR CONCENTRATION:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

IS THIS CONSISTENT WITH A

GENERAL EQUATION FOR A FLOWING, REACTING SYSTEM?

$$\frac{\partial C_A}{\partial t} + \bar{u} \cdot \bar{\nabla} C_A = D \nabla^2 C_A - r_A(C_A)$$

IN THIS EQUATION D IS MOLECULAR DIFFUSIVITY

BUT WE CAN GENERALIZE THIS TO (A) TURBULENT FLOW

$$D + D_t(y)$$

(B) PACKED BED FLOW

D_a = AXIAL DISPERSION COEFFICIENT

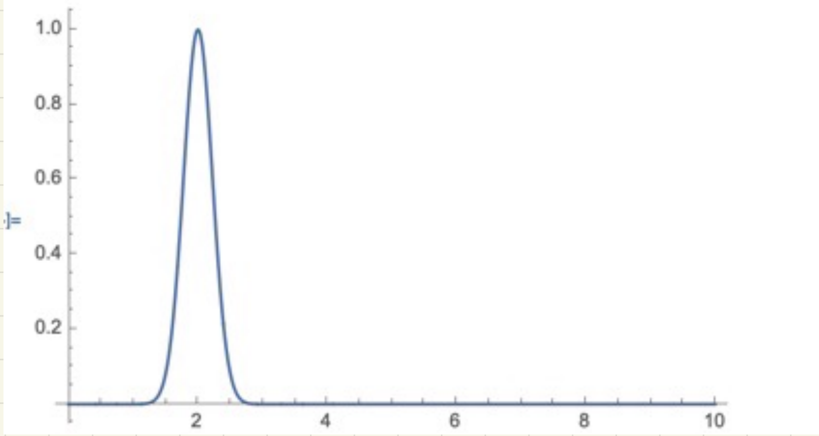
SO WE WRITE FOR A 1 DIMENSIONAL FLOW:

$$\frac{\partial C_i}{\partial t} + u \frac{\partial C_i}{\partial z} = D_a \frac{\partial^2 C_i}{\partial z^2}$$

$$\underbrace{\frac{\partial C_A}{\partial t} + u_z \frac{\partial C_A}{\partial z}}_{\text{TRAVELING WAVE}} = \underbrace{D_a \frac{\partial^2 C_A}{\partial z^2}}_{\text{DISPERSION}}$$

THESE TOGETHER TRACK A DISTURBANCE THROUGH REACTOR

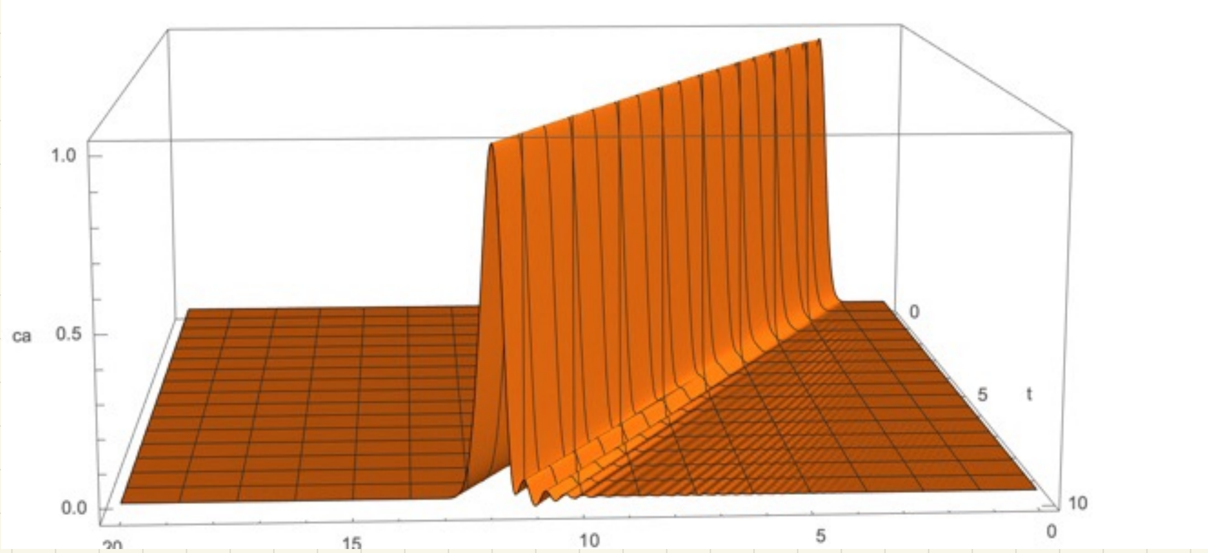
```
Plot[Exp[-(2 - x)^2 10], {x, 0, 10}, PlotRange → All]
```



INITIAL CONDITION

SOLVE WITH NO DISPERSION, $D_a = 0$

```
Plot3D[asol01 // Evaluate, {x, 0, 20}, {t, 0, 10}, Exclusions → None, PlotRange → All,
 AxesLabel → {"x", "t", "ca"}, PlotPoints → 200]
```

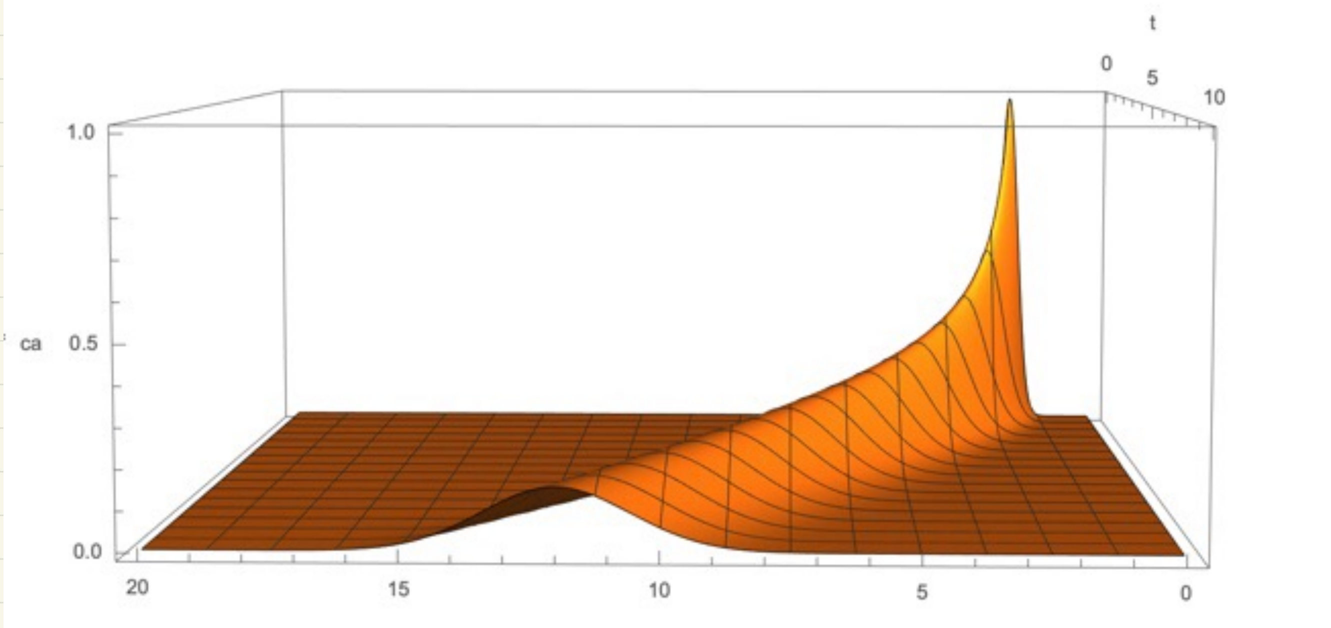


PULSE JUST TRAVELS DOWN BED WITH NO CHANGE OF SHAPE

"TRAVELING WAVE"

NOW SOLVE INCLUDING DISPERSION!

```
Plot3D[asol01 // Evaluate, {x, 0, 20}, {t, 0, 10}, Exclusions → None, PlotRange → All,
  AxesLabel → {"x", "t", "ca"}, PlotPoints → 200]
```



DISTURBANCE SPREADS AS IT TRAVELS

NOW CONSIDER OUR EQUATION!

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial z} = D_a \frac{\partial^2 c_i}{\partial z^2}$$

NON DIMENSIONALIZE:

$$\Theta \equiv \frac{t}{\langle t \rangle} = \frac{tu}{L}$$

$$Z \equiv \frac{z}{L}$$

$$Pe_a \equiv \frac{Lu}{D_a}$$ PECLET NUMBER

WE CAN WRITE:

$$\frac{\partial C_i}{\partial \theta} + \frac{\partial C_i}{\partial Z} = \frac{1}{Pe_a} \frac{\partial^2 C_i}{\partial Z^2}$$

WE WILL GET A SOLUTION IN A FRAME OF REFERENCE MOVING AT SPEED OF FRONT

$$\Theta \Longleftrightarrow \frac{z}{u}$$

$$\frac{\partial c}{\partial t} = \frac{1}{Pe} \frac{\partial^2 c}{\partial z^2}$$

$$Pe \equiv \frac{uL}{D_a} \qquad \frac{\text{CONVECTIVE FLOW}}{\text{DISPERSION}}$$

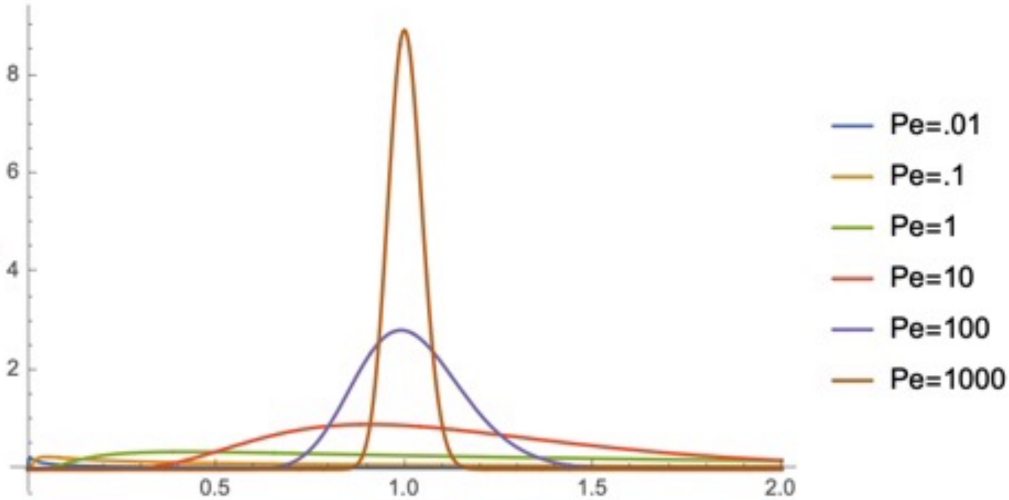
CONSIDERING $t = \dfrac{z}{u}$

A SOLUTION CAN BE OBTAINED FOR AN INITIAL PULSE

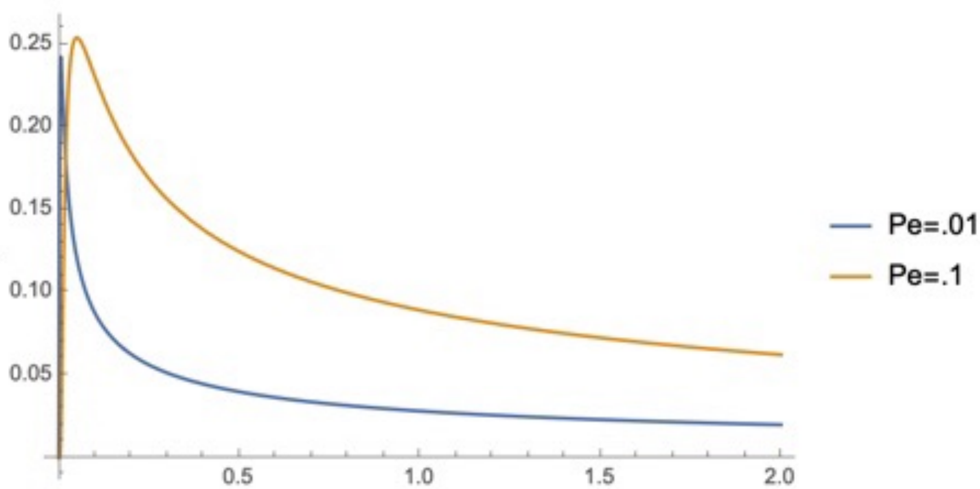
$$C_i = \left(\frac{Pe_a}{4\pi\theta}\right)^{1/2} \exp\left[\frac{-(1-\theta)^2 Pe_a}{4\theta}\right]$$

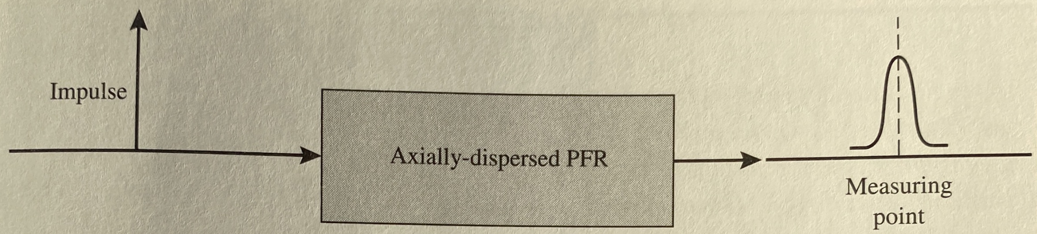
$$= E(\theta) = \left(\frac{Pe_a}{4\pi\theta}\right)^{1/2} \exp\left[\frac{-(1-\theta)^2 Pe_a}{4\theta}\right]$$

```
Plot[Evaluate[{ddans /. {pe → .01}, ddans /. {pe → .1}, ddans /. {pe → 1},
   ddans /. {pe → 10}, ddans /. {pe → 100}, ddans /. {pe → 1000}}], {θ, 0, 2},
 PlotRange → All, PlotLegends → {"Pe=.01", "Pe=.1", "Pe=1", "Pe=10", "Pe=100", "Pe=1000"}]
```

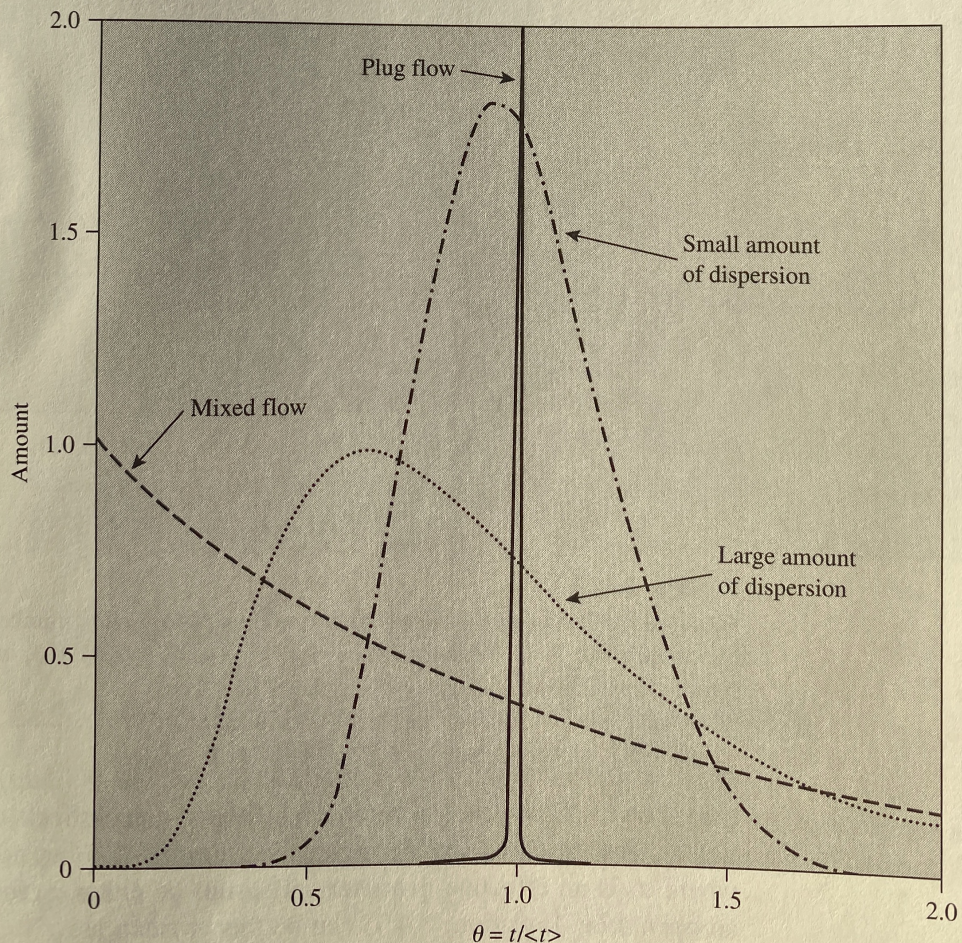



```
Plot[Evaluate[{ddans /. {pe → .01}, ddans /. {pe → .1}}], {θ, 0, 2}, PlotRange → All,
 PlotLegends → {"Pe=.01", "Pe=.1"}]
```




Impulse
Axially-dispersed PFR
Measuring point

(a)


Plug flow
Small amount of dispersion
Mixed flow
Large amount of dispersion
Amount
2.0
1.5
1.0
0.5
0
0
0.5
1.0
1.5
2.0
$\theta = t/<t>$

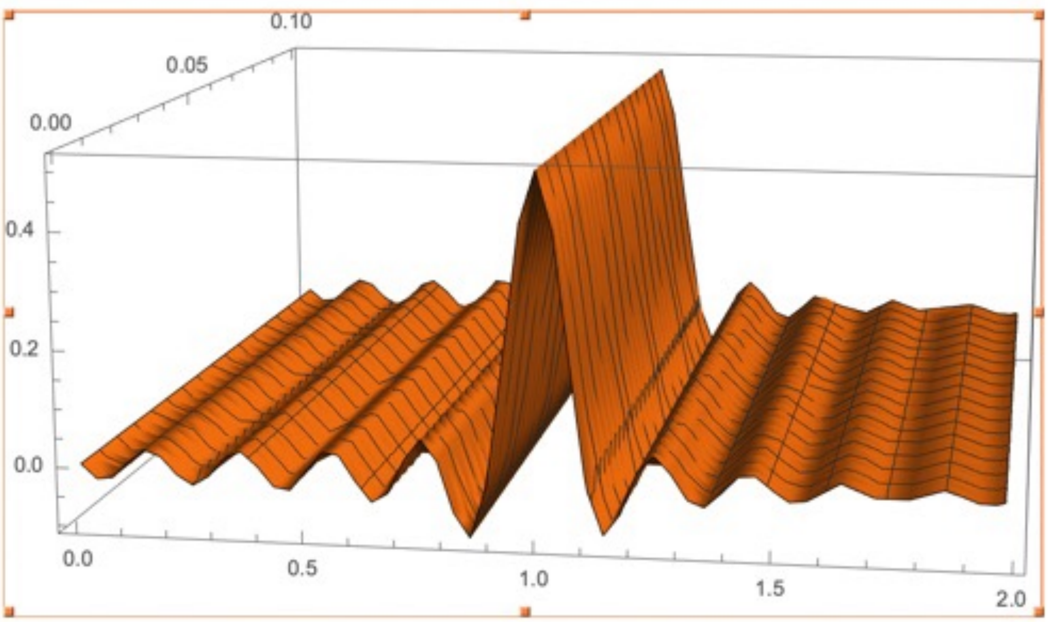
$\alpha = \frac{1}{Pe}$

```
sol = DSolve[{heqn, ic, bc}, u[x, t], {x, t}]
```

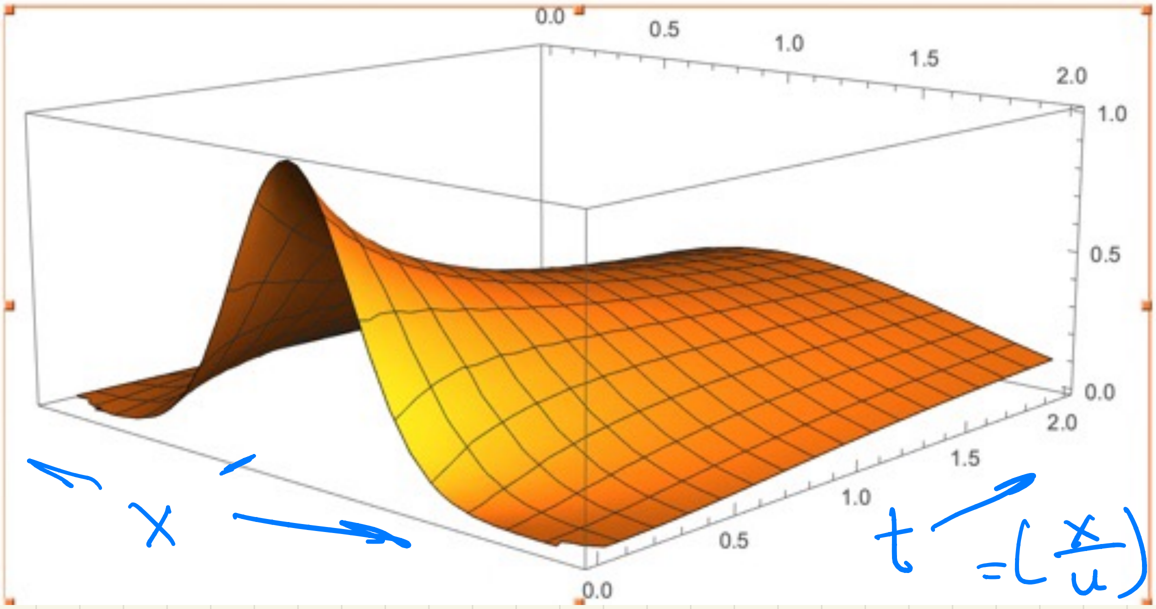
$$\left\{\left\{u[x,t] \to \sum_{K[1]=1}^{\infty} \frac{1}{20\sqrt{pe}} e^{-\frac{1}{100}\pi^2 t\,\alpha\,K[1]^2-\frac{\pi K[1]\,(40\,i\,pe+\pi K[1])}{400\,pe}} \sqrt{\pi}\left(\mathrm{Erfi}\left[\frac{20\,i\,pe+\pi K[1]}{20\sqrt{pe}}\right]-\mathrm{Erfi}\left[\frac{-180\,i\,pe+\pi K[1]}{20\sqrt{pe}}\right]+ e^{\frac{1}{5} i\pi K[1]}\left(\mathrm{Erfi}\left[\frac{-20\,i\,pe+\pi K[1]}{20\sqrt{pe}}\right]-\mathrm{Erfi}\left[\frac{180\,i\,pe+\pi K[1]}{20\sqrt{pe}}\right]\right)\right)\mathrm{Sin}\left[\frac{1}{10}\pi\,x\,K[1]\right]\right\}\right\}$$

```
asol01 = (u[x, t] /. %99[[1]] /. {∞ → 100} // Activate) /. {pe → 1000, α → 1 / 1000};

Plot3D[asol01 // Evaluate, {x, 0, 2}, {t, 0, .1}, Exclusions → None, PlotRange → All]
```



```
asol01 = (u[x, t] /. %99[[1]] /. {∞ → 100} // Activate) /. {pe → 10, α → 1 / 10};
Plot3D[asol01 // Evaluate, {x, 0, 2}, {t, 0, 2}, PlotRange → All]
```



$Pe = 10$ DISTURBANCE SPREADS WITHIN A SHORT DISTANCE

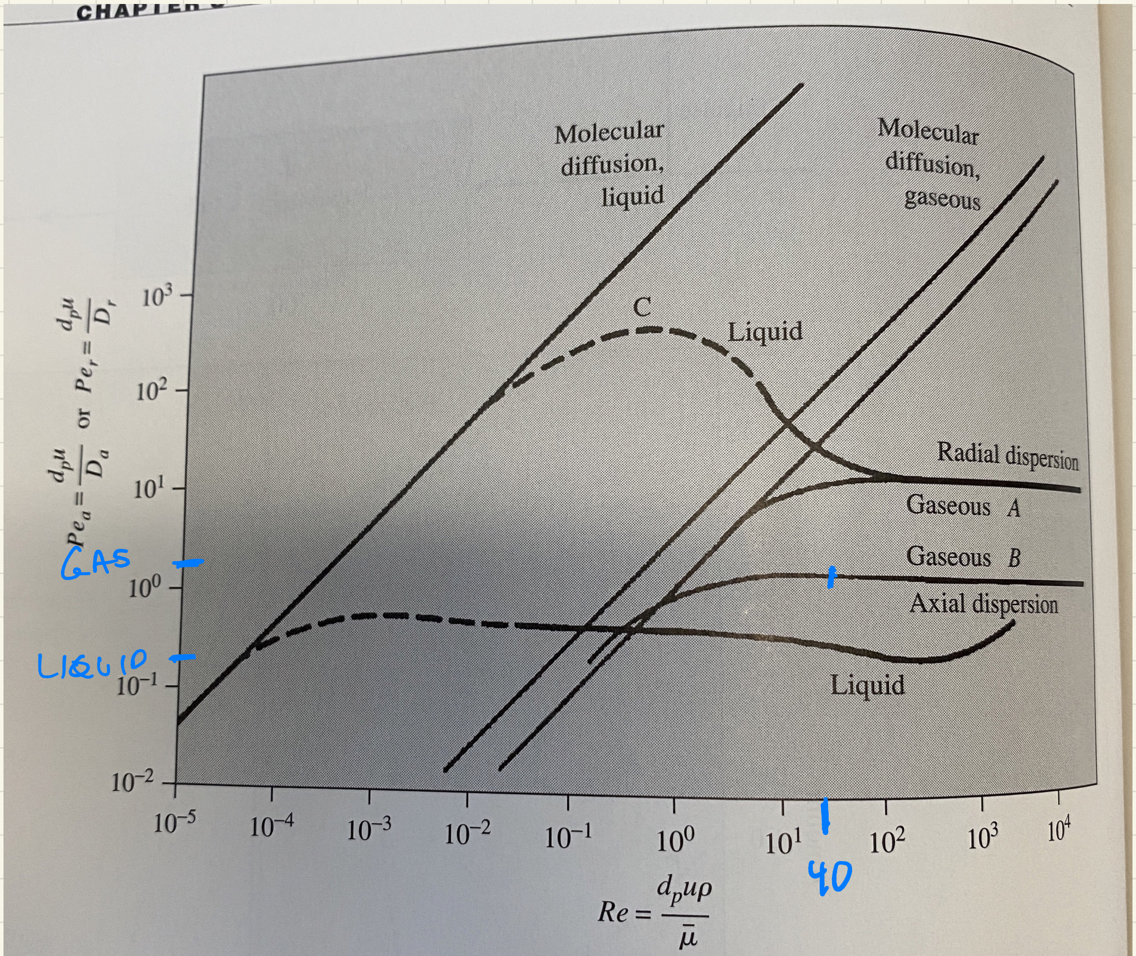


Figure 8.4.3 |
Axial and radial Peclet numbers as a function of Reynolds number for packed-beds. [Adapted from R. H. Wilhelm, *Pure App. Chem.*, **5** (1962) 403, with permission of the International Union of Pure and Applied Chemistry.]

$$Pe \equiv \frac{d_p u}{D_a} \qquad Re \equiv \frac{d_p u \rho}{\mu}$$

$Re > 40$ "TURBULENT"

DISPERSION WITH REACTION

WE PICK THE EQUATION!

$$D_a \frac{d^2 C_A}{dz^2} - u \frac{dC_A}{dz} - k C_A = 0$$

$$y = \frac{C_A}{C_A^0}, \quad Z = \frac{z}{L}, \quad Pe_a = \frac{uL}{D_a}$$

$$\frac{1}{Pe_a} \frac{d^2 y}{dZ^2} - \frac{dy}{dZ} - \frac{kL}{u} y$$

BC'S

$Z = -\infty \quad y = 1$

$Z = \infty \quad y = \text{FINITE}$

$Z = 0 \quad y(0_-) = y(0_+) = y(0)$

$Z = 1 \quad y(1_-) = y(1_+)$

$$uC_A\Big|_{0^-} = \left[uC_A - D_a\frac{dC_A}{dz}\right]_{0^+}$$

$$\frac{dC_A}{dz}\Big|_{L^-} = 0$$

WE CAN SOLVE