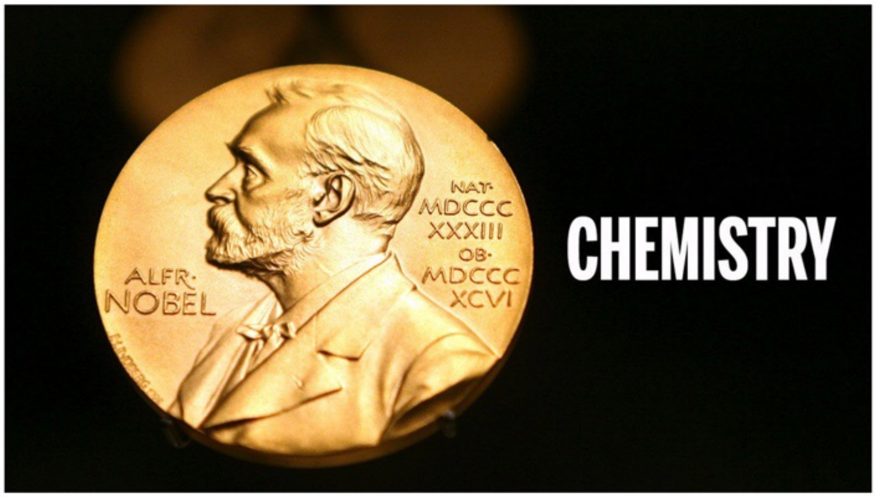
CBE 40445
10/7/20

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

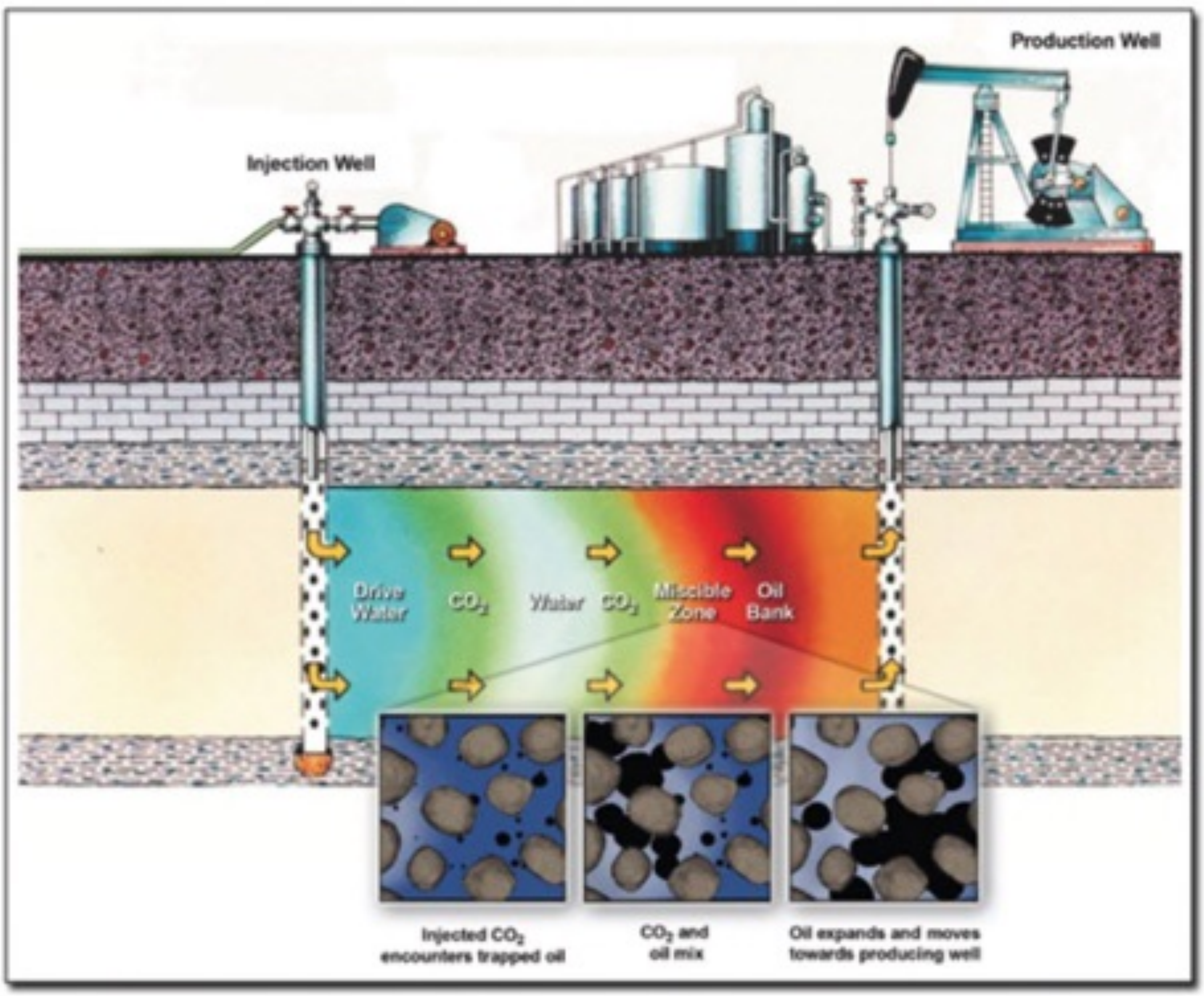
SHARE

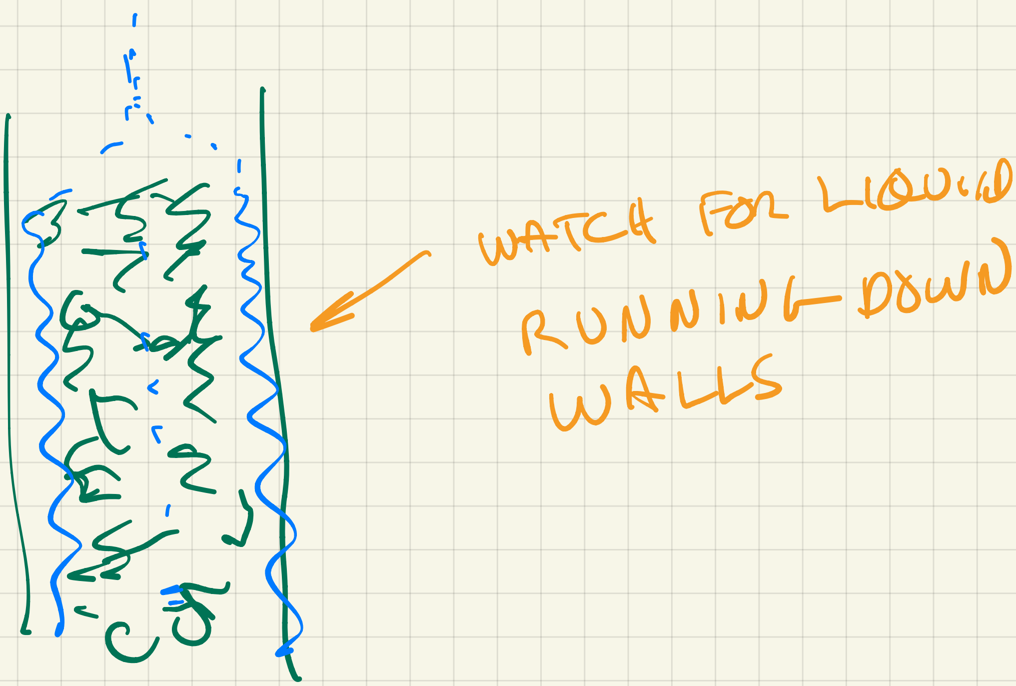


KAY NIETFELD/PICTURE-ALLIANCE/DPA/AP IMAGES

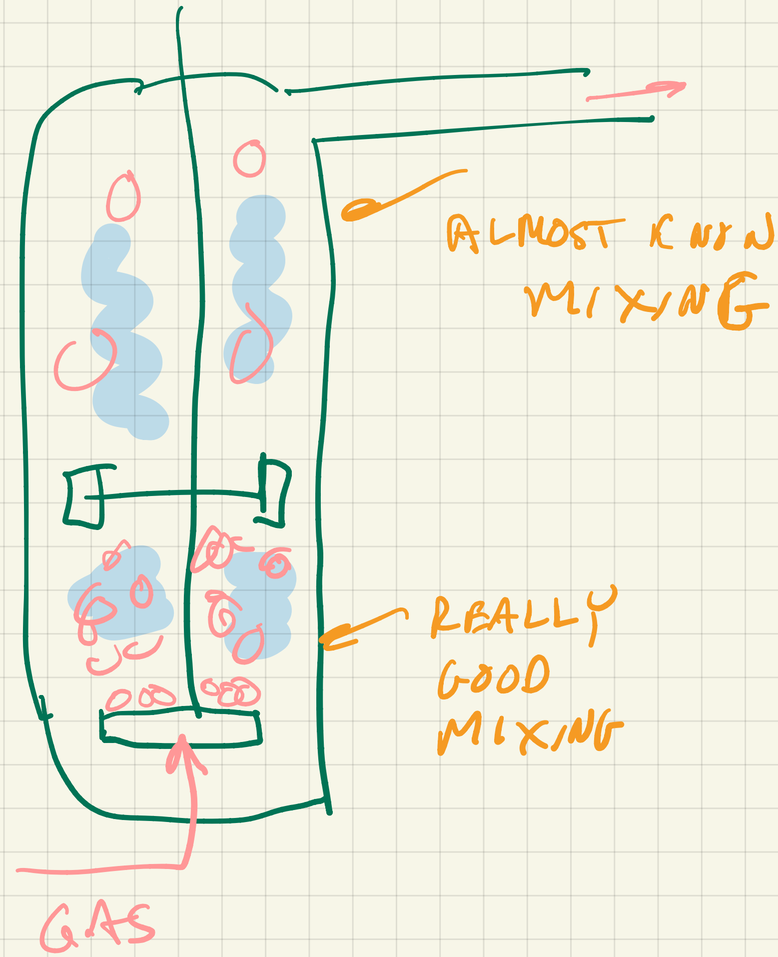
CRISPR, the revolutionary genetic "scissors," honored by Chemistry Nobel

By Science News Staff | Oct. 7, 2020 , 6:10 AM


Production Well
Injection Well
Drive Water
CO_2
Water
CO_2
Miscible Zone
Oil Bank
Injected CO_2 encounters trapped oil
CO_2 and oil mix
Oil expands and moves towards producing well


WATCH FOR LIQUID
RUNNING DOWN
WALLS


MOST GAS BY PASSES
NO PACKING


ALMOST KNOWN MIXING
REALLY GOOD MIXING
GAS

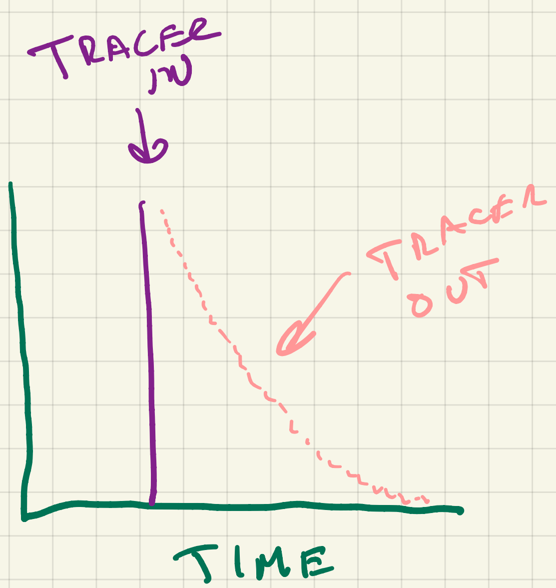
FOR REACTORS:

WHAT IS IDEAL?

CSTR → COMPOSITION + TEMPERATURE ARE UNIFORM IN REACTOR

→ EACH FLUID ELEMENT MIXED DOWN TO MOLECULAR SCALE

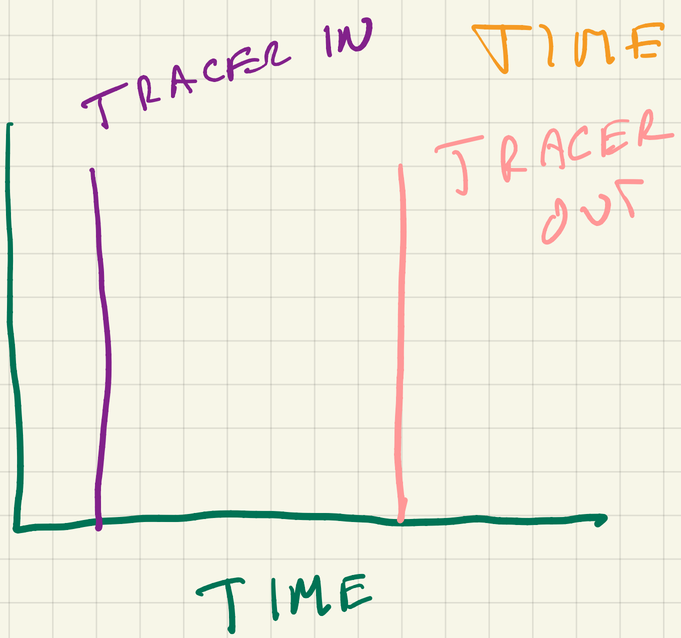
→ NEXT MOLECULE OUT IS IN NO WAY CORRELATED TO WHEN IT ENTERED



PFR – A PACKET OF FLUID ENTERS AT A SPECIFIC TIME AND DOES NOT MIX WITH FLUID AHEAD OR BEHIND IT

COMPOSITION + POSSIBLY TEMPERATURE CHANGES ALONG REACTOR

NEXT MOLECULE OUT IS DETERMINED BY TIME OF ENTRY



THESE IDEALIZATIONS LEAD TO VERY DIFFERENT PREDICTIONS OF REACTION OUTCOME

$$A \rightarrow M \qquad r = k C_A$$

$$\tau = \frac{V}{F}$$

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

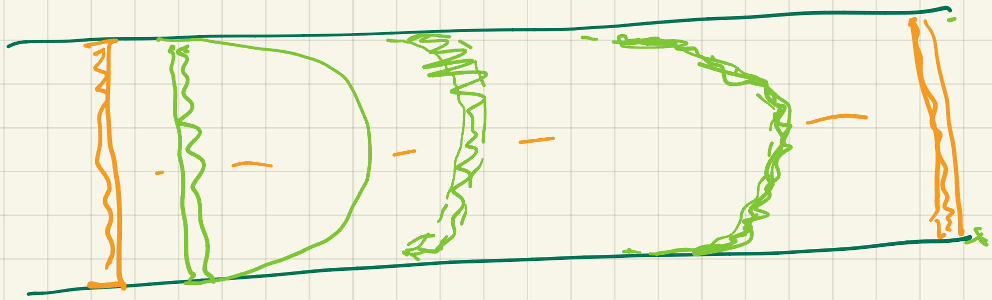
PLUG FLOW $$\frac{C_A}{C_{A0}} = \exp(-k\tau)$$

FOR 1ST ORDER, JUST 1 REACTION, THE DIFFERENCE JUST THE AMOUNTS OF A + M.

FOR SEQUENTIAL OR PARALLEL REACTIONS, THE DIFFERENCE COULD BE PRODUCT MIX.

A SIMPLE CASE THAT CAN BE QUANTIFIED

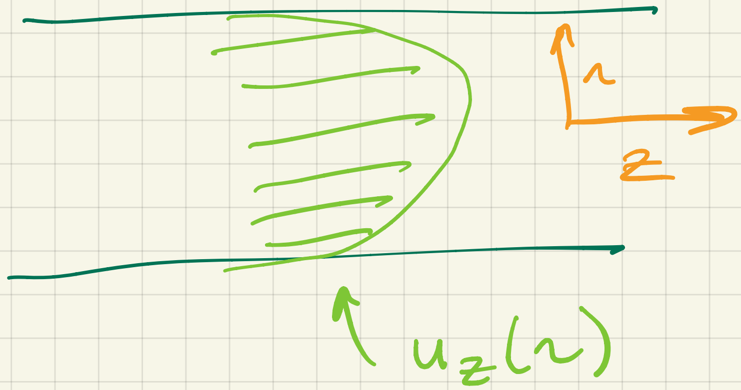
OPEN PIPE REACTOR



IF "PLUG FLOW" THEN

IF LAMINAR FLOW, CENTER OF PIPE WOULD EXIT FIRST

HOW DOES THIS AFFECT THE CONCENTRATION OF OUR FAVORITE A → M REACTION



REACTION AND DIFFUSION IN A FLOWING SYSTEM

$$\frac{dF_A}{dV_r} = -kC_A$$

$$\frac{d\,qC_A}{dV_r} = \frac{q}{A_t}\frac{dC_A}{dz} = \frac{u_z A_c}{A_c}\frac{dC_A}{dz}$$

$$u_z\frac{dC_A}{dz} = -kC_A$$

BUT MORE GENERALLY:

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

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

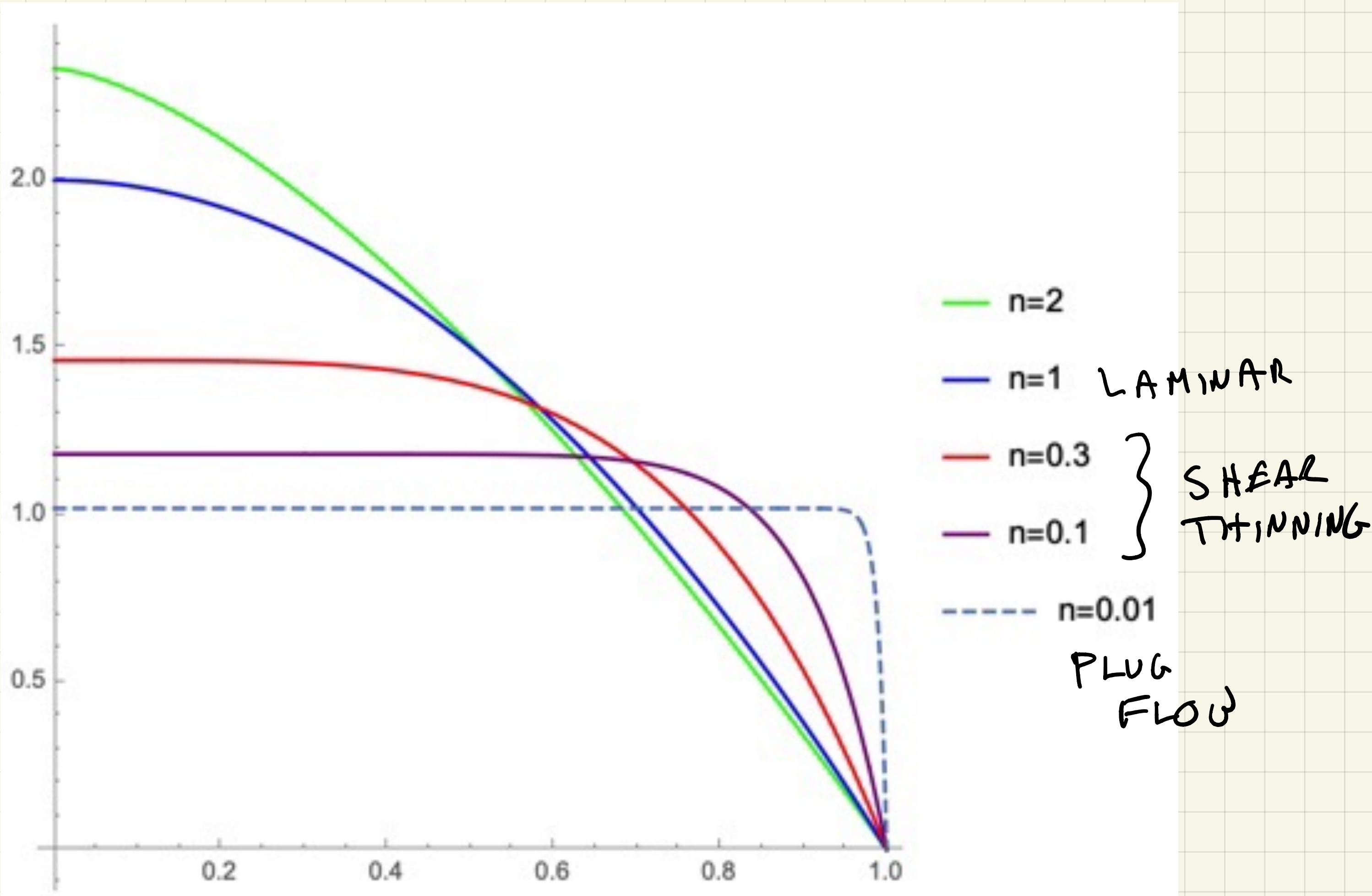
$$u_z \frac{dC_A}{dz} = -kC_A$$

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

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

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

POWER-LAW VELOCITY PROFILES



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

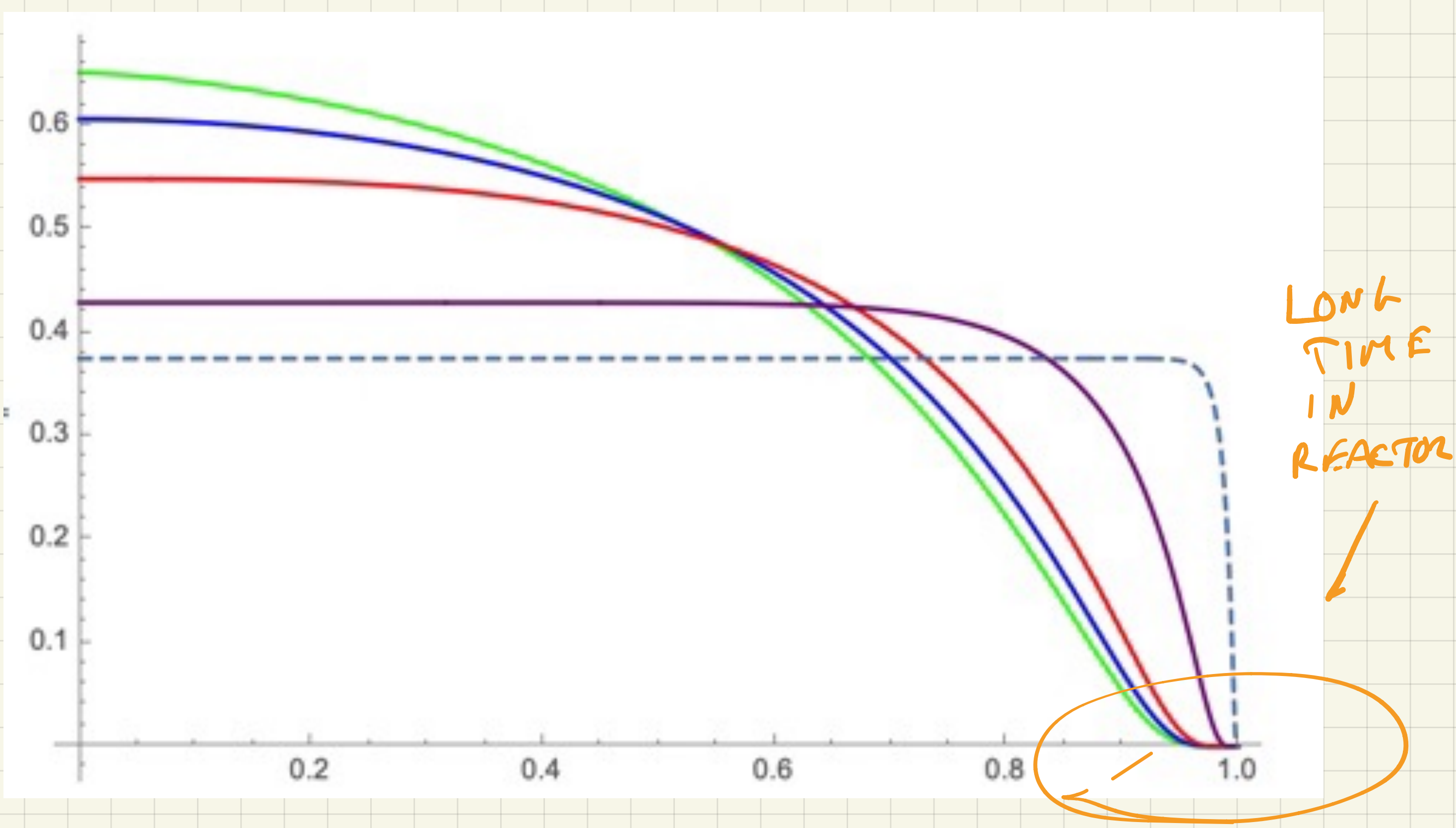
$$\bar{u} = \frac{2^{-1/n}\, n \left(R^{\frac{1}{n}+2} - \frac{n\, R^{\frac{1}{n}+2}}{2\,n+1}\right) \left(\frac{\text{dpdz}}{K}\right)^{1/n}}{n+1}$$

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

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

FOR FLOW REACTOR

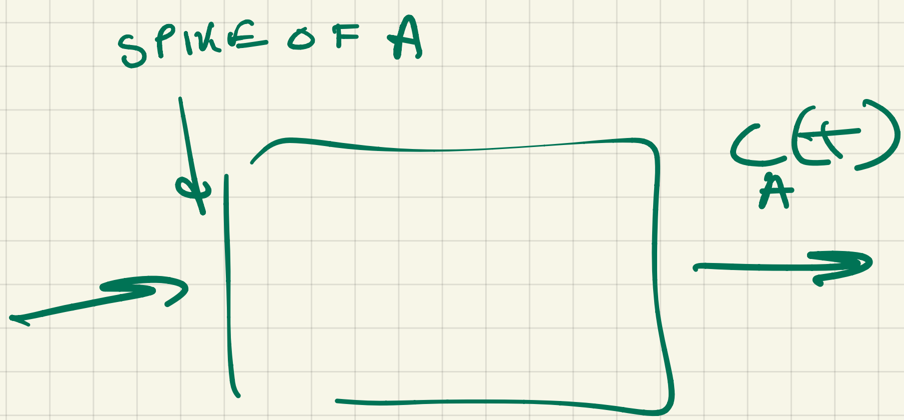
n	$\bar{C}_A^{EXIT}$
2	.453
1	.443
.5	.429
.3	.416
.1	.392
.01	.371



HOW TO QUANTIFY "IDEALITY"

RESISIDENCE TIME DISTRIBUTION

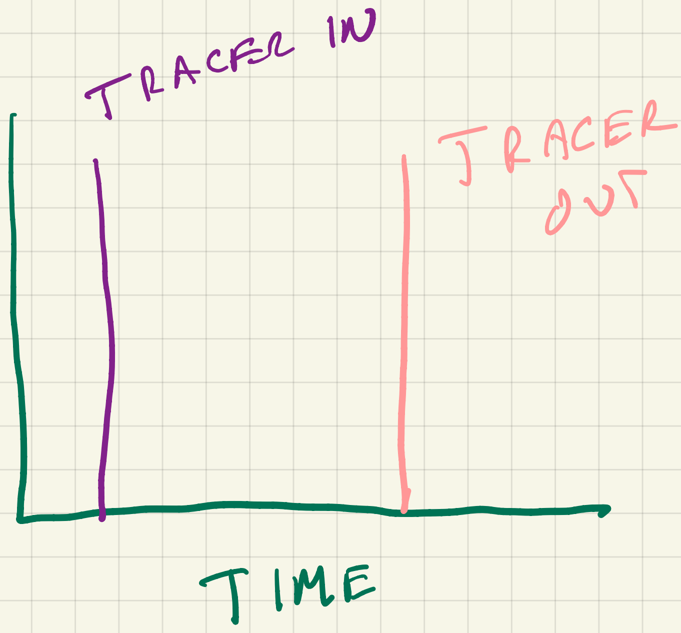
$E(t) \rightarrow$ EXIT TIMES OF TRACER SPECIES (= NOMINAL FLUID ELEMENTS)



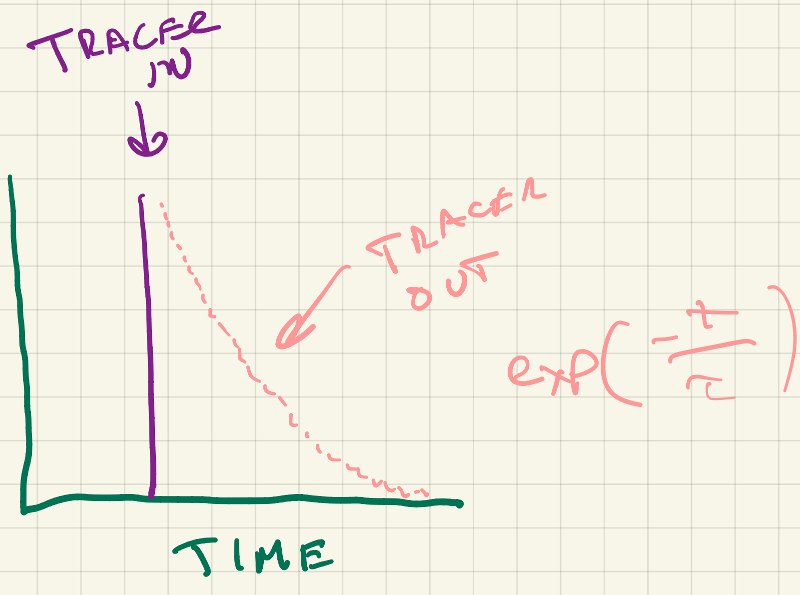
$$E(t) = \frac{C_A(t)}{\int_0^\infty C_A(\bar{t})\,d\bar{t}}$$

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

PFR



CSTR



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

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

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

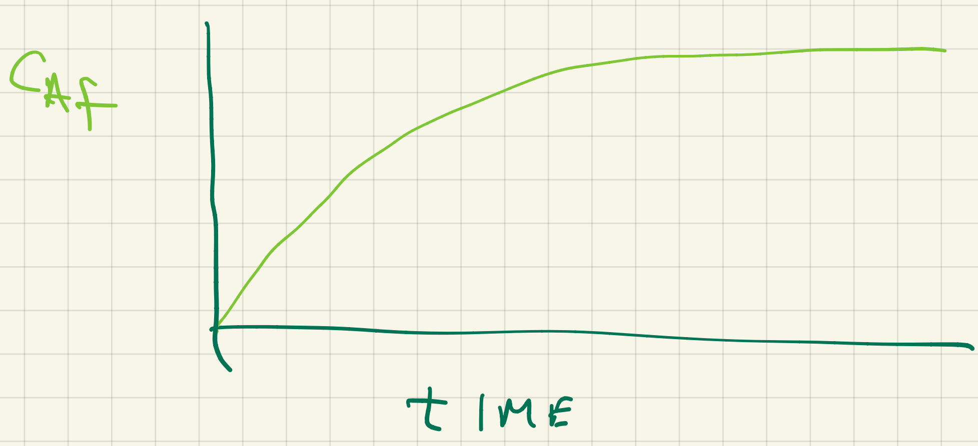
$$\frac{dC_A}{\left(C_A - C_{Af}\right)} = -\frac{q}{V}\,dt$$

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

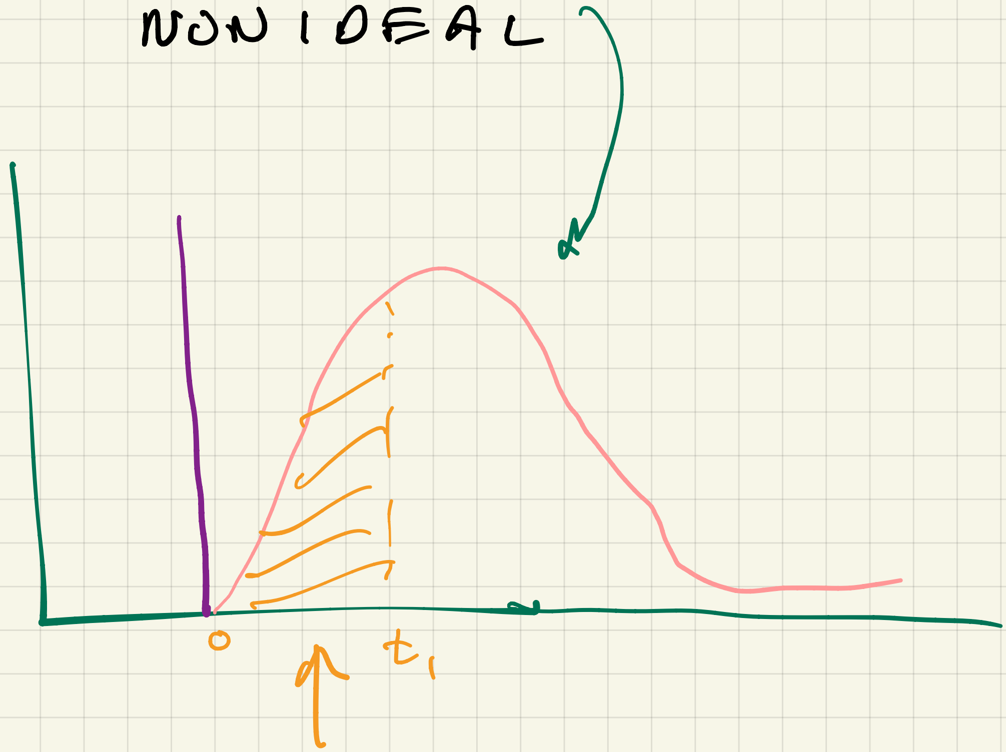
$C_A^0 = 0$

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

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



MORE LIKELY NONIDEAL



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

HOW DOES AN RTD DISTRIBUTION ACTALLY AFFECT CONVERSION?

[MEAN CONCENTRATION OF REACTANT AT REACTOR OUTLE] =

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)

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

$$C_A = C_A^0 \exp[-kt]$$

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

INSERT EXPRESSION FOR $E(t)$

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

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

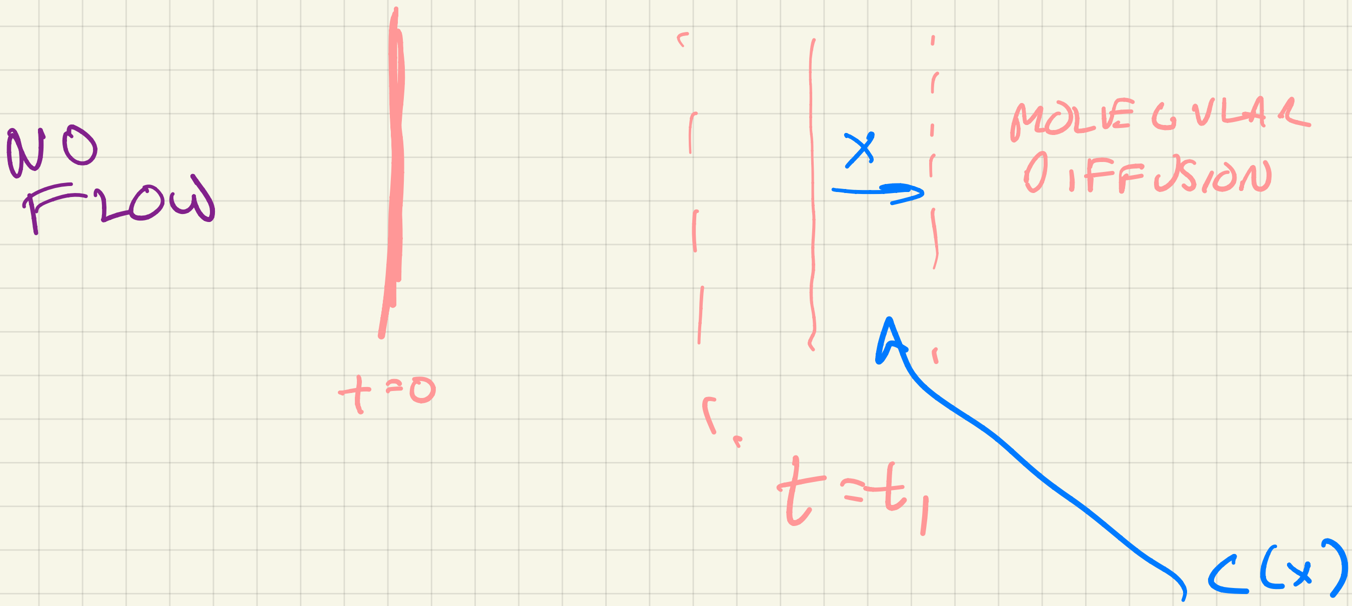
WE INTEGRATE:

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

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

EFFECT OF AXIAL DISPERSION

WE KNOW THAT IDEALIZATION OF SPIKE IN $\Rightarrow$ SPIKE OUT WILL NOT OCCUR EVEN FOR A FLAT VELOCITY PROFILE



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

AS NOTED ABOVE FOR A FLOWING 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_A 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:

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

NON DIMENSIONALIZE:

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

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

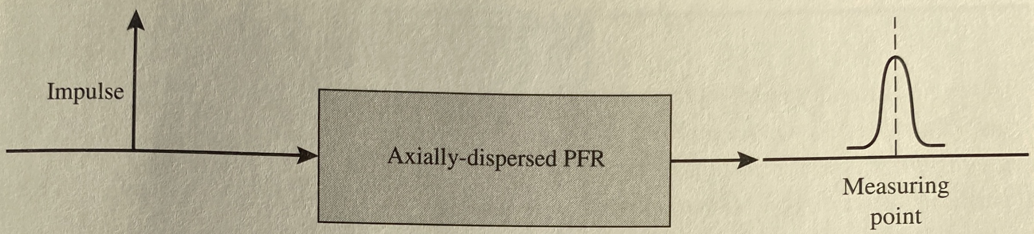
$$Pe_a \equiv \frac{L u}{D_a}$$ PECLET NUMBER

WE CAN WRITE:

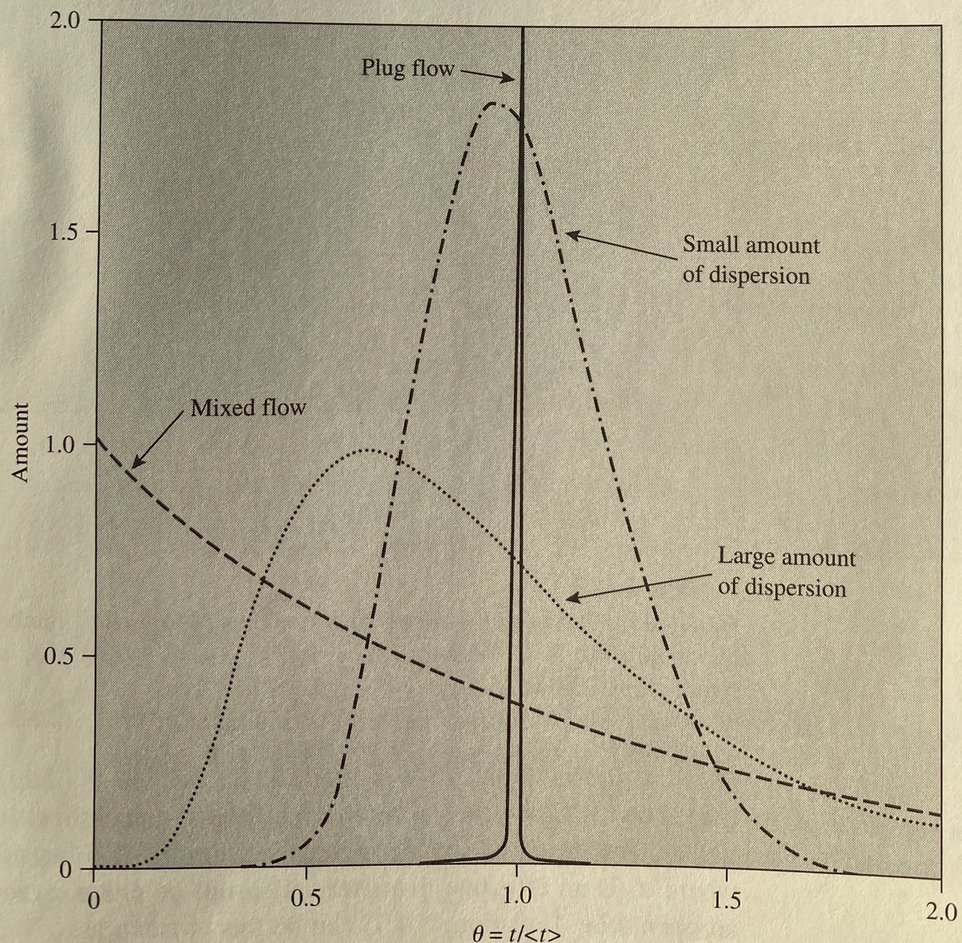
$$\frac{\partial C_i}{\partial \theta} + \frac{\partial C_i}{\partial Z} = \frac{1}{Pe_a} \frac{\partial^2 C_i}{\partial Z^2}$$

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

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


Impulse
Axially-dispersed PFR
Measuring point

(a)


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