CHE 504
ADVANCED [CHE] REACTOR DESIGN

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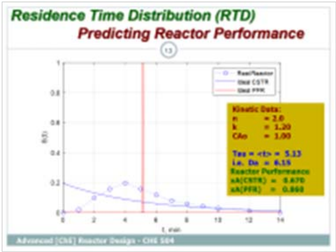
FALL 2020 [COURSE # 5336]
MW 6:00 – 7:50 PM
REMOTE DELIVERY



Residence Time Distribution (RTD)

Significance of Mixing

- For a 1st order reaction:

$$-r_A = kC_A^n = k\left[C_A^o\left(1-x_A\right)\right]^n$$

Concentration does not affect the rate of conversion, so RTD is sufficient to predict conversion

- But concentration does affect conversion in other (non-linear) scenarios, so we need to know the degree of mixing in the reactor

- RTD provides information on how long material has been in the reactor
- RTD does not provide information about the exchange of matter within the reactor (i.e., mixing)!
  - ✓ **Macromixing:** produces a distribution of residence times without specifying how molecules of different age encounter each other and are distributed inside of the reactor
  - ✓ **Micromixing:** describes how molecules of different residence time encounter each other in the reactor

Residence Time Distribution (RTD)

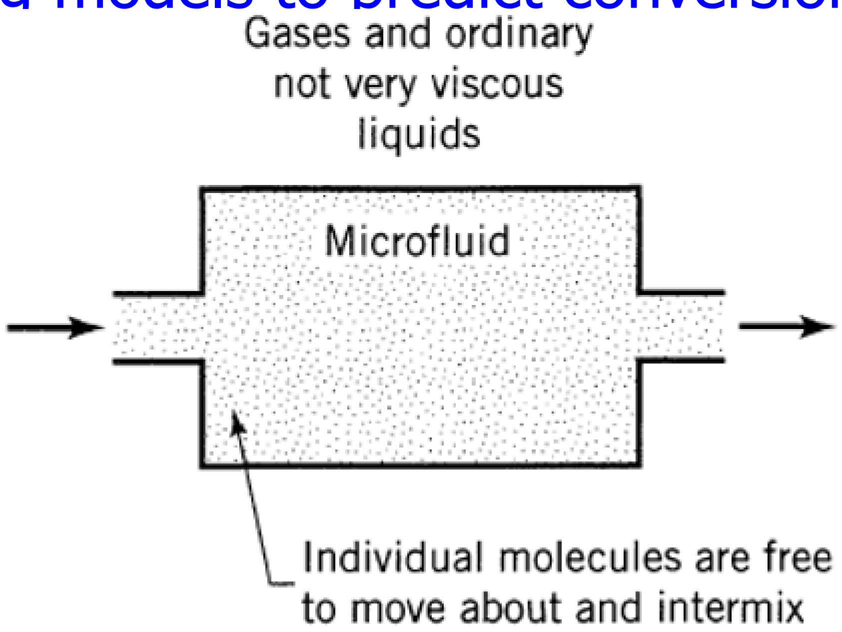
Quality of Mixing

- ✓ RTDs alone
  are not sufficient to determine reactor performance
- ✓ Quality of mixing is also required

Goal: Use RTD and micromixing models to predict conversion in real reactors

2 Extremes of Fluid Mixing

Maximum mixedness: molecules are free to move anywhere, like a microfluid. This is the extreme case of early mixing



Residence Time Distribution (RTD)

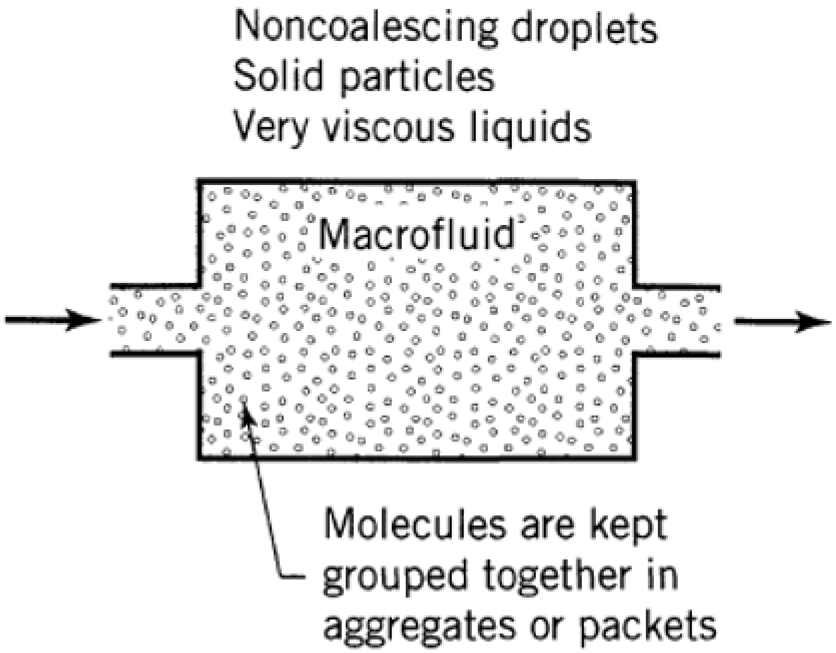
Quality of Mixing

- ✓ RTDs alone
  are not sufficient to determine reactor performance
- ✓ Quality of mixing is also required

Goal: Use RTD and micromixing models to predict conversion in real reactors

2 Extremes of Fluid Mixing

Complete segregation: molecules of a given age do not mix with other globules. This is the extreme case of late mixing



Advantages [and Responsibilities] of ...
Hands-on/Active Learning

I hear and I forget,
I see and I remember,
<u>I do</u> and I understand!

Confucius
(551-479 BCE)

Residence Time Distribution (RTD)

Predicting Reactor Performance

An isothermal pulse test on a piece of reaction equipment gave the following results: The output concentrations rose linearly from zero to 0.5 μmol/dm³ in 5 min, then fell linearly to zero in 10 min after reaching the maximum value.

(a) Calculate in tabular form the values of $E(t)$ and $F(t)$ at 1-min intervals. Sketch these functions.

(b) What is the mean residence time? If the flow were 150 gal/min, what would be the total reactor volume? (*Ans.:* t_m = 6.67 min, V = 1000 gal.)

A second-order reaction with kC_{A0} = 1.2 min^{-1} at 325 K is carried out in the system.

(c) If the reactor were plug flow with the same flow and volume, what would be the conversion? (*Ans.:* X = 0.889.)

(d) If the reactor were a CSTR with the same flow and volume, what would be the conversion? (*Ans.:* X = 0.703.)

$$\tau = \frac{V}{Q^o}$$

$$Da = \frac{\tau}{\tau_{rxn}} = \tau \underbrace{k\left(C_A^o\right)^{n-1}}_{\frac{1}{\tau_{rxn}}}$$

$$Da \Rightarrow \text{Reactor Performance?} \begin{cases} \text{CSTR} \\ \text{or} \\ \text{PFR} \end{cases}$$

Reactor Performance

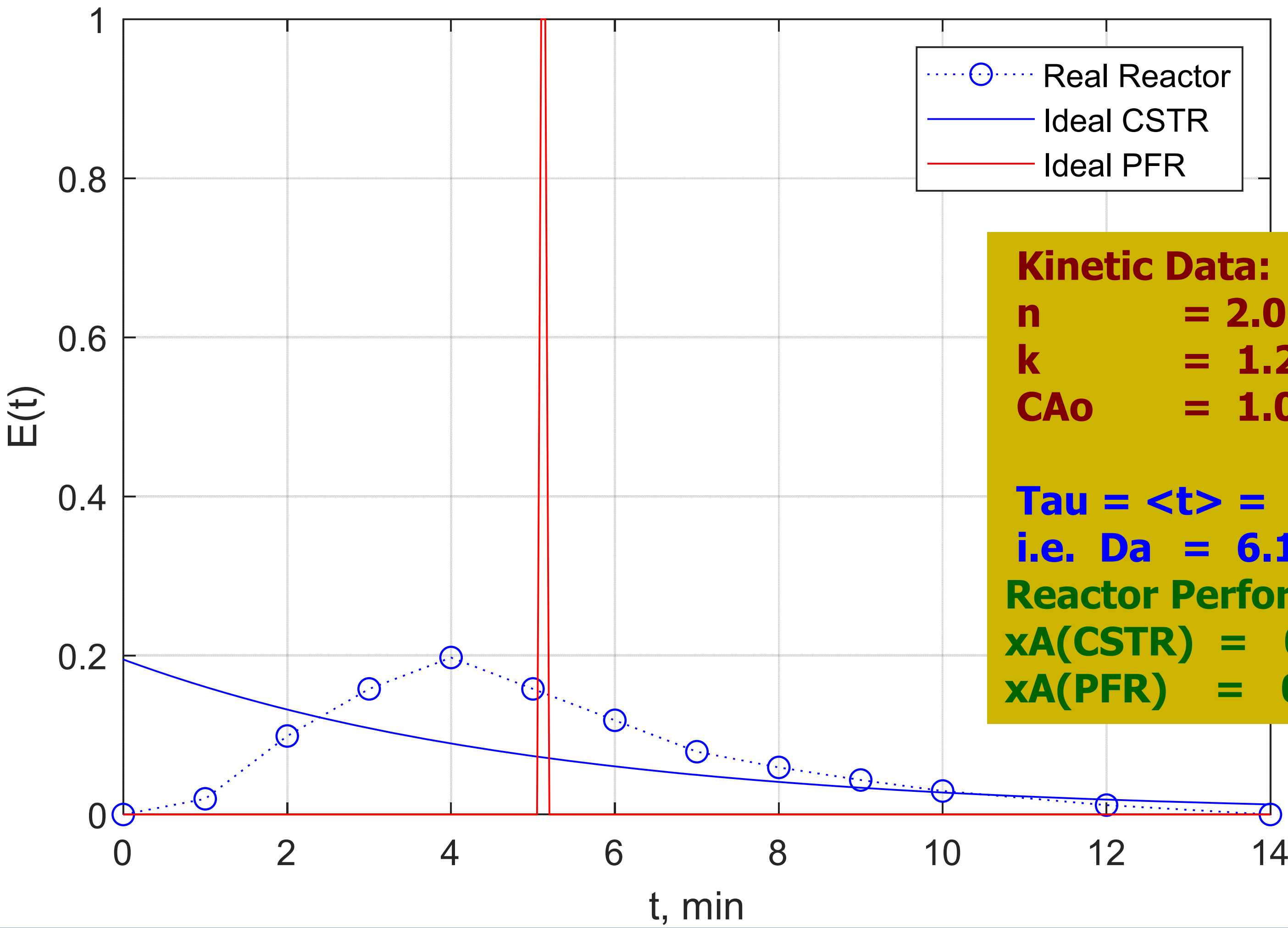
Da = 8.0

xA(CSTR) = 0.703

xA(PFR) = 0.889

Residence Time Distribution (RTD)

Predicting Reactor Performance



Kinetic Data:

n = 2.0

k = 1.20

CAo = 1.00

Tau = <t> = 5.13

i.e. Da = 6.15

Reactor Performance

xA(CSTR) = 0.670

xA(PFR) = 0.860

Residence Time Distribution (RTD)

Segregation Model

An isothermal pulse test on a piece of reaction equipment gave the following results: The output concentrations rose linearly from zero to 0.5 μmol/dm³ in 5 min, then fell linearly to zero in 10 min after reaching the maximum value.

(a) Calculate in tabular form the values of $E(t)$ and $F(t)$ at 1-min intervals. Sketch these functions.

(b) What is the mean residence time? If the flow were 150 gal/min, what would be the total reactor volume? (*Ans.:* t_m = 6.67 min, V = 1000 gal.)

A second-order reaction with kC_{A0} = 1.2 min⁻¹ at 325 K is carried out in the system.

(c) If the reactor were plug flow with the same flow and volume, what would be the conversion? (*Ans.:* X = 0.889.)

(d) If the reactor were a CSTR with the same flow and volume, what would be the conversion? (*Ans.:* X = 0.703.)

(e) If the flow were completely *segregated* with the $F(t)$ above, what would be the conversion? (*Ans.:* X = 0.86.)

$$\tau = \frac{V}{Q^o}$$

$$Da = \frac{\tau}{\tau_{rxn}} = \tau \underbrace{k\left(C_A^o\right)^{n-1}}_{\frac{1}{\tau_{rxn}}}$$

$$Da \Rightarrow \text{Reactor Performance?} \begin{cases} \text{CSTR} \\ \text{or} \\ \text{PFR} \end{cases}$$

Reactor Performance

Da = 8.0

xA(CSTR) = 0.703

xA(PFR) = 0.889

xA(MACRO) = ?

Residence Time Distribution (RTD)

Segregation Model

Example 16–1 Constructing the C(t) and E(t) Curves

A sample of the tracer hytane at 320 K was injected as a pulse into a rea
concentration was measured as a function of time, resulting in the data

t (min)	0	0.5	1	2	3	4	5	6	7	8	9	10	12	14
C (g/m^3)	0	0.6	1.4	5	8	10	8	6	4	3	2.2	1.5	0.6	0

TABLE E16-1.1 TRACER DATA

Pulse input

The measurements represent the exact concentrations at the times listed and not average values between the various sampling tests.

(a) Construct a figure showing the tracer concentration $C(t)$ as a function of time.

(b) Construct a figure showing $E(t)$ as a function of time.

Kinetic Data:
n = 2.0
k = 1.20
CAo = 1.00

RTD Analysis
Tau = <t> = 5.13
i.e. Da = 6.15

Reactor Performance
xA(CSTR) = 0.670
xA(PFR) = 0.860
xA(MACRO) = ?

CHE 504 Advanced [ChE] Reactor Design
Open for Questions … ?