ChE445_Seminar5_Winter2020_Solution

February 11, 2020

Q 1. Again review of 345: conversion in an ideal PFR. 20 pts

(adapted from Fogler's 4th Ed. Elements of Chemical Reaction engineering). $2NOCl \rightarrow 2NO + Cl_2$ The second-order gas-phase reaction is carried out in a steady-state isothermal isobaric ideal PFR. Pure NOCl is fed with an inlet flow rate of $2.26 * 10^{-5} \frac{mol}{s}$ and initial concentration of $0.283 \frac{mol}{L}$. The rate constant with respect to A is $267L/(mol.s)$. Find reactor volume to decrease the exit molar flow rate of $NOCl$ to $0.33910^{-5} \frac{mol}{s}$.

$2NOCl \rightarrow 2NO + Cl_2$

$A \rightarrow B + \frac{1}{2}C$

Stoichiometry Table where $X = X_A = \frac{F_{A0} - F_A}{f_{A0}} = \frac{2.26 - 0.339}{2.26} = 0.85$

Species	Initial	Change	Final
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	0	$F_{A0}X$	$F_B = F_{A0}X$
C	0	$0.5F_{A0}X$	$F_C = 0.5F_{A0}X$
Total	$F_{T0} = F_{A0}$	$\frac{1}{2}F_{A0}X$	$F_{A0}(1 + \frac{1}{2}X)$

At $P, T = cte$, $Q = Q_0 \frac{F_T}{F_{T0}} = Q_0(1 + \frac{1}{2}X)$

rate law for 2nd order reaction:

$-r_A = k_A C_A^2$

$C_A = \frac{F_A}{Q} = \frac{F_{A0}(1-X)}{Q_0(1+\frac{1}{2}X)} = C_{A0}\frac{1-X}{1+\frac{1}{2}X}$

Therefore:

$-r_A = k_A (C_{A0}\frac{1-X}{1+\frac{1}{2}X})^2$

Mole Balance for an ideal PFR:

$V = F_{A0} \in_0^X \frac{dX}{-r_A}$

$V = F_{A0} \int_0^X \frac{(1+0.5X)^2}{kC_{A0}^2(1-X)^2} dX$

Integration rule: $\int_0^X \frac{(1+\epsilon X)^2\, dX}{(1-X)^2} = 2\epsilon(1+\epsilon)ln(1-x) + \epsilon^2 X + \frac{(1+\epsilon)^2 X}{1-X}$

$V = \frac{2.26*10^{-5}}{267*0.283^2}(2*0.5*1.5*ln(1-0.85) + 0.5^2*0.85 + \frac{(1.5)^2*0.85}{1-0.85}) = 1.07*10^{-5}\ L$ (microreactor)

0.0.1 CH E 445, Midterm Exam Fall 2018. 45 minutes. Weight: 24/100.

Q1. A gas-phase irreversible reaction $2A + B \rightarrow C$ occurs in an ideal isobaric isothermal PFR and 80% conversion of A is reached. The feed contains $1\frac{mol}{m^3}$ of A, $5\frac{mol}{m^3}$ of B and $4\frac{mol}{m^3}$ of inerts. The reaction is 2^{nd} order to A and 0^{th} order to B. Rate constant is $3\frac{m^3}{mols}$.

1a. Calculate mean residence time.

1b. Is the space time higher or lower that the mean residence time? Explain.
Limiting reactant is A so:
$A + \frac{1}{2}B \rightarrow \frac{1}{2}C$
Stoichiometry Table where $X = X_A$

Species	Initial	Change	Final
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	$5F_{A0}$	$-0.5F_{A0}X$	$F_B = F_{A0}(5-0.5X)$
C	0	$0.5F_{A0}X$	$F_C = 0.5F_{A0}X$
I	$4F_{A0}$	0	$4F_{A0}X$
Total	$F_{T0} = 10F_{A0}$	$-F_{A0}X$	$F_{A0}(10-X)$

$\frac{F_T}{F_{T0}} = \frac{10-X}{10} = 1 - 0.1X$
At $P, T = cte$: $\frac{Q}{Q_0} = 1 - 0.1X$
At $P, T = cte$: $\bar{t} = C_{A0}\int_0^X \frac{dX}{-r_A(1+\epsilon X)}$
Rate law: $-r_a = kC_A^2C_B^0 = kC_A^2 = k\frac{F_A^2}{Q^2} = k\frac{F_{A0}^2(1-X)^2}{Q_0^2(1-0.1X)^2} = k\frac{C_{A0}^2(1-X)^2}{(1-0.1X)^2}$
$\bar{t} = \frac{C_{A0}}{k.C_{A0}^2}\int_0^X \frac{(1-0.1X)^2}{(1-X)^2(1-0.1X)}dX$
$\bar{t} = \frac{1}{kC_{A0}}\int_0^X \frac{1-0.1X}{(1-X)^2}dX$
$\bar{t} = \frac{1}{3*1}\frac{0.9}{1-0.8} + 0.1 * ln\frac{1}{1-0.8} = \frac{3.76}{3} = 1.25\ s$
$\tau = V/Q_0 =$
since $Q < Q_0$, $(Q = Q_0(1-0.1X))$ then $\tau < \bar{t}$

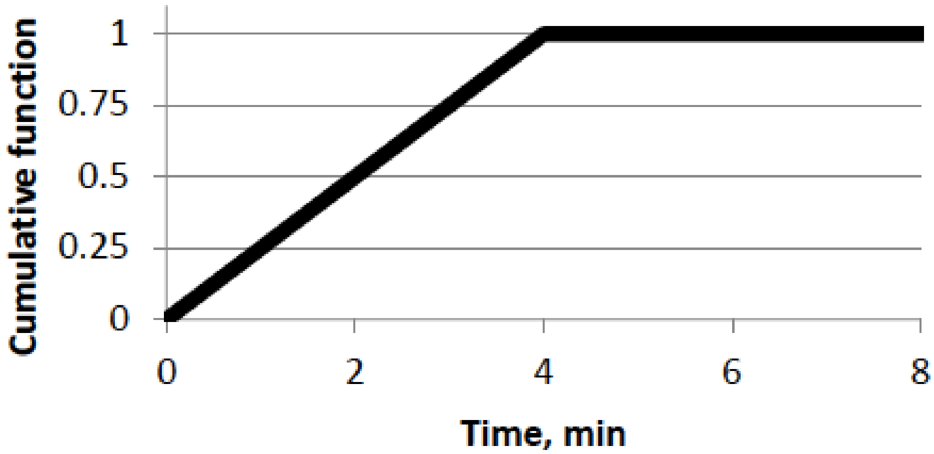
Q2. 25/100 pts

What fraction of the material spends between 2 and 8 minutes in a liquid-phase ideal CSTR with space time of 4 minutes?

Cumulative function for an ideal CSTR:
$F = 1 - e^{-t/\tau}$
up to 8 min: $F = 1 - e^{-8/4} = 0.865$
up to 2 min: $F = 1 - e^{-2/4} = 0.393$
Between: F(10)-F(2)= 0.472

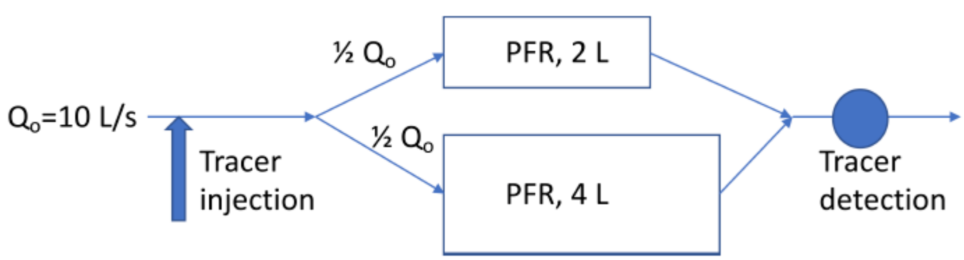
Q3. 25/100 pts

Predict conversion using segregation model for a zero-order liquid phase reaction $A \rightarrow B$ with rate constant of $5mol/(Lmin)$, C_{A0} of $10mol/L$ using the given cumulative distribution function:



S5Q3.png

Answer
$\bar{X} = \int_0^\infty X(t)E(t)dt$
$-r_A = k$
X from CVBR: $\frac{dX}{dt} = \frac{-r_A}{C_{A0}} = \frac{k}{C_{A0}}$
$\int_0^X dX = \frac{k}{C_{A0}} \int_0^t dt$
$X = \frac{k}{C_{A0}} t$
From the plot: $F(t) = 0.25t \quad 0 \leq t \leq 4$ else$= 0$.
$F(t) = \frac{dF(t)}{dt}$
$E(t) = 0.25 \quad 0 \leq t \leq 4$ else$= 0$.
$\bar{X} = \int_0^4 \frac{0.25k}{C_{A0}} t dt = \frac{0.25*5}{10} \frac{1}{2} t^2 [0 \rightarrow 4] = 1$
Q 4. 25/100 pts
A pulse of tracer is injected in a liquid flow which is equally divided between two ideal PFRs:
4a. Plot the tracer concentration at the point of detection as a function of time.
4b. Plot cumulative distribution function at the point of detection as a function of time. For both graphs in 4a and 4b, clearly indicate relevant numerical values and how they were calculated.

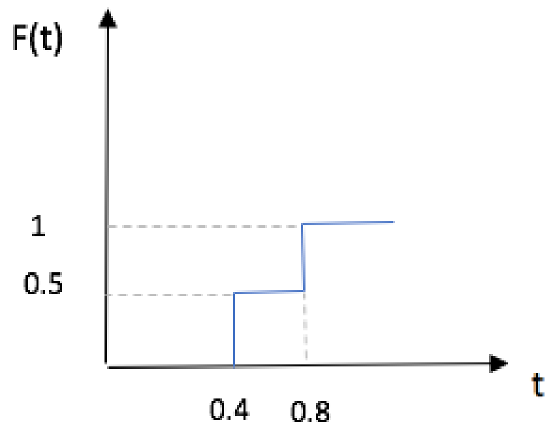


S5Q4.png

Answer
Ideal PFR
2L PFR: $\tau = \frac{V}{Q_0} = \frac{2L}{5L/s} = 0.4\ s$

4L PFR: $\tau = \frac{V}{Q_0} = \frac{4}{5} = 0.8\ s$

b) since flow is divided in 50% half of the tracer will leave at $0.4s$ and the rest at $0.8s$.



S5Q4-2.png

0.0.2 CH E 445, Midterm Exam Fall 2019. 45 minutes.

Q1. 25/100 pts.

A gas-phase 1st-order irreversible reaction $A \rightarrow 2B$ occurs in an ideal isobaric isothermal CSTR at $5s$ space-time. 80% conversion of A is reached. The feed contains $7mol/m3$ of A, $1mol/m3$ of B and $2mol/m3$ of inerts.

Calculate mean residence time in this ideal reactor.

Answer.

Stoichiometry Table where $X = X_A$

Species	Initial	Change	Final
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	$\frac{1}{7}F_{A0}$	$2F_{A0}X$	$F_B = F_{A0}(\frac{1}{7}+2X)$
I	$\frac{2}{7}F_{A0}$	0	$\frac{2}{7}F_{A0}X$
Total	$F_{T0} = \frac{10}{7}F_{A0}$	$F_{A0}X$	$F_{A0}(\frac{10}{7}+X)$

$Q = Q_0\frac{F_T}{F_{T0}} = \frac{Q_0(\frac{10}{7}+X)}{\frac{10}{7}}$

$\bar{t} = \int_0^V \frac{dV}{Q} = \frac{V}{Q_{exit}} = \frac{V}{Q_0}\frac{10/7}{10/7+X} = 3.205\ s$

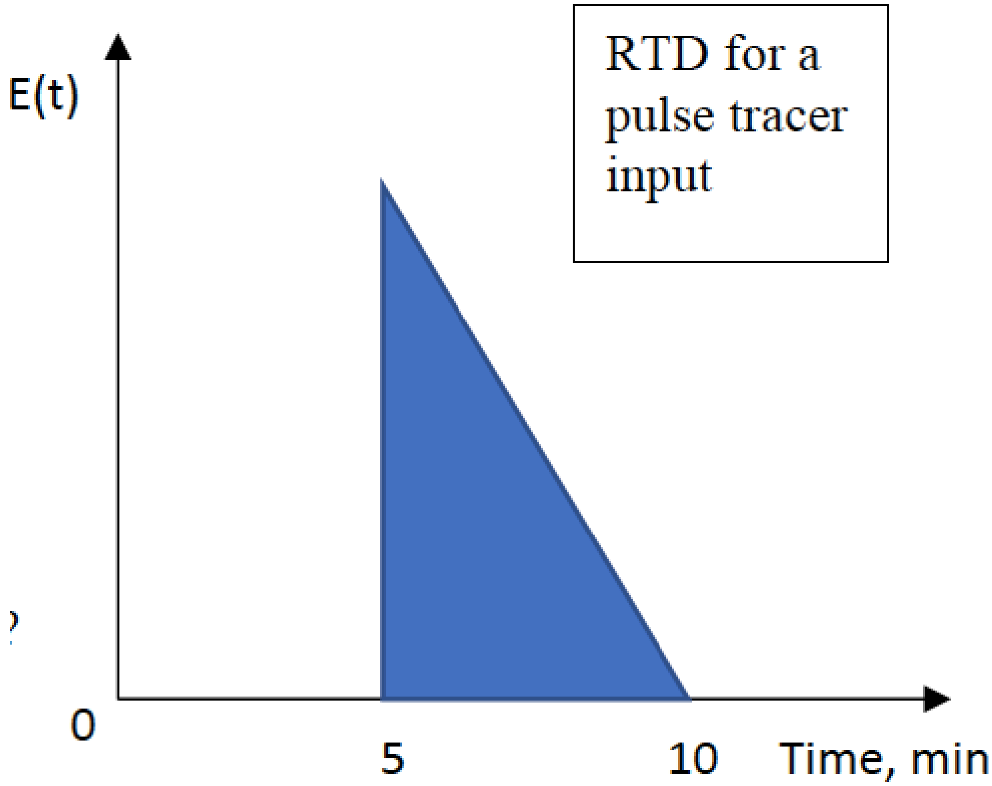
Q2. 25/100 pts

A pulse tracer input was used to determined RTD function in a constant-density flow reactor (see the Figure). All tracer has left by 10 minutes.

2a). Calculate the maximum value of the E(t) function. **10 pts**

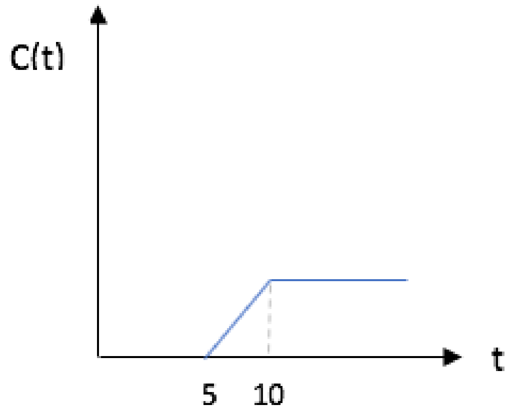
2b). What is the maximum achieved value of F(t) function? Explain. **5 pts**

2c). Sketch the exit tracer concentration vs. time if a step tracer input is performed on the same reactor at the same volumetric flow rate. Mark all known numerical values. **10 pts**



S5Q119.png

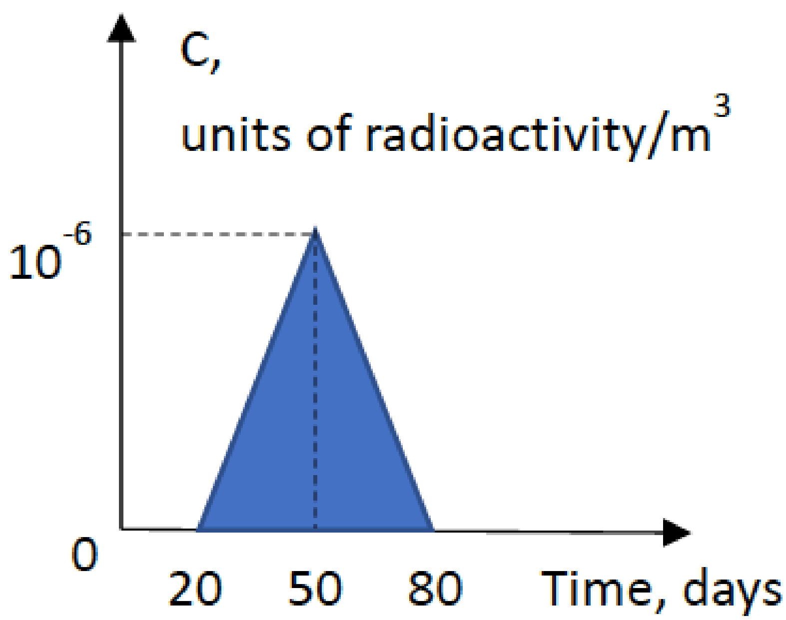
Answer
2a). $\int_0^\infty E(t)dt = 1$ so area under the graph$= 1$
$1 = \frac{1}{2}X(10-5)$
$X = 0.4$
2b). Since all tracer has left the reactor, $F(t)_{max} = 1$
2c). Step tracer input:
The $F(t)$ plot would be as :



S5Q219.png

no tracer upto 5 min. The tracer reaches ts maxium value by $10 min$

Q3. 20/100 pts A radioactive waste with half-life time of 100 years was dumped into a river. The flowing waters ($20010^6 m3/day$) are monitored downstream for this particular radioisotope. The data are shown in the Figure below:



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3a). How many radioactive units of this isotope were dumped? 5 pts

3b). What is the volume of the river between the monitoring point and the point of introduction of the waste? 10 pts

3c). Why is the half-life time of the isotope is mentioned? (1-sentence answer). 5 pts

Answer

3a) $\int_0^\infty C(t)dt = Area\ under\ the\ triangle = 30 * 10^{-6}\ \frac{u.r.}{m^3} days$

$30 * 10^{-6} * Q = 30 * 10^{-6} \frac{u.r.}{m^3} days * 200 * 10^6 \frac{m^3}{day} = 6000\ u.r.$

3b) $\tau = \frac{V}{Q_0}$ here $\tau = \bar{t} = 50\ days$

$V = 50 * 200 * 10^6 = 10^{10}\ m^3$

3c) It does not convert within this time of 80days, so it can be considered as a non-reactive tracer.

Q4. 30/100 pts

Based on RTD measurements, a real flow reactor can be modelled as a combination of one ideal PFR ($8L$) followed by one ideal CSTR ($4L$) in series. The volumetric flow rate of the liquid feed is $2L/s$.

4a). Sketch the RTD function of the real reactor. Show and justify all known numerical values on both axes. **15 pts**

4b). Find mean residence time in the real reactor. **5 pts**

4c). Imagine now if 25% of the PFR volume is "dead zones". Sketch the RTD function of the real reactor. Show and justify all known numerical values on both axes. **10 pts**

Answer

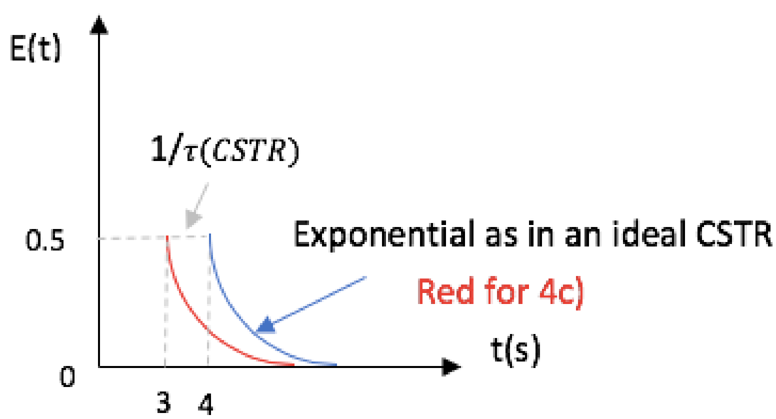
4a) $\tau_{PFR} = \frac{V}{Q_0} = \frac{8}{2} = 4\ s$

$\tau_{CSTR} = \frac{4}{2} = 2\ s$

PFR only delays the ideal exit from CSTR.

4b) $\bar{t} = \tau = 4 + 2 = 6\ s$

4c) For PFR $\tau_{new,PFR} = \frac{0.75*8L}{2L/s} = 3\ s$ τ_{CSTR} the same.



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