ChE445_HW2_Winter2020_Solution_and_Code

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Predicting conversion in non-ideal reactors (part 1)

Q1. Again review of 345: build a stoichiometric table. 40 pts

Consider a gaseous feed: $C_{A0} = 100 mol/L$, $C_{B0} = 200 mol/L$, $C_{inerts,0} = 100 mol/L$ to a steady-state isothermal isobaric ideal PFR. At the reactor exit $C_A = 40 mol/L$.

The gas-phase reaction is:
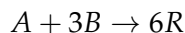
$$A + 3B \rightarrow 6R$$

Find X_B and X_A. (Use any method and any approach to build a stoichiometric table). (Hint: these conversions are connected via exit flow rates)

Find a limiting reactant (LR) in $A + 3B \rightarrow 6R$

$$\frac{A}{B} = \frac{1}{2}\frac{mol}{mol}$$

So B is the limiting reactant, this means that there is not enough B to convert all A

Therefore we can rewrite the reaction to have , 1 as the coefficient for the LR.

$$\frac{1}{3}A + B \rightarrow 2R$$
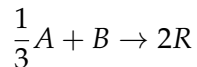
Stoichiometric table where $X = X_B$, $X = \frac{F_{B0} - F_B}{F_{B0}}$

Species	Initial	Change	Final
A	$F_{A0} = \frac{1}{2}F_{B0}$	$-\frac{1}{3}F_{B0}X$	$F_A = F_{B0}(\frac{1}{2} - \frac{1}{3}X)$
B	F_{B0}	$-F_{B0}X$	$F_B = F_{B0}(1 - X)$
R	0	$2F_{B0}X$	$F_C = 2F_{B0}X$
inert	$F_{I0} = \frac{1}{2}F_{B0}$	0	$F_I = \frac{1}{2}F_{B0}$
Total	$F_{T0} = 2F_{B0}$	$\frac{2}{3}F_{B0}X$	$2F_{B0}(1 + \frac{1}{3}X)$

$$C_A = \frac{F_A}{Q}$$

$$Q = \frac{Q_0}{F_{T0}}F_T \quad at \quad P, T = CTE$$

$$C_A = \frac{F_{B0}(\frac{1}{2} - \frac{1}{3}X)2F_{B0}}{Q_0 2 F_{B0}(1 + \frac{1}{3}X)} = C_{B0}\frac{\frac{1}{2} - \frac{1}{3}X}{1 + \frac{1}{3}X} = 200[\frac{mol}{L}] = 40\frac{mol}{L}$$
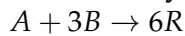
$$X = X_B = 0.75$$

Using the stoichiometric table, moles of A reacted (change) $= \frac{1}{3}F_{B0}X = \frac{1}{3} * 0.75$

$$X_A = \frac{moles\ of\ A\ reacted}{moles\ of\ A\ fed} = \frac{0.25F_{B0}}{0.5F_{B0}} = 0.5$$

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Another way of solving the same problem

$A + 3B \rightarrow 6R$

Stoichiometric table

Species	Initial	Final
A	F_{A0}	F_A
B	$F_{B0} = 2F_{A0}$	$F_{B0} - 3(F_{A0} - F_A) = 3F_A - F_{A0}$
R	0	$6(F_{A0} - F_A)X$
inert	$F_{I0} = F_{A0}$	F_{A0}
Total	$F_{T0} = 4F_{A0}$	$6F_{A0} - 2F_A$

$$C_A = \frac{F_A}{Q}$$

$$Q = \frac{Q_0}{F_{T0}}F_T \quad at \quad P, T = CTE$$

$$C_A = 40$$

$$40 = \frac{F_A.4F_{A0}}{Q_0(6F_{A0} - 2F_A)} = \frac{4 * F_A * 100}{6F_{A0} - 2F_A}$$

$$\frac{F_{A0}}{F_A} = 2$$

$$X_A = 0.5$$

Using the stoichiometric table

$$\frac{F_B}{F_{B0}} = \frac{3F_A - F_{A0}}{2F_{A0}} = \frac{3}{2.2} - \frac{1}{2} = 0.25$$

$$X_B = 0.75$$

Q2. Laminar flow reactor and 2nd order reaction. 35 pts

RTD measurements were performed in a flow reactor of $5L$ volume at a constant fluid flow rate of $2.5L/s$. The reactor was found to behave as a laminar flow reactor. It is to be used to perform a $2nd$ order constant-density reaction with $kC_{A0} = 15s^{-1}$ at the same flow rate.

Predict the maximum possible conversion in the reactor (i.e., use the segregation micromixing model because the overall reaction order is above 1).

To solve, use a trapezoidal rule to estimate the required integral.

Let us use $\Delta t = 0.01$ s and $t_{max} = 20s$. (The small enough interval and the large enough final point in the tail gives a more accurate result). To report, do not print out the Excel file, but show all relevant equations, and report the numerical values for $E(t)$ and $X(t)$ at 5s, as well as the final predicted conversion.

Segregation model:

$$\bar{X} = \int_0^\infty X(t)E(t)dt$$

$$CVBR : C_{A0}\frac{dX}{dt} = -r_A = kC_{A0}(1-X)^2$$

$$\int_0^X \frac{dX}{(1-X)^2} = kC_{A0}\int_0^t dt$$

$$\frac{X}{1-X} = kC_{A0}t$$

$$X = \frac{kC_{A0}t}{1+kC_{A0}t}$$

$E(t)$ comes from the LFR:

$$\tau = \frac{V}{Q_0} = \frac{5}{2.5} = 2 \text{ s}$$

$$E(t) = 0, \quad t < \frac{\tau}{2}(\tau < 1s)$$

$$E(t) = \frac{\tau^2}{2t^3} = \frac{2}{t^3}, \quad t \geq \frac{\tau}{2}(\tau \geq 1s)$$

Calculate $E(t)$, $X(t)$, and $X(t).E(t)$. Then using the trapezoidal rule, for example, $(t_4 - t_3)$:

$\frac{E_3X_3+E_4X_4}{2}$

$\sum$ =conversion= 0.965

Values at 5s:

$X(t) = 0.987$ $E(t) = 0.016$

```python
import numpy as np
V=5 #L
Q0=2.5 #L/s

Tau=V/Q0
print ("{0:.1f}".format(Tau),'(s)')
```

2.0 (s)

```python
import math
import matplotlib.pyplot as plt

t=np.linspace(0.,20,2000)
E=np.zeros(len(t))
```

3

```
for i in range(0,len(t)):
    if  t[i]>(Tau/2):
        E[i]=(pow(Tau,2)/2)/pow(t[i],3)
    else:
        E[i]=0

plt.plot(t,E)
plt.ylabel('E, 1/s')
plt.xlabel('Time, s')
```

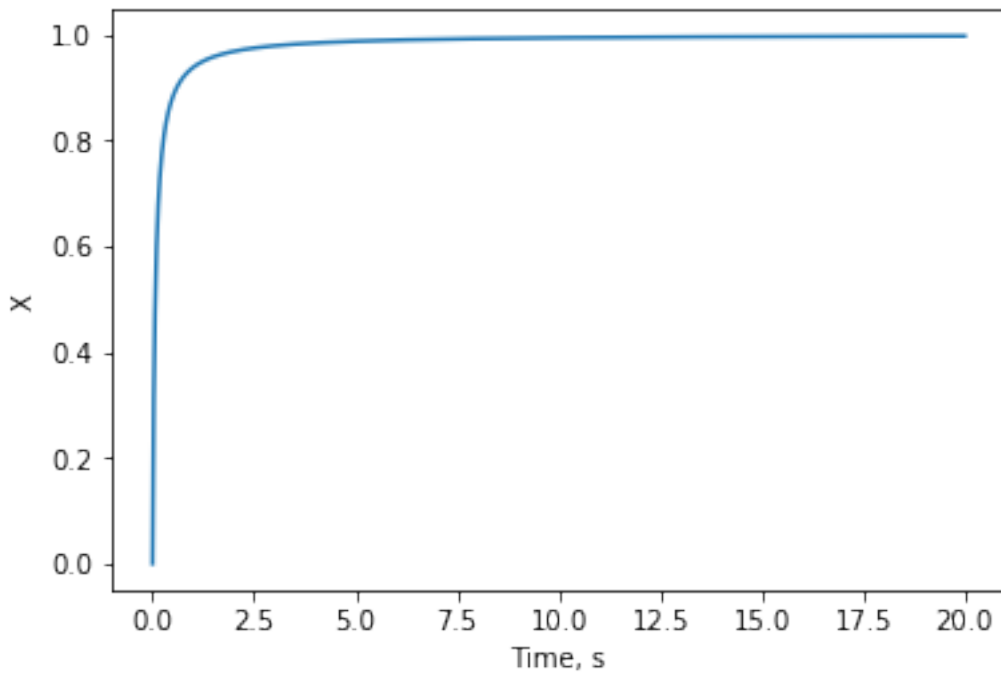[2]: Text(0.5, 0, 'Time, s')

[3]:
```
kCA0=15 #S^{-1}

X=kCA0*t/(1+kCA0*t)

plt.plot(t,X)
plt.ylabel('X')
plt.xlabel('Time, s')
```
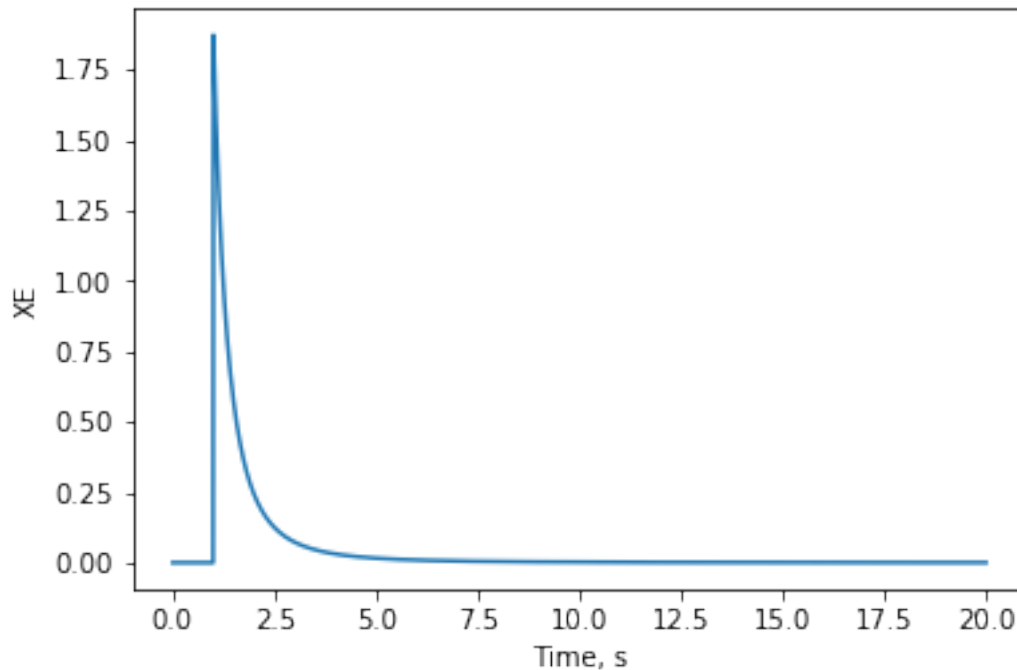
[3]: Text(0.5, 0, 'Time, s')

[4]:
```
XE=X*E

plt.plot(t,XE)
plt.ylabel('XE')
```

```
plt.xlabel('Time, s')
```

[4]: Text(0.5, 0, 'Time, s')

[5]:
```
import scipy.integrate as integrate

Conv = integrate.trapz(XE, t)
print ("{0:.3f}".format(Conv), '=Conversion')
```

0.964 =Conversion

Q3. Dead zones in a CSTR. 5 pts
In problem 2, seminar 2, what is the volume of dead zones in the reactor?
τ_{real} CSTR with dead zones $= \frac{V_{SD}[Active]}{Q_0}$

$$1.7s = \frac{V_{SD}}{5}$$

$$V_{SD} = 8.5L$$

$$V_{dead} = 10L - 8.5 = 1.5L$$

Q 4. A real-life case. 20 pts (4 pts for each subquestion).
So far, we used hypothetical tracer concentrations with profiles which are easily described by simple correlations for learning purposes. In reality, the $C(t)$ profiles look more similar as shown in this problem (depending on the reactor performance).

5

Read the following sections from a real-life study from Esso Research Laboratories: Industrial and Engineering Chemistry Process Design and Development, Volume 3 (1964), p. 381 (posted on eClass):

Introduction
Determination of Residence-Time-Distribution
Application to a Commercial Desulfurization Reactor

Answer the following questions (short, 1-2 sentences each):

4-a). What tracer was used for the RTD measurements? What was the reactor feed?

4-b). What method was used (pulse or step)?

4-c). Is the reactor perfectly mixed?

4-d). The RTD measurements revealed some problems: what were they and how this could be deducted from, for example, Figure 6?

4-e). What was done to fix the problem and which Figure represents the cured reactor?

4-a)

Feed: liquid Oil and H_2 gas.

Tracer: Octadecane tagged with radioactive ^{14}C.

4-b)

Pulse

4-c)

No. The reactor approaches a PFR behavior.

4-d

Comparing Figs 4 and 6, in Fig. 6 there is a peak at $0 time$ (indicates by-passing) and a large tracer amount leaving after 20 minutes.

The catalyst was not packed property and the catalyst bed shifted at the startup.

4-e

The catalyst was repacked. The RTD of the cured reactor is shown in Fig. 7.

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