# CBE 142: Chemical Kinetics \& Reaction Engineering 

Midterm \#2<br>November 6 ${ }^{\text {th }} 2014$

This exam is worth 100 points and $20 \%$ of your course grade. Please read through the questions carefully before giving your response. Make sure to SHOW ALL YOUR WORK and BOX your final answers!

Name: $\qquad$
Student ID: $\qquad$
Section (Day/GSI) that you attend: $\qquad$

You are allowed one $8.5^{\prime \prime} \times 11^{\prime \prime}$ sheet of paper (front and back), a calculator and a ruler for this exam. Any additional paper you wish to be graded must have your NAME and STUDENT ID written on each page.

| Problem | Max Points | Points Earned |
| :---: | :---: | :---: |
| 1 | 5 |  |
| 2 | 30 |  |
| 3 | 30 |  |
| 4 | 10 |  |
| 5 | 25 |  |

$\qquad$

## Problem \#1 (5 points)

The following two liquid-phase reactions occur in parallel and isothermally. One produces a desired product ( D ) and the other produces an undesired product $(\mathrm{U})$.

$$
\begin{array}{lll}
\mathrm{A}+\mathrm{B} & \rightarrow \mathrm{D} & r_{D}=k_{D} C_{A} C_{B}^{1 / 4} \\
\mathrm{~A}+\mathrm{B} & \rightarrow \mathrm{U} & r_{U}=k_{U} C_{A}^{1 / 2} C_{B}^{2}
\end{array}
$$

In both schemes below, the total amount of A and B fed into the system are the same. From the standpoint of favorable product distribution, which one of these two reactor setup schemes would be best? Circle your answer and take a few sentences to explain your answer.


## Problem \#2 (30 points)

Consider the following liquid-phase reaction:

$$
\mathrm{A} \rightarrow 3 \mathrm{C} \quad-r_{A}=k
$$

Pure A enters a non-ideal flow reactor at temperature $T_{0}$ and molar feed rate $\mathrm{F}_{\mathrm{A} 0}$. A non-ideal flow reactor means the reactor is nether a CSTR nor a PFR.

Known system parameters:
$\mathrm{F}_{\mathrm{A} 0}=20 \mathrm{~mol} / \mathrm{min}$
$\Delta \mathrm{H}_{\mathrm{rx}}(@ 300 \mathrm{~K})=-12000 \mathrm{~J} / \mathrm{mol}$ of A
$\mathrm{k}(@ 300 \mathrm{~K})=0.6 \mathrm{~mol} / \mathrm{L} \cdot \mathrm{min}$
$\mathrm{E} / \mathrm{R}=1000 \mathrm{~K}$

$$
\begin{aligned}
& \mathrm{T}_{0}=350 \mathrm{~K} \\
& \mathrm{C}_{\mathrm{pA}}=45 \mathrm{~J} / \mathrm{mol} \cdot \mathrm{~K} \\
& \mathrm{C}_{\mathrm{pC}}=15 \mathrm{~J} / \mathrm{mol} \cdot \mathrm{~K}
\end{aligned}
$$

a) (7 points) For a given outlet conversion of $X_{A}=0.5$, how much heat needs to be removed per minute from the system to maintain isothermal reactor operation?
b) ( 5 points) For a given outlet conversion of $X_{A}=0.5$, under adiabatic reactor operation, what is the temperature of the outlet stream?
c) (8 points) Consider if this reaction were carried out in an adiabatic CSTR, what is the required volume of reactor to achieve $\mathrm{X}_{\mathrm{A}}=0.5$ ?
d) (10 points) Now consider if this reaction were to be carried out in an adiabatic PFR. Show graphically whether the volume required to reach $X_{A}=0.5$ will be either higher, lower, or stay the same compared with your answer in part (c). Use a Levenspiel Plot and 2 sentences to give a physical explanation of your comparison. Answers without a correct explanation receive no credit.

## Problem \#3 (30 points)

Consider the elementary, reversible, exothermic liquid-phase reaction:

$$
\mathrm{A} \leftrightarrow \quad \mathrm{~B}
$$

This reaction is carried out in a CSTR equipped with a jacketed heat exchanger. Species A is fed into the reactor with a molar feed rate of $\mathrm{F}_{\mathrm{A} 0}$, temperature $\mathrm{T}_{0}$ and volumetric flow of $\mathrm{v}_{0}$.

Known system parameters:
$\mathrm{V}_{\text {CSTR }}=10 \mathrm{~L}$

$$
\mathrm{C}_{\mathrm{pA}}=\mathrm{C}_{\mathrm{pB}}=10 \mathrm{cal} / \mathrm{mol} \cdot \mathrm{~K}
$$

$\mathrm{v}_{0}=2 \mathrm{~L} / \mathrm{min}$
$\mathrm{F}_{\mathrm{A} 0}=1 \mathrm{~mol} / \mathrm{min}$
$\Delta \mathrm{H}_{\mathrm{rxn}}(@ 360 \mathrm{~K})=-11 \mathrm{kcal} / \mathrm{mol}$ of A
$\mathrm{T}_{\text {ambient }}=315 \mathrm{~K}$
$\mathrm{T}_{0}=340 \mathrm{~K}$
$\mathrm{UA}=40 \mathrm{cal} / \mathrm{min} \cdot \mathrm{K}$

The heat generated term $(\mathrm{G}(\mathrm{T}))$ has already been found and plotted for you.

$$
G(T)=\frac{\tau k}{1+\tau k\left(1+\frac{1}{K_{c}}\right)}
$$


a) (6 points) Write an expression for the heat removal term $R(T)$ as a function of only temperature and numerical values. What is the slope and $x$-intercept?
b) (4 points) Draw $R(T)$ on the plot based on your answer in part (a). Indicate on the plot the location of the steady state operating temperatures. What are these temperatures?
c) (5 points) Suppose you are operating at the middle steady state and suddenly there is a small decrease in the reactor operating temperature due to a surge in the heat exchanger coolant. Explain in 1-2 sentences what you would expect to happen to conversion and temperature after the spike and why.
d) (15 points) You decide to operate your reactor to reach maximum conversion. Keeping all other values the same, what must your new UA be in order to achieve this?

## Problem \#4 (10 points)

Consider the elementary, irreversible, exothermic liquid-phase reaction:

$$
\mathrm{A} \rightarrow \mathrm{~B}
$$

This reaction is carried out in a jacketed steady-state CSTR. Species A is fed into the reactor with a molar feed rate of $\mathrm{F}_{\mathrm{A} 0}$ and volumetric flowrate of $\mathrm{v}_{0}$. Below are given system parameters and a plot of reactor temperature $(\mathrm{T})$ versus feed temperature $\left(\mathrm{T}_{0}\right)$.

Known system parameters:
$\mathrm{V}_{\text {CSTR }}=100 \mathrm{~L}$
$\mathrm{v}_{0}=20 \mathrm{~L} / \mathrm{min}$
$\Delta \mathrm{H}_{\mathrm{rxn}}(@ 350 \mathrm{~K})=-32 \mathrm{~kJ} / \mathrm{mol}$ of A
$\mathrm{UA}=36 \mathrm{~kJ} / \mathrm{min} \cdot \mathrm{K}$
$\mathrm{C}_{\mathrm{pA}}=\mathrm{C}_{\mathrm{pB}}=20 \mathrm{~J} / \mathrm{mol} \cdot \mathrm{K}$
$\mathrm{T}_{\text {ambient }}=300 \mathrm{~K}$
$\mathrm{k}(@ 350 \mathrm{~K})=0.02 \mathrm{~min}^{-1}$
$\mathrm{E} / \mathrm{R}=18000 \mathrm{~K}$

a) (2 points) Initially, you have a feed temperature of 400 K . You increase it 15 K and then drop it 35 K . What temperature is the reactor operating at?
b) (8 points) What is the rate of heat generated per mole of species A for a reactor operating under part (a) conditions?

## Problem \#5 (25 points)

A chemical engineer equipped with only an accurate thermometer and a stopwatch is charged with determining the rate constant, $\mathbf{k}$, of an exothermic, elementary reaction:

$$
\mathrm{A} \rightarrow \mathrm{~B}
$$

This reaction occurs in a liquid phase, wall-cooled, BSTR. The approach of the chemical engineer is to measure the initial rate of temperature change with respect to time (ie. at very low conversions), such that the system acts as in a differential-reactor regime. The reactor is initially charged with pure A and is at a temperature $\mathrm{T}_{0}$. Assume the same molar volume for liquid-phase $A$ and $B$.

Known system parameters:
$\mathrm{V}_{\mathrm{BSTR}}=1 \mathrm{~m}^{3}$

$$
\Delta \mathrm{H}_{\mathrm{rxn}}\left(@ 25^{\circ} \mathrm{C}\right)=-100 \mathrm{~J} / \mathrm{mol} \text { of } \mathrm{A} \quad \mathrm{C}_{\mathrm{pB}}=25.90 \mathrm{~J} / \mathrm{mol} \cdot{ }^{\circ} \mathrm{C}
$$

$$
\mathrm{UA}=25 \mathrm{~W} /{ }^{\circ} \mathrm{C}
$$

$$
\mathrm{T}_{\text {ambient }}=25^{\circ} \mathrm{C}
$$

$$
\begin{aligned}
& \mathrm{C}_{\mathrm{pA}}=25.00 \mathrm{~J} / \mathrm{mol} \cdot{ }^{\circ} \mathrm{C} \\
& \mathrm{C}_{\mathrm{pB}}=25.90 \mathrm{~J} / \mathrm{mol} \cdot{ }^{\circ} \mathrm{C} \\
& \mathrm{~T}_{0}=125{ }^{\circ} \mathrm{C} \\
& \mathrm{~N}_{\mathrm{A} 0}=\text { moles of A in reactor initially }=12500 \mathrm{~mol}
\end{aligned}
$$

a) (5 points) Write an expression for $-\mathrm{r}_{\mathrm{A}} \mathrm{V}$ under these differential conditions in terms of k , and parameters provided above.
b) (20 points) Using the measured rate of temperature change given by:

$$
\frac{d T}{d t}_{\text {initial }}=0.01^{\circ} \mathrm{C} / \mathrm{s}
$$

calculate k at $125^{\circ} \mathrm{C}$.

