CBE3223 – Kinetics and Reactor Design

Final Exam

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Please be sure to print your name, Net ID #, instructor, the subject "CBE-UY-3223", and the date on the first page of your examination solution. Please be sure to upload all your solutions as a single electronic file (including any derivations, explanations, or calculated answers).

This is an untimed exam that must be submitted within 24 hours. Please note that you are expected to complete all solutions, from scratch to final draft, on your own and within the 24-hour window. You are expected to follow the **NYU Tandon Student Code of Conduct** and **NYU's Policy on Academic Integrity for Students**. You are not allowed to communicate the questions or any solutions to this examination with anyone until after the completion of the 24-hour window, i.e., not until after 1pm ET on May 13, 2021.

If you have any questions for clarification while taking the examination, then you may either chat with the instructor in Zoom during the 120 min examination period that begins at 1pm ET on May 12, 2021, or you may email the instructor outside this time but within the 24-hour window.

Problem	%
1	15
2	10
3	10
4	20
5	15
6	5
7	10
8	15
9	4
Total	**104**

1. The elementary gas-phase reaction,

$$A + B \leftrightarrow 2C$$
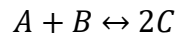
is carried out in a packed-bed reactor with no pressure drop in which the feed is equimolar in A and B.

a. **(5%)** Derive an expression for the equilibrium conversion, X_e, solely as a function of the equilibrium concentration constant, K_C.

b. **(5%)** Given that $K_C = 1200$ @ 305 K and $\Delta H_{Rx} = -15$ kcal/mol, sketch the trend of X_e as a function of the temperature for a feed temperature of 315 K if $C_{PA} = C_{PB} = C_{PC}$.

c. **(5%)** On the same graph, identify the adiabatic equilibrium conversion and the adiabatic equilibrium temperature when $C_{Pi} = 25$ cal/mol/K.

2. **What's wrong with these codes?** Shown below are excerpts of MATLAB codes for four different reactor designs for an elementary, reversible isomerization in which pure A is fed to each reactor. Identify the reactor type, the heat exchange method, and any errors in each code.

A. (2.5%)

```
% Explicit equations
Cao = 2.0;
k = 16.1 * exp(E / R * (1 / 350 - 1 / T));
Kc = 5.07 * exp(dH / R * (1 / 315 - 1 / T));
raprime = 0 - (k * Cao * (1 - ((1 + 1 / Kc) * X)));
Xe = Kc / (1 - Kc);
CPo = 147;
dH = -33400;
FAo = 20.0;
Ua = 5000*0;
m = 500;
Cpc = 31;
E = 65000;
R = 8.314;
rhob = 1.9;
alpha = 0.0002;
epsilon = 0;
To = 320;
% Differential equations
dTadW = Ua * (T - Ta) / (m * Cpc);
dTdW = (raprime * dH - (Ua / rhob * (T - Ta))) / (CPo * FAo);
dXdW = 0 - (raprime / FAo);
dpdW = 0 - alpha / 2 / p * (1 + X) * (T / To);
```

B. (2.5%)

```
% Explicit equations
Cao = 2.0;
k = 16.1 * exp(E / R * (1 / 350 - 1 / T));
Kc = 5.07 * exp(dH / R * (1 / T - 1 / 315));
ra = 0 - (k * Cao * (1 + ((1 + 1 / Kc) * X)));
Xe = Kc / (1 + Kc);
CPo = 147;
dH = -33400;
FAo = 20.0;
Ua = 5000;
m = 500;
Cpc = 31;
E = 65000;
R = 8.314;
% Differential equations
dTadV = Ua * (T - Ta) / (m * Cpc);
dTdV = ((Ua * (T - Ta)) - ra * dH) / (CPo * FAo);
dXdV = 0 - (ra / FAo);
```

C. (2.5%)

```
% Explicit equations
Cao = 2.0;
k = 16.1 * exp(E / R * (1 / 350 - 1 / T));
Kc = 5.07 * exp(dH / R * (1 / 315 - 1 / T));
ra = 0 - (k * Cao * ((1 + 1 / Kc) * X));
Xe = Kc / (1 + Kc);
CPo = 147;
dH = -33400;
FAo = 20.0;
Ua = 5000;
m = 500;
Cpc = 31;
E = 65000;
R = 8.314;
% Differential equations
dTadV = 0* Ua * (T - Ta) / (m * Cpo);
dTdV = (ra * dH - ((T - Ta))) / (CPo * FAo);
dXdV = 0 - (ra / FAo);
```

D. (2.5%)

```
% Explicit equations
Cao = 2.0;
k = 16.1 * exp(E / R * (1 / 350 - 1 / T));
Kc = 5.07 * exp(-dH * (1 / 315 - 1 / T));
raprime = 0 - (k * Cao * (1 - ((1 + 1 / Kc) * X)));
Xe = Kc / (Kc - 1);
CPo = 147;
dH = -33400;
FAo = 20.0;
Ua = 5000;
m = 500;
Cpc = 31;
E = 65000;
R = 8.314;
rhob = 1.9;
alpha = 0.0002;
epsilon = 0;
To = 320;
% Differential equations
dTadW = Ua / rhob * (Ta - T) / (m * Cpc);
dTdW = (raprime * dH - (Ua / rhob * (T - Ta))) / (CPo * FAo);
dXdW = 0 - (raprime / FAo);
dpdW = 0 - alpha / 2 * (1 + epsilon * X) * (T / To);
```
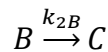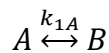
3. **(10%)** The elementary liquid phase reactions,

$$A \overset{k_{1A}}{\longleftrightarrow} B$$

$$B \overset{k_{2B}}{\longrightarrow} C$$

take place in a CSTR. Derive an expression for G(T) as a function of C_{A0}, k_{1A}, k_{2B}, K_C, τ, ΔH_{Rx1A}, and ΔH_{Rx2B}. HINT: lump together parameters and define,

$$Y = \left(\frac{\tau k_{1A}}{1 + \tau k_{2B} + \dfrac{\tau k_{1A}}{K_C}} \right) \left(\frac{1}{1 + \tau k_{1A}} \right)$$

4. Let's revisit Living Example Problem 12-6 discussed in Chapter 12.

   a. **(10%)** What would be the new overall selectivity $\tilde{S}_{B/C}$ if the heat exchanger suddenly failed while operating at the maximum overall selectivity?

   b. **(5%)** If the autoignition temperature of the reaction solvent is 550°C, then should the operators be concerned of a possible explosion? Please explain your answer.

c. **(5%)** What would be the maximum overall selectivity $\tilde{S}_{B/C}$ for safe operation of the reactor without any heat exchanger?

5. Let's revisit the T2 Laboratories explosion discussed in Chapter 13 (Living Example Problem 13-6). Please answer the following questions and be sure to use equations and calculations to justify your answers. [HINT: Run the simulation and use the conditions at 3 hours of reaction time].

   a. **(5%)** Would the explosion have occurred had the operators used an inert solvent instead of diglyme?

   b. **(5%)** What if the diglyme was diluted by half its initial concentration with an inert solvent? Would the explosion have occurred?

   c. **(5%)** Would the explosion have occurred had the operators been able to get the heat exchanger working after 3 hours of adiabatic operation?

6. **(5%)** The conversion from an adiabatic PBR is shown below as a function of temperature.
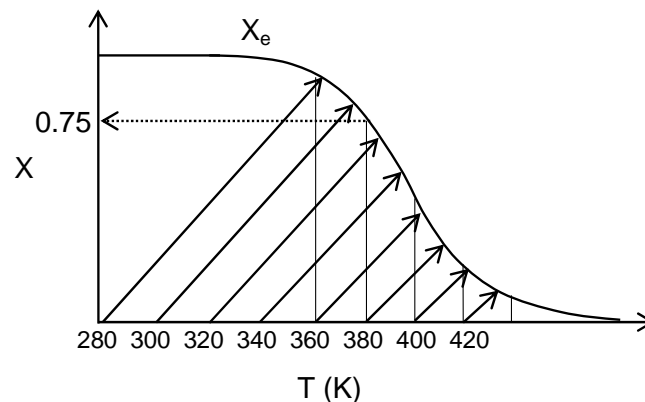
Which of the following statements are **TRUE**? Circle the correct statement(s).

   A. The reaction could be a first order endothermic reaction carried out with a very large heat exchanger attached to the reactor.
   B. If the reaction is carried out adiabatically in a CSTR, the ratio $F_{A0}/(-r_A)$ will decrease and then increase as the conversion increases.
   C. For a small but fixed reactor length, one is more likely to achieve the maximum conversion for an entering temperature of 420 K than an entering temperature of 280 K.
   D. 75% conversion could be achieved for a first order reaction by adding a very large heat exchanger on the PBR with a very large area for an entering temperature of 380 K.
   E. 75% conversion could be achieved for a first order reaction by increasing the inerts by a factor of 100 or greater for an entering temperature of 400 K.

7. **(10%)** The following elementary, liquid-phase reaction is carried out in a CSTR with a heat exchanger:

$$A \leftrightarrow B$$

Should the operators be concerned of a possible runaway reaction if the reactant feed was suddenly shutoff while operating at a steady-state temperature of 393.7 K? Assume the feed consists of pure A, neglect any shaft work, the volume of the liquid does not change, the coolant mass flow rate is very high, and the conversion X = 0.457 at the time the feed was shutoff.

Additional information:
  $k = 1.0$ min^{-1} at 375 K
  $E = 40,000$ cal/mol
  $K_C = 100$ at 375 K
  $\Delta H_{Rx}^o = -75,000$ cal/mol
  $N_{A0} = 100$ mol
  $T_a = 310$ K
  $UA = 3,700$ cal/min/K
  $C_{PA} = C_{PB} = 40$ cal/mol/K

8. **(15%)** Please indicate whether each of the following statements is true ("T"), false ("F"), or that one can't tell from the information given ("CT"). Please write the correct answer on your answer sheet. **[2.5% for each correct answer].**

  T   F   CT   Consider the reversible endothermic adiabatic reaction, A $\leftrightarrow$ B, carried out in a PFR. Decreasing the feed temperature using a heat exchanger will increase the adiabatic temperature and conversion.

  T   F   CT   Failure to account for the heat of mixing of reactants could result in overestimation of an adiabatic batch reactor temperature, which could lead to a runaway reaction.

  T   F   CT   The temperature at which a fraction-of-a-degree decrease results in a dropdown to a lower stable steady-state is called the extinction temperature.

  T   F   CT   A heat exchange failure in a semi-batch reactor fitted with a cooling jacket, in which an exothermic reaction takes place, will lead to a run-away reaction.

  T   F   CT   Consider an exothermic irreversible reaction carried out in a laminar flow reactor with a heat exchanger. Decreasing the overall heat transfer coefficient may result in an increase in the conversion near the reactor's wall.

  T   F   CT   Lack of knowledge of the reaction chemistry and temperature control problems are among the leading causes of accidents with batch reactors in chemical manufacturing.

9. **(4%) Extra credit:** Derive an expression for the equilibrium constant $K_C(T)$ solely as a function of $K_C(T_1)$, ΔC_P, $\Delta H_{Rx}^o(T_R)$, T, T_1, T_R, and the gas constant R for the following reaction:

$$2A + B \leftrightarrow C$$