Chemical Kinetics and Reaction Engineering

MIDTERM EXAMINATION II
Friday, April 9, 2010

The exam is 100 points total and 20% of the course grade.

Please read through the questions carefully before giving your response.

Question Number	Your Points	Possible Points
1		40
2		30
3		30
Total		100

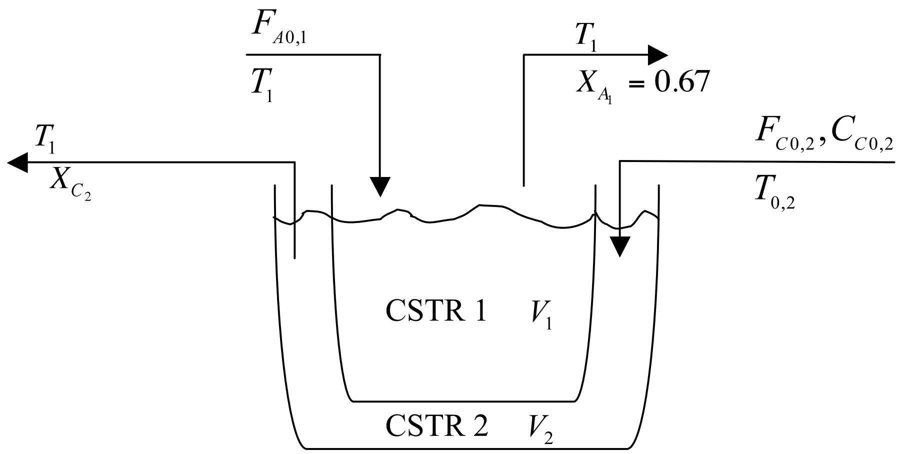
Name:____

SID:____

You are allowed one 8.5" x 11" sheet of paper and a calculator for this exam.

Problem 1 CSTRs in Thermal Equilibrium (40 points)

Two steady-state, liquid-phase CSTRs are placed in thermal equilibrium with each other, meaning that heat transfer is so rapid between the two reactors that both are at a fixed temperature T_1. The overall system comprising both CSTR 1 and CSTR 2 is adiabatic meaning that there is no heat transfer to the external surroundings.



In CSTR 1, the following elementary, exothermic reaction takes place:

$$A \xrightarrow{k_1} B \qquad \Delta H^0_{R1} = -50\,\text{kJ mol}^{-1};\ k_1 = 0.4\ \text{min}^{-1} \text{ at } 425\ \text{K}$$

Pure A enters CSTR 1 at a molar rate $F_{A0,1}$ = 50 mol min^{-1}, and temperature T_1.

In CSTR 2 ($V_2 = 100\ L$), the following elementary, endothermic reaction takes place:

$$C \xrightarrow{k_2} D \qquad \Delta H^0_{R2} = 25\,\text{kJ mol}^{-1};\ k_2 = 0.5\ \text{min}^{-1} \text{ at } 425\ \text{K}$$

Pure C ($C_{C0,2}$ = 3 mol L^{-1}) enters CSTR 2 at a molar rate $F_{C0,2}$, and temperature $T_{0,2}$.

All species have a heat capacity C_p = 45 J mol^{-1} K^{-1} that is independent of temperature. Neglect any shaft work for both CSTRs.

(a) If CSTR 2 is operated isothermally ($T_{0,2} = T_1$), what must be the inlet molar flow rate $F_{CO,2}$? (15 points)

(b) Suppose now that $T_{0,2} < T_1$. Write the equation that is needed to solve for the new inlet molar flow rate $F_{CO,2}$ such that both reactors are maintained at a steady-state temperature T_1, in terms of variables provided above. ***Do not solve*** ***– just write the single equation that can be used to solve for*** $F_{CO,2}$. How do you expect $F_{CO,2}$ to change qualitatively compared to part (a)? Explain why in one sentence – longer answers will be penalized (25 points)

Problem 2 Wall-Cooled Differential Reactor (30 points)

The following gas-phase elementary reaction,

$2B \rightarrow C$ $\qquad\qquad$ $k = A \exp\left(-\frac{E_a}{RT}\right)$

is to be carried in a isobaric wall-cooled, steady state differential reactor. Reactant B is fed to the reactor at a temperature T_0, a molar flow rate F_{B0}, and a volumetric flow rate ν_0. The conversion of B is X=0.01, and the temperature of the outlet stream is T. The pre-exponential factor, A, and activation energy, E_a, are known for this reaction. Also, the reaction is highly exothermic, with a known enthalpy of reaction of ΔH^0_{rxn}.

Due to the differential nature of the reactor, there are no temperature gradients in the system. That is to say, the temperature is uniform throughout the reactor at a value of T. The heat transfer coefficient of the reactor is UA, and the heat capacities are $C_{P,B}$ and $C_{P,C}$, where $C_{P,C}=2C_{P,B}$.

(a) Derive an expression for the residence time, τ_0, of the reactor in terms of variables given in the problem statement. (10 points)

(b) Would your expression for part (a) be the same if $X = 0.9$? Explain in less than 2 sentences. (10 points)

(c) What is the temperature of the cooling fluid, T_{amb}, required to operate under the conditions in part (a)? Express your answer in terms of variables given in the problem statement. Also, sketch a plot of T_{amb} vs. ΔH^0_{rxn}, and provide an expression for the intersection of the curve with the y-axis (10 points)

Problem 3 Surface-Catalyzed Reaction (30 points)

For the overall reaction A + B → ½ D, consider the following mechanism for a surface catalyzed reaction:

		$\underline{\sigma_i}$
(1)	$A + S \xleftrightarrow{K_A} A{*}S$	1
(2)	$A{*}S + B \xleftrightarrow{K_B} C{*}S$	1
(3)	$2\,C{*}S \xrightarrow{k_C} D{*}S + S$	½
(4)	$D{*}S \xleftrightarrow{K_D} D + S$	1

where S represents vacant surface sites, A*S, C*S and D*S represent surface-bound intermediates, and A, B and D represent stable gas-phase species. Step (3) in the series is irreversible, while all other reactions in the series are quasi-equilibrated. The total surface concentration of sites of the catalyst is known and is C_T.

a) Derive an expression for the rate of reaction in terms of readily measurable quantities P_A, P_C, P_D, C_T and appropriate equilibrium and rate constants. (15 points)

b) What is the rate expression if S is the most abundant surface intermediate (MASI)? (7.5 points)

c) If C*S is MASI, then the overall reaction rate is $r = 2k_c K_B K_A P_B P_A C_T$. In this case, derive an expression for the apparent activation energy of the system, $E_{app,}$ in terms of the activation energies and heats of adsorption of the relevant reaction steps and components, respectively. (7.5 points)