Chemical Kinetics and Reaction Engineering

MIDTERM EXAMINATION II
Friday, April 17, 2009

The exam is 110 points total and 20% of the course grade.

Please read each question carefully.

*Only answers written in the **blue book** will be graded.*
(Except for any work shown in the graph for problem 1c)

Question Number	Your Points	Possible Points
1		40
2		35
3		35
Total		110

Name:____

SID:____

Problem 1 (40 points)

Please provide concise answers (and explanations) to these three unrelated (to each other) questions:

(a) The following endothermic, reversible gas-phase reaction occurs in a plug-flow reactor of volume V, with a pure A inlet stream entering at a fixed v_0, C_{A0}, T_0 and P_0:

$$\boldsymbol{2A \rightleftarrows 2B + C} \qquad\qquad \Delta H_R, C_{Pj} \neq f(T)$$

The PFR operates isothermally at T_0 and isobarically at P_0. Explain how and why the equilibrium conversion would change in the following cases:

(i) The PFR is operated isothermally at T_0 but is filled with an inert packing that results in a significant pressure drop across the reactor. *(5 points)*

(ii) The PFR is operated isobarically at P_0 and adiabatically. *(5 points)*

(b) Comment (in <200 words and perhaps a couple of useful equations) about what the long-chain approximation (LCA) is and why it is a reasonable approximation, for what types of reactions it is applicable, and how it is implemented to simplify rate equations that are derived from sequences of elementary steps. *(10 points)*

(c) Consider the liquid-phase reaction: $\boldsymbol{A + B \rightarrow C}$

$$\Delta H_R = -5\ kJ/mol$$

$$C_{PA} = 7\ J/mol\text{-}K \qquad C_{PB} = 3\ J/mol\text{-}K \qquad C_{PC} = 10\ J/mol\text{-}K \qquad C_{Pj} \neq f(T)$$

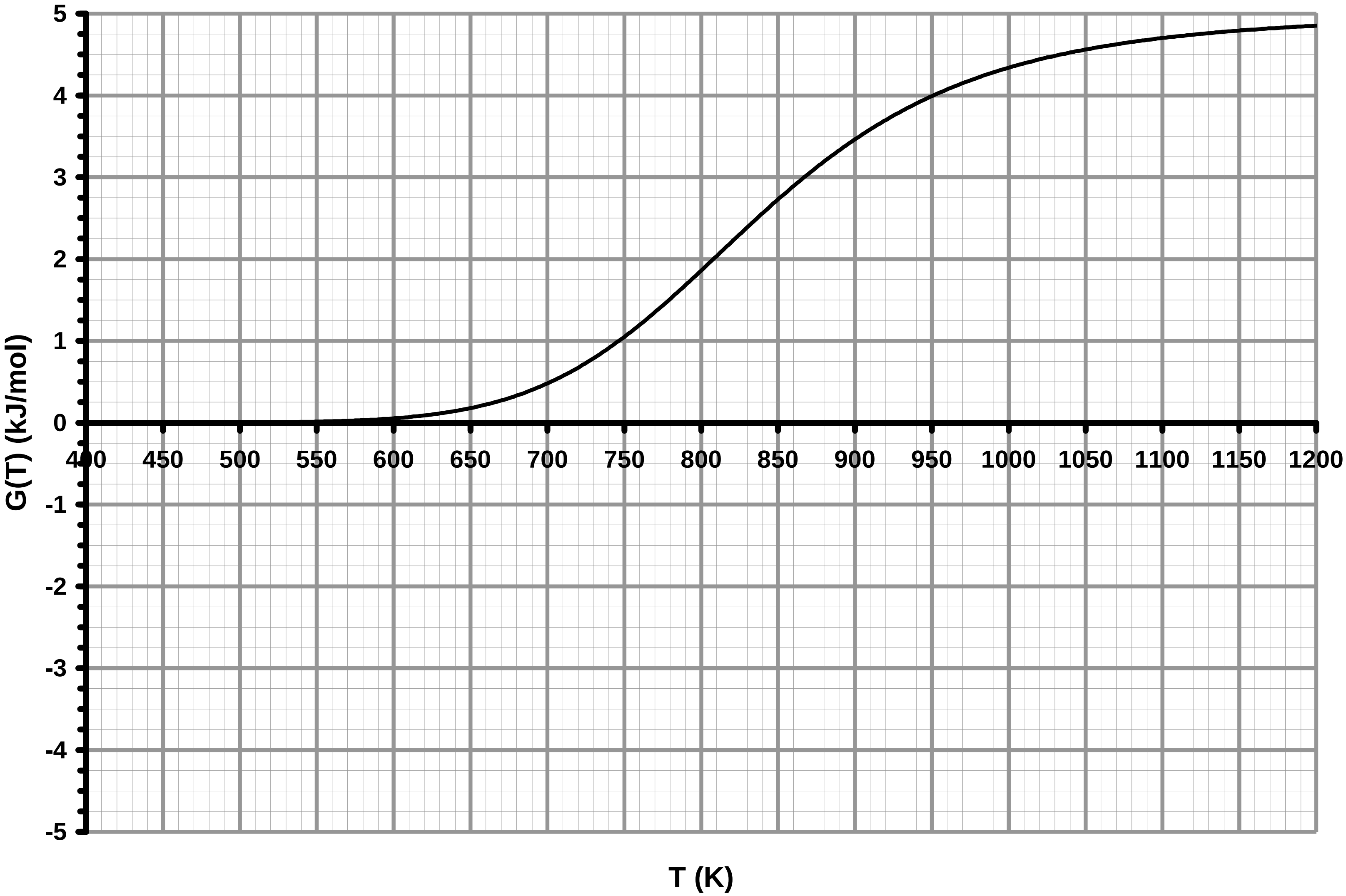
This reaction occurs in a wall-cooled CSTR ($V=10\ dm^3$), with $UA = 10\ W/K$ and $T_a = T_0$. The inlet stream is an equimolar mixture of A and B, entering at $v_0 = 100\ dm^3/min$ and $F_{T0} = 10\ mol/s$.

Use the G(T) plot (provided on the next page) to answer the following questions:

(i) Determine the extinction and ignition temperatures (provide numbers) when the coolant is shut off and the reactor becomes adiabatic. On the plot, draw and label the R(T) curves for ignition and extinction and circle the bifurcation points. *(10 points)*

(ii) Sketch a G(T) curve for an endothermic reaction on the plot and show (explain) whether multiple steady-states are possible in this case. *(5 points)*

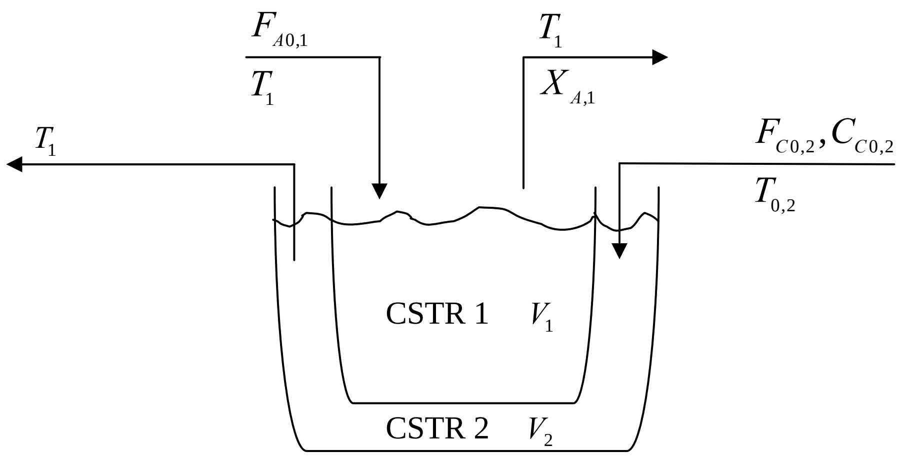
(iii) If the coolant is turned on, does the extinction temperature increase or decrease? Why? *(5 points)*



G(T) (kJ/mol)
5
4
3
2
1
0
-1
-2
-3
-4
-5
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050
1100
1150
1200
T (K)

Problem 2 (35 points)

Two CSTRs are placed in perfect thermal contact with each other and have no other heat transfer to the surroundings.



In CSTR 1, the following elementary, ***liquid-phase*** reaction takes place:

$A \xrightarrow{k_1} B$ $\Delta H^0_{R1} = -50\,\text{kJ mol}^{-1}$; k_1 = 0.5 min^{-1} at 500 K

Pure A enters CSTR 1 at a molar rate $F_{A0,1}$ = 100 mol min^{-1}, and temperature T_1 = 500 K. The reactor is isothermal at T_1 with a residence time τ_1 = 2 min.

In CSTR 2 ($V_2 = 100\ L$), the following elementary, ***liquid-phase*** reaction takes place:

$C \xrightarrow{k_2} D$ $\Delta H^0_{R2} = 25\,\text{kJ mol}^{-1}$; k_2 = 1 min^{-1} at 500 K

Pure C ($C_{C0,2} = 5\ mol/L$) enters CSTR 2 at a molar rate $F_{C0,2}$, and temperature $T_{0,2}$. The reactor is held at the same temperature T_1.

All species have a heat capacity C_p = 30 J/mol-K $\neq f(T)$.

(a) Determine the conversion of A in the exit stream of CSTR 1. *(5 points)*

(b) When CSTR 2 is operated isothermally ($T_{0,2} = T_1$), determine the inlet molar rate of C to CSTR 2 that is required to hold both reactor temperatures at T_1. *(20 points)*

(c) Suppose that the inlet temperature for CSTR 2 has decreased ($T_{0,2} < T_1$). Write the equation, only in terms of variables provided above, needed to solve ***(but do not solve)*** for the new inlet molar rate of C required to maintain both reactor temperatures at T_1. How will the inlet molar rate of C change compared to part (b)? Why? *(10 points)*

Problem 3 (35 points)

A gas-phase catalytic reaction ($A_2 \longrightarrow 2B$) proceeds in a PFR via the elementary steps:

$A_2 + 2S \rightleftarrows A-S + A-S$	K_1; quasi-equilibrated
$A-S \longrightarrow B-S$	k_2; irreversible
$B-S \rightleftarrows B+S$	k_3, k_{-3}; reversible

(a) Derive a rate equation for the rate of formation of B in terms of gas-phase concentrations (or pressures) of A_2 and B for the case of step 3 reversible but not quasi-equilibrated. *(15 points)*

(b) Simplify the equation in (a) for the case of (A-S) and (B-S) as MASI and step 3 in quasi-equilibrium. *(10 points)*

(c) An irreversible side reaction ($A-S+A-S \longrightarrow C+2S$) forms the undesired product C with a rate constant k_4. The selectivity is defined as r_B/r_C. *(10 points)*

(i) Would recycle in the PFR increase or decrease selectivity? Why?

(ii) The activation energy for step 2 is higher than for step 4 and B and C both form via exothermic reactions. Would an adiabatic or an isothermal reactor (at the same inlet temperature) give a higher selectivity? Why?

(iii) The selectivity increases with increasing concentration of B. Why?