Instructions

1. Write your name at the top of each answer sheet and on the front page of the exam questions.
2. Start each problem at the top of a new page.
3. The exam consists of three equally weighted problems.
4. Useful integrals and equations are listed beginning on page 5.
5. Return the exam questions or you will receive a grade of zero.

R = 82.06 cm^3-atm/gmole-K; R = 1.987 cal/gmole-K

The van't Hoff relation is $\frac{\partial \ln K}{\partial T} = \frac{\Delta H^\circ}{RT^2}$

Problem 1

An adiabatic CSTR with a first-order, liquid-phase reaction

$$\mathrm{A} \longrightarrow \mathrm{B}, \qquad r = kc_A \tag{1}$$

operates at the conditions shown below

Parameter	Value	Units
T_f	298	°K
c_{Af}	3.5	kmol/m^3
Q_f	60×10^{-6}	m^3/s
ΔH_R	-2.09×10^8	J/kmol
$\hat{C}_p$	4.19×10^3	J/kg °K
ρ	10^3	kg/m^3
V_R	18×10^{-3}	m^3
k	$4.48 \times 10^6 \quad \exp(-7550/T)$	s^{-1}; T in °K

One of the steady-state operating temperatures is 341.1 K. Determine if this is stable or unstable.

Problem 2

An adiabatic plug flow reactor is used for the reversible gas phase reaction.

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{B} \tag{2}$$

where

$$r_1 = k_1 c_A \qquad k_1 = A_1 \exp(E_1/RT) \qquad r_{-1} = k_{-1} c_B$$

The kinetic constants, thermodynamic data and inlet conditions are listed below. You may assume the heat capacity and heat of reaction are independent of temperature.

Item	Units	Value
A_1	$\sec^{-1}$	5×10^{13}
E_1	cal/gmol-K	33,112
A_{-1}	$\sec^{-1}$	3.6×10^{22}
E_{-1}	cal/gmol-K	58,112
ΔH_R	cal/gmol	-25,000
C_{pA}	cal/gmol-K	63
C_{pB}	cal/gmol-K	63
C_{pI}	cal/gmol-K	100
Q_f	cm^3/sec	3880
T_f	K	473
N_{Af}	gmol/sec	0.10
P	atm	1

The molar flowrates of A and B (N_A and N_B) are plotted in Figure 1 and the temperature is plotted in Figure 2 versus reactor volume as increasing amounts of an inert are added to the feed. The inert is added as a fraction of the inlet molar flowrate of A where this fraction ranges from 0.0 to 0.6. Note that the molar flowrates of A and B cross each other when the fraction is 0.4, such that the final molar flowrate of B is greater than the final molar flowrate of A. Using the data listed above, and supported by calculations you deem appropriate, and Figures 1 and 2 answer the following questions.

(a) Why does the curve for N_A decrease and reach a different constant value as the fraction of inert is increased from 0.00 to 0.40?

(b) Why does the volume for N_A to reach the constant value increase as the fraction of inert is increased from 0.00 to 0.40?

(c) Do you think the curve corresponding to a fraction of 0.60 for N_A will reach a constant value? Why?

(d) Why does the maximum reactor temperature decrease as the fraction of inert is increased from 0.00 to 0.40?

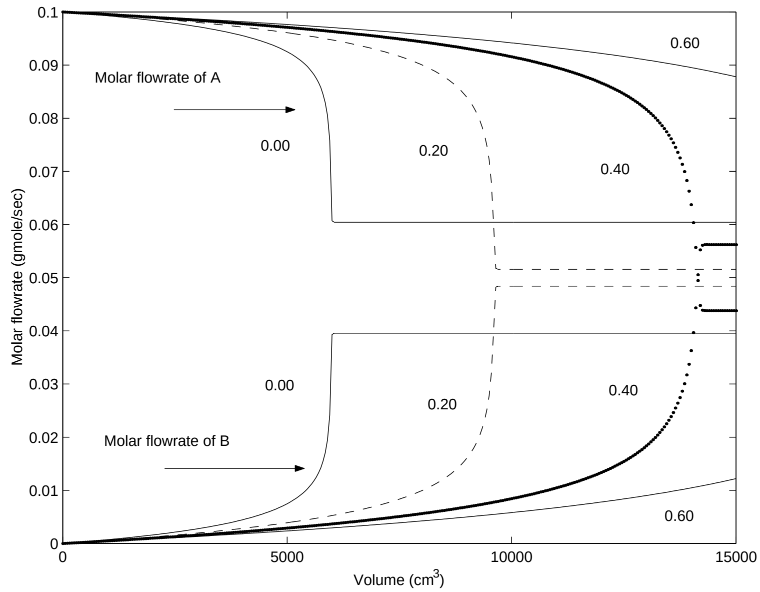

Figure 1: Molar flowrates of A and B versus reactor volume for increasing multiples of inert, i.e. the curve labeled 0.20 refers to $N_{If} = 0.02 \times N_{Af}$.

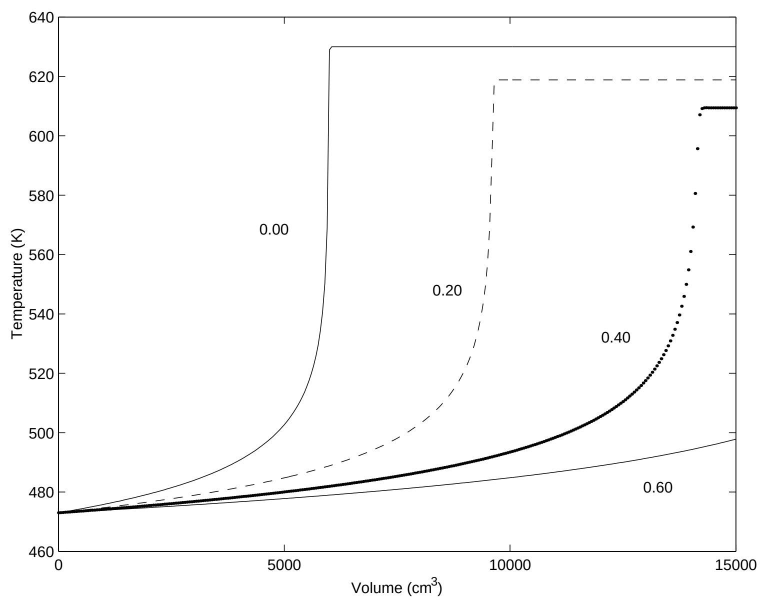

Figure 2: Temperature versus volume for increasing multiples of inert, i.e. the curve labeled 0.20 refers to $N_{If} = 0.02 \times N_{Af}$.

Problem 3

The reaction

$$H_2 + Br_2 \rightleftharpoons 2HBr$$

serves as one of the classics to illustrate how statements of mass action, such as listed above, actually proceed by a series of elementary reactions. Use the mechanism of elementary reactions presented below and the concepts developed in the text and in class to show that the rate of HBr formation (R_{HBr}) is given by

$$R_{\mathrm{HBr}} = \frac{k c_{H_2} c_{Br_2}^{0.5}}{1 + k' \frac{c_{HBr}}{c_{Br_2}}}$$

where k and k' are effective rate constants **AND** relate these effective rate constants to the rate constants for the individual elementary reactions. Note the first reaction, which is reversible, cannot be treated as at equilibrium. Also, Br and H atoms are reaction intermediates. List any assumptions you make,

$$Br_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2Br$$

$$Br + H_2 \xrightarrow{k_2} H + HBr$$

$$H + Br_2 \xrightarrow{k_3} Br + HBr$$

$$H + HBr \xrightarrow{k_4} H_2 + Br$$