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 6.
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

The gas phase, first-order reaction

$$\mathrm{A} \longrightarrow \mathrm{B} + \mathrm{C} \qquad r = kc_A \qquad k = 14.2 \ \mathrm{sec}^{-1}$$

will be carried out in a constant pressure, isothermal plug flow reactor. The feed is pure A at a temperature of 525 K and a molar flowrate of $N_{Af} = 140$ gmol/s. The reactor volume is $V_R = 1 \times 10^6$ cm^3.

(a) By what percentage does the conversion of A change if the pressure is increased from 1.25 atm to 2.50 atm?

(b) Does your answer to the first part make sense? Please explain.

Problem 2

An adiabatic batch reactor is used for the liquid phase reaction.

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

where

$$r = k_1 c_A - k_{-1} c_B \qquad k_1 = A_1 \exp(-E_1/RT) \qquad k_{-1} = A_{-1} \exp(-E_{-1}/RT)$$

The kinetic constants, thermodynamic data and initial conditions are listed below. You may assume the heat capacity and heat of reaction are independent of temperature and that the density is constant.

Item	Units	Value
A_1	hr^{-1}	75.96×10^{15}
E_1	cal/gmol	30,400
A_{-1}	hr^{-1}	48.45×10^{17}
E_{-1}	cal/gmol	33,600
ΔH_R	cal/gmol	-12,700
$\hat{C}_p$	cal/g-K	0.25
T_o	K	358
ρ	$\mathrm{g/cm^3}$	0.9
c_{Ao}	$\mathrm{gmol/cm^3}$	5×10^{-3}

The concentrations of A and B (c_A and c_B) are plotted in Figure 1 and the temperature is plotted in Figure 2 versus reactor time.

(a) Develop a relationship that allows you to compute the reactor temperature versus the concentration of A. Using this, compute the temperature when $c_A = 3.5 \times 10^{-3}$ $\mathrm{gmol/cm^3}$.

(b) Why to do the curves for the concentration reach a constant value after about 5 hours?

(c) Why does the temperature increase to a constant value after about 5 hours?

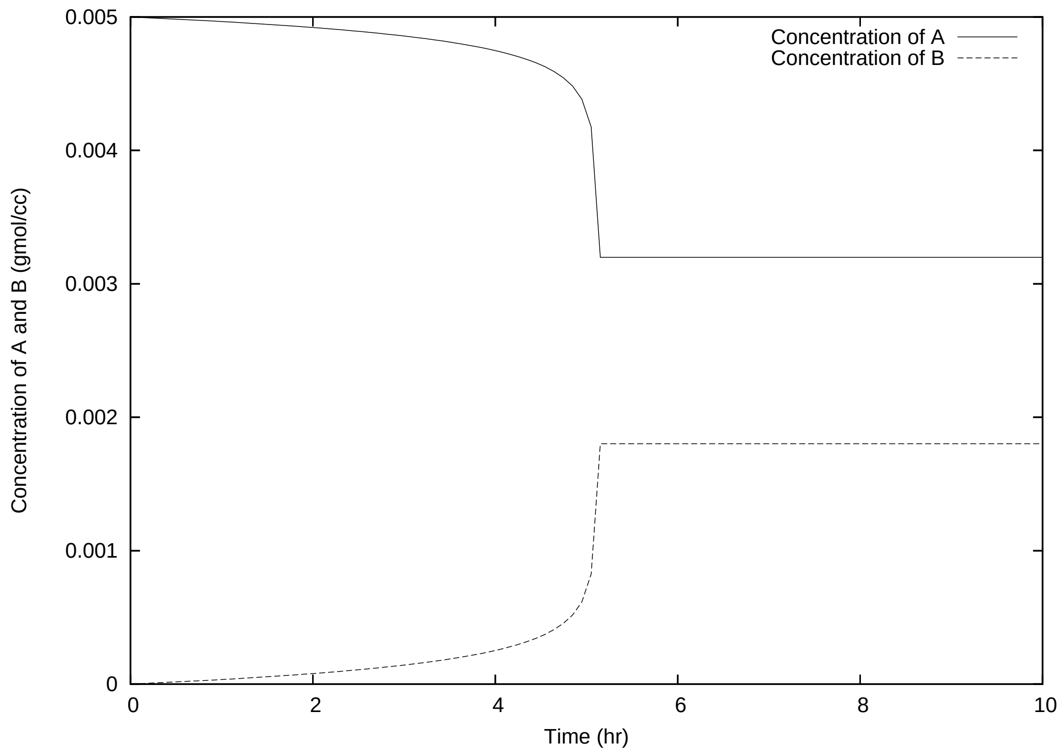

Figure 1: Concentration of A and B versus time

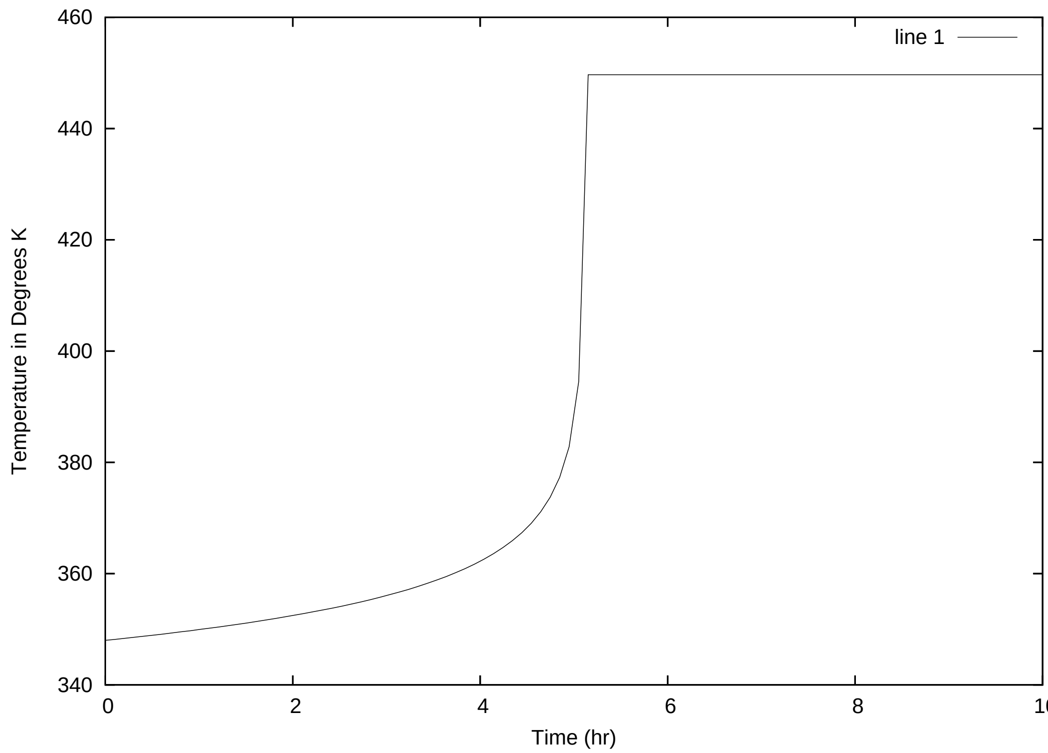

Figure 2: Temperature versus time

Problem 3

Consider the liquid phase reaction in a nonadiabatic, nonisothermal CSTR.

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C}$$

$$r = \left(16.96 \times 10^{12} \times \exp\left(\frac{-32,400\mathrm{Btu/lbmole}}{RT}\right)\mathrm{hr}^{-1}\right) \times c_A$$

For the reactor conditions listed below, the reactor operates at 570 R. Determine if this is a stable operating condition. You may assume the thermodynamic properties do not change with temperature.

Compound	C_p (Btu/lbmole-F)	H_f (Btu/lbmole)
A	35	-66,600
B	16	-123,000
C	46	-226,000
Inert	19.5	-

Variable	Value
V_R	40.1 ft^3
Q_f	326.34 ft^3/hr
T_a	55 F
U	80 Btu/hr-ft^2-F
A	30 ft^2
N_{Af}	43.03 lbmole/hr
N_{Bf}	802.8 lbmole/hr
N_{Cf}	0 lbmole/hr
N_{If}	71.87 lbmole/hr
T_f	75 F

Batch Reactor

$$\frac{d(V_R c_j)}{dt} = \sum_{i}^{n_{rxns}} \nu_{ij} r_i V_R$$

$$\frac{dT}{dt} = \frac{UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R}{V_R \sum_j^{n_{components}} c_j C_{pj}}$$

Plug Flow Reactor

$$\frac{d(Qc_j)}{dV} = \sum_{i}^{n_{rxns}} \nu_{ij} r_i$$

$$\frac{dT}{dV} = \frac{\frac{2}{R} U(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri}}{Q \sum_j^{n_{components}} c_j C_{pj}}$$

Stirred Tank Reactor

$$\frac{d(V_R c_j)}{dt} = Q_f c_{jf} - Q c_j + \sum_{i}^{n_{rxns}} \nu_{ij} r_i V_R$$

$$\frac{dT}{dt} = \frac{UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R + Q_f \sum_j^{n_{components}} c_{jf}(H_{jf} - H_j)}{V_R \sum_j^{n_{components}} c_j C_{pj}}$$

Continuous Stirred Tank Reactor (constant phase)

$$0 = Q_f c_{jf} - Q c_j + \sum_{i}^{n_{rxns}} \nu_{ij} r_i V_R$$

$$0 = UA(T_a - T) - \sum_{i}^{n_{rxns}} r_i \Delta H_{Ri} V_R + \sum_{j}^{n_{components}} Q_f c_{jf} \int_T^{T_f} C_{pj} dT$$

$$\int \frac{1}{a+bx}dx = \frac{1}{b}\ln(a+bx)$$

$$\int (a+bx)^n\,dx = \frac{(a+bx)^{n+1}}{(n+1)b} \qquad ;n \neq -1$$

$$\int \frac{dx}{(a+bx)(a'+b'x)} = \frac{1}{ab'-a'b}\ln\left(\frac{a'+b'x}{a+bx}\right)$$

$$\int \frac{a+bx}{a'+b'x}dx = \frac{bx}{b'} + \frac{ab'-a'b}{b'^2}\ln(a'+b'x)$$

$$\int \frac{(a+bx)^m}{(a'+b'x)^n}dx = \frac{-1}{(n-1)b'}\left[\frac{(a+bx)^m}{(a'+b'x)^{n-1}} - mb\int \frac{(a+bx)^{m-1}}{(a'+b'x)^{n-1}}dx\right]$$

$$\int x^m(a+bx)^n\,dx = \frac{x^{m+1}(a+bx)^n}{m+n+1} + \frac{an}{m+n+1}\int x^m(a+bx)^{n-1}\,dx$$

Simpson's three-eighth's rule for numerical integration:

$$\int_{X_0}^{X_3} f(X)dX = \frac{3h}{8}\left[f(X_0)+3f(X_1)+3f(X_2)+f(X_3)\right]$$

where:

$$h = \frac{X_3-X_0}{3} \qquad X_1 = X_0+h \qquad X_2 = X_0+2h$$

Integration of $N+1$ points, where N is even:

$$\int_{X_0}^{X_N} f(X)dX = \frac{h}{3}\left[f_0+4f_1+2f_2+4f_3+2f_4+\ldots+4f_{(N-1)}+f_N\right]$$

where:

$$h = \frac{X_N-X_0}{N}$$