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 problems. NOTE: They are not equally weighted.
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

[**40 POINTS**] An adiabatic PFR will be used for the gas phase reaction

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{D} + \mathrm{E} \qquad r = kP_\mathrm{A}P_\mathrm{B} \qquad k = 200,000\exp(-14,000/T)$$

The units for the rate are lbmoles/hr-ft^3, P_j is in atm and T is in °R. The feed enters at 500 °F and 2 atm total pressure. The inlet molar feed rate of B is $N_{\mathrm{B}f} = 0.17$ lbmole/hr. The feed only contains A and B at a molar ratio of 3:1 A:B (i.e., the molar flow rate of A is 3 times the molar flow rate of B). The heat of reaction is $\Delta H_r = -58,000$ Btu/lbmole and the molar average heat capacity of the fluid phase is $\tilde{C}_p = 95$ Btu/lbmole-R. You may assume ΔH_r and $\tilde{C}_p$ remain constant.
Determine the reactor volume required to realize a conversion of B of 85% ($x_B = 0.85$).

Problem 2

[**40 POINTS**] The following liquid-phase reaction will take place in a CSTR

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C} \qquad r = kc_A$$

The feed enters at 75 °F, a total volumetric flow of $Q_f = 226.34$ ft^3/hr, and consists of a mixture of A and B having molar flow rates of $N_{Af} = 35$ lbmol/hr and $N_{Bf} = 500$ lbmol/hr. The remaining process parameters are listed in the table below. You may assume the thermodynamic properties are constant with temperature. This reactor has one unstable and two stable operating conditions and you are to find the upper stable operating condition; use $T = 800$ R and/or $c_A = 0.1 \times c_{Af}$ as your initial guess for a solution. If you elect a trial and error solution, make four iterations and quit after telling us what your next guess would be in the event your solution has not converged.

Variable	Value	Units
C_{pA}	35	Btu/lbmol-R
C_{pB}	18	Btu/lbmol-R
C_{pC}	46	Btu/lbmol-R
H_{fA}	-60,000	Btu/lbmol
H_{fB}	-100,000	Btu/lbmol
H_{fC}	-386,000	Btu/lbmol
V_R	50	ft^3
T_a	85	°F
U	500	Btu/hr-ft^2-R
A	40	ft^2
k	$9.0 \times 10^{12} \exp(-19,628/T)$	hr^{-1}; T in Rankine

NOTE The problem had an error and was pulled from the exam statement.

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

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

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

Continuous Stirred Tank Reactor (constant phase)

$$0 = Q_f c_{jf} - Qc_j + \sum_i^{n_{rxns}} \nu_{ij} r_i V_R$$

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

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

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

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

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

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

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

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:

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