CE 329, Fall 2015
Second Mid-Term Exam

You may only use pencils, pens and erasers while taking this exam. You may **NOT** use a calculator. You may not leave the room for any reason; if you do, you must first turn in your exam, and you will not be permitted to resume taking the exam.

This exam is printed on two-sided pages; there are 5 short answer questions, each worth 5 points and three problems worth 25 points each for a total of 100 points. Answer All questions, including the short answer questions, in the blue book that has been provided to you. When the exam ends, put these sheets inside your blue book and turn both in.

For the problems you only need to fully show what equations to use and to fully explain how to use them to obtain the requested answer. You do not need to perform any calculations, and you do not need to perform any algebra beyond that needed to obtain the equations to be solved. If you need to use numerical methods to answer a question, provide the information listed below

Numerical Methods

If you need to fit a linear model to data, you must state that it is necessary to fit a model to the data numerically and you must explicitly identify (a) the specific linear model being fit to the data, (b) the response and set variables in the model and (c) the parameters in the model. Then you must (d) show how to calculate the value of each response and set variable for an arbitrary data point. Once you have provided that information, you may assume that the correlation coefficient, the best value of each model parameter and its 95% confidence interval and either a model plot or a parity plot and residuals plots have been found using appropriate numerical software, and you may use those results as you need to complete the problem.

If the solution to a problem involves solving a set of non-linear algebraic equations, you must state that it is necessary solve a set of non-linear algebraic equations numerically and you must (a) explicitly identify the equations to be solved and an equal number of unknowns to be solved for by writing the equations in the form, $0 = f_i$(unknowns list) = expression. You then must (b) show how to calculate every quantity that appears in those functions, assuming you are given values for the unknowns. Once you have provided (a) and (b), you may assume that the values of the unknowns have been found numerically, and you may use those values as needed to complete the problem.

If the solution to a problem involves solving a set of initial value ordinary differential equations, you must state that it is necessary to solve a set of initial value ODEs numerically and you must (a) explicitly identify the equations to be solved, the independent variable and the dependent variables by writing the equations in the form, (derivative i) = f_i(independent variable, dependent variable list) = expression. Then you must list values or show how to calculate (b) initial values of the independent and dependent variables, (c) the final value of either the independent variable or one of the dependent variables and (d) every quantity that appears in those functions, assuming you are given values for the independent and dependent variables. Once you have provided (a), (b) and (c), you may assume that the

final values of the remaining independent and dependent variables have been found numerically, and you may use those values as needed to complete the problem.

If the solution to a problem involves solving a set of boundary value ordinary differential equations, you must state that it is necessary to solve a set of boundary value ODEs numerically and you must (a) explicitly identify the equations being solved, the independent and dependent variables in those equations and the boundaries of the range of the independent variable over which the equations are to be solved, (b) list values or show how to calculate boundary conditions for each dependent variable; the number of boundary conditions for a particular dependent variable must equal the highest order of derivative of that dependent variable appearing in the equations being solved and (c) list values or show how to calculate every quantity in the equations being solved other than the derivatives, assuming you are given values for the independent and dependent variables. Once you have provided (a), (b) and (c), you may assume that the value of each dependent variable and its first derivative with respect to the independent variable is known at any position between the boundaries, and you may use those values as needed to complete the problem.

Indefinite Integrals

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

$$\int \frac{dx}{x^2(a+bx)} = -\frac{1}{ax} + \frac{b}{a^2}\ln\left(\frac{a+bx}{x}\right); \; \int \frac{dx}{x(a+bx)} = -\frac{1}{a}\ln\left(\frac{a+bx}{x}\right); \; \int \frac{dx}{(a+bx)^2} = -\frac{1}{b(a+bx)};$$

$$\int \frac{x^2\,dx}{a+bx} = \frac{1}{b^3}\left[\frac{1}{2}(a+bx)^2 - 2a(a+bx) + a^2\ln(a+bx)\right];; \; \int \frac{x\,dx}{(a+bx)^2} = \frac{1}{b^2}\left[\ln(a+bx) + \frac{a}{a+bx}\right];$$

$$\int \frac{x^2\,dx}{(a+bx)^2} = \frac{1}{b^3}\left[a+bx - 2a\ln(a+bx) - \frac{a^2}{a+bx}\right]; \; \int \frac{x\,dx}{a+bx} = \frac{x}{b} - \frac{a}{b^2}\ln(a+bx);$$

Thermodynamic Relationships

$$\Delta H_j^0(298\text{ K}) = \sum_{\substack{i=\text{ all} \\ \text{species}}} v_{i,j}\Delta H_{f,i}^0(298\text{ K}) = \sum_{\substack{i=\text{ all} \\ \text{species}}} v_{i,j}\left(-\Delta H_{c,i}^0(298\text{ K})\right); \; K_j(T) = \prod_{\substack{i=\text{all} \\ \text{species}}} a_i^{v_{i,j}} ;$$

$$\Delta H_j^0(T) = \Delta H_j^0(298\text{ K}) + \sum_{\substack{i=\text{ all} \\ \text{species}}}\left(v_{i,j}\int_{298K}^{T} \hat{C}_{p,i}\,dT\right); \Delta G_j^0(298\text{ K}) = \sum_{\substack{i=\text{all} \\ \text{species}}} v_{i,j}\Delta G_{f,i}^0(298\text{ K});$$

$$K_j(298\text{ K}) = \exp\left\{\frac{-\Delta G_j^0(298\text{ K})}{R(298K)}\right\}; K_j(T) = K_j(298\text{ K})\exp\left\{\int_{298\text{ K}}^{T} \frac{\Delta H_j^0(T)}{RT^2}\,dT\right\}; \; a_i = \frac{y_i P}{1\text{ atm}};$$

$$a_i = \frac{y_i \varphi_i P}{1\text{ atm}}; \; a_i = \gamma_i x_i; \; a_i = x_i; \; a_i = h_i x_i$$

Rate, Composition and Reaction Progress Relationships

$$\xi_j = \frac{\left(n_i - n_i^0\right)_j}{\nu_{i,j}} \; ; \; \dot{\xi}_j = \frac{\left(\dot{n}_i - \dot{n}_i^0\right)_j}{\nu_{i,j}} \; ; \; n_i = n_i^0 + \sum_{j=1}^{N_{ind}} \nu_{i,j}\xi_j \; ; \; f_k = \frac{n_k^0 - n_k}{n_k^0} \; ; \; r_j = \frac{r_{i,j}}{\nu_{i,j}} = \frac{1}{V}\frac{d\xi_j}{dt} \; ;$$

$$g_k = \frac{f_k}{\left(f_k\right)\big|_{equil}} = \frac{n_k^0 - n_k}{n_k^0 - \left(n_k\right)\big|_{equil}} \; ; C_i = \frac{n_i}{V} \; ; C_i = \frac{\dot{n}_i}{\dot{V}} \; ; \dot{V} = \frac{\dot{n}_{total}RT}{P} \; ; \dot{V} = \dot{V}^0 \left(\frac{constant}{\rho}\right) ; P = \frac{n_{total}RT}{V} \; ;$$

$$P = \frac{\dot{n}_{total}RT}{\dot{V}} \; ; P_i = \frac{n_i RT}{V} \; ; P_i = \frac{\dot{n}_i RT}{\dot{V}} \; ; P_i = y_i P \; ; \; \mu = \frac{r_g}{C_{cells}}$$

Elementary Reaction Relationships

$$r_{AB-forward} = N_{Av}\sigma_{AB}C_A C_B \sqrt{\frac{8k_B T}{\pi\mu}}\exp\left(\frac{-E_j}{RT}\right) \; ; \; r_{AA-forward} = N_{Av}\sigma_{AA}C_A^2 \sqrt{\frac{2k_B T}{\pi\mu}}\exp\left(\frac{-E_j}{RT}\right) \; ;$$

$$r_{ABC-forward} = 8N_{Av}\sigma_{AB}\sigma_{BC}lC_A C_B C_C \sqrt{\frac{2k_B T}{\pi}}\left(\frac{1}{\mu_{AB}} + \frac{1}{\mu_{BC}}\right)\exp\left(\frac{-E_j}{RT}\right) \; ;$$

$$r_{j-forward} = \frac{q_{\ddagger}}{Nq_{AB}q_C}\left\{\frac{k_B T}{h}\right\}\exp\left(\frac{-\Delta E_0^0}{k_B T}\right)\left[AB\right]\left[C\right] \; ;$$

$$r_j = k_{j,f}\prod_{\substack{i=all \\ reactants}}\left[i\right]^{-\nu_{i,j}} - k_{j,r}\prod_{\substack{i=all \\ products}}\left[i\right]^{\nu_{i,j}} = k_{j,f}\left(\prod_{\substack{i=all \\ reactants}}\left[i\right]^{-\nu_{i,j}}\right)\left(1 - \frac{\prod_{\substack{i=all \\ species}}\left[i\right]^{\nu_{i,j}}}{K_{j,eq}}\right) \; ; \; r_{i,j} = \sum_{\substack{s=all \\ steps}}\nu_{i,s}r_s \; ; \; r_j = r_{s_{rd}} \; ;$$

$$r_{RI,j} = \sum_{\substack{s=all \\ steps}}\nu_{RI,s}r_s = 0 \; ; C_{cat}^0 = C_{cat,free} + \sum_{\substack{i=all \\ catalyst \\ complexing \\ species}}\nu_{cat,i}C_{cat,i} \; ; \; C_{i_{surf}} = C_{sites}\theta_i \; ; \; \theta_{vacant} + \sum_{\substack{i=all \\ adsorbed \\ species}}\theta_i = 1$$

Age Function Relationships

$$F(\lambda) = \frac{w_t - w_0}{w_f - w_0} \; ; \; F(\lambda) = 1 - \exp\left\{\frac{-\lambda}{\bar{t}}\right\} \; ; \; F(\lambda) = \frac{\dot{M}\int_{t_0}^{t'}\left[w_{out}(t) - w_0\right]dt}{m_{tot}} \; ; \; \begin{array}{l} F(\lambda) = 0 \text{ for } t < \bar{t} \\ F(\lambda) = 1 \text{ for } t \geq \bar{t} \end{array} \; ;$$

$$x_{total} = \sum_{x=0}^{x=\infty}xN(x) \; ; \; x_{total} = \int_{x=0}^{x=\infty}x\,dN(x) \; ; \; y_{total} = \sum_{x=0}^{x=\infty}y(x)N(x) \; ; \; y_{total} = \int_{x=0}^{x=\infty}y(x)dN(x) \; ;$$

$$N_{total} = \sum_{x=0}^{x=\infty}N(x) \; ; \; N_{total} = \int_{x=0}^{x=\infty}dN(x) \; ; \; y_{average} = \frac{\sum_{x=0}^{x=\infty}y(x)N(x)}{\sum_{x=0}^{x=\infty}N(x)} \; ; \; y_{average} = \frac{\int_{x=0}^{x=\infty}y(x)dN(x)}{\int_{x=0}^{x=\infty}dN(x)}$$

Reactor Relationships

$$\tau = \frac{V}{\dot{V}^0} \ ; \ SV = \frac{1}{\tau} \ ; \ \frac{dn_i}{dt} = V \left(\sum_{\substack{j=\text{all} \\ \text{reactions}}} v_{i,j} r_j \right) ;$$

$$\dot{Q} - \dot{W} = \left(\sum_{\substack{i=\text{all} \\ \text{species}}} n_i \hat{C}_{p,i} \right) \frac{dT}{dt} + V \left(\sum_{\substack{j=\text{all} \\ \text{reactions}}} r_j \Delta H_j \right) - V \frac{dP}{dt} - P \frac{dV}{dt} \ ; \ \dot{n}_i^0 + V \sum_{\substack{j=\text{all} \\ \text{reactions}}} v_{i,j} r_j = \dot{n}_i + \frac{d}{dt} \left(\frac{\dot{n}_i V}{\dot{V}} \right) ;$$

$$\dot{Q} - \dot{W} = \sum_{\substack{i=\text{all} \\ \text{species}}} \left(\dot{n}_i^0 \int_{T^0}^{T} \hat{C}_{p-i} \, dT \right) + V \sum_{\substack{j=\text{all} \\ \text{reactions}}} \left(r_j \Delta H_j (T) \right) + V \left(\sum_{\substack{i=\text{all} \\ \text{species}}} \frac{\dot{n}_i \hat{C}_{p-i}}{\dot{V}} \right) \frac{dT}{dt} - P \frac{dV}{dt} - V \frac{dP}{dt} \ ;$$

$$\frac{\partial \dot{n}_i}{\partial z} = \frac{\pi D^2}{4} \left[\left(\sum_{\substack{j=\text{all} \\ \text{reactions}}} v_{i,j} r_j \right) - \frac{\partial}{\partial t} \left(\frac{\dot{n}_i}{\dot{V}} \right) \right] \ ; \ \frac{\partial P}{\partial z} = -\frac{G}{g_c} \left(\frac{4}{\pi D^2} \right) \frac{\partial \dot{V}}{\partial z} - \frac{2 f G^2}{\rho D} \ ;$$

$$\frac{\partial P}{\partial z} = -\frac{1-\varepsilon}{\varepsilon^3} \frac{G^2}{\rho \Phi_s D_p g_c} \left[\frac{150(1-\varepsilon)\mu}{\Phi_s D_p G} + 1.75 \right] ;$$

$$\pi D U \left(T_e - T \right) = \frac{\partial T}{\partial z} \left(\sum_{\substack{i=\text{all} \\ \text{species}}} \dot{n}_i \hat{C}_{p-i} \right) + \frac{\pi D^2}{4} \left(\sum_{\substack{j=\text{all} \\ \text{reactions}}} r_j \Delta H_j \right) + \frac{\pi D^2}{4} \left[\frac{\partial T}{\partial t} \left(\sum_{\substack{i=\text{all} \\ \text{species}}} \frac{\dot{n}_i \hat{C}_{p-i}}{\dot{V}} \right) - \frac{\partial P}{\partial t} \right] ;$$

$$\frac{dn_i}{dt} = \dot{n}_i + V \sum_{\substack{j=\text{all} \\ \text{reactions}}} v_{i,j} r_j \ ;$$

$$\dot{Q} - \dot{W} = \sum_{\substack{i=\text{all} \\ \text{species}}} \dot{n}_i \left(\hat{h}_i - \hat{h}_{i,stream} \right) + \frac{dT}{dt} \sum_{\substack{i=\text{all} \\ \text{species}}} \left(n_i \hat{C}_{pi} \right) + V \sum_{\substack{j=\text{all} \\ \text{reactions}}} \left(r_j \Delta H_j \right) - \frac{dP}{dt} V - P \frac{dV}{dt} \ ;$$

$$-D_{ax} \frac{d^2 C_i}{dz^2} + \frac{d}{dz} \left(u_s C_i \right) = \sum_{\substack{j=\text{all} \\ \text{reactions}}} v_{i,j} r_j \ ; \ D_{er} \left(\frac{\partial^2 C_i}{\partial r^2} + \frac{1}{r} \frac{\partial C_i}{\partial r} \right) - \frac{\partial}{\partial z} \left(u_s C_i \right) = \sum_{\substack{j=\text{all} \\ \text{reactions}}} v_{i,j} r_j \ ;$$

$$\lambda_{er} \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) - u_s \rho_{fluid} \tilde{C}_{p,fluid} \frac{\partial T}{\partial z} = \sum_{\substack{j=\text{all} \\ \text{reactions}}} r_j \Delta H$$

Other Relationships

$$\sum_{\substack{i=all \\ species}} \dot{n}_{i,hot} \int_{T_{hot,in}}^{T_{hot,out}} \hat{C}_{p,i}\, dT + \sum_{\substack{i=all \\ species}} \dot{n}_{i,cold} \int_{T_{cold,in}}^{T_{cold,out}} \hat{C}_{p,i}\, dT = 0 \; ; \quad \sum_{\substack{i=all \\ species}} \dot{n}_{i,hot} \int_{T_{hot,in}}^{T_{hot,out}} \hat{C}_{p,i}\, dT + UA\Delta T = 0 \; ;$$

$$\Delta T_{AM} = \frac{T_{cold,out}+T_{hot,out}}{2} - \frac{T_{cold,in}+T_{hot,in}}{2} \; ; \quad \Delta T_{LM} = \left(\frac{\left(T_{hot,out}-T_{cold,in}\right)-\left(T_{hot,in}-T_{cold,out}\right)}{\ln\left\{\frac{\left(T_{hot,out}-T_{cold,in}\right)}{\left(T_{hot,in}-T_{cold,out}\right)}\right\}} \right) \; ;$$

$$\Delta T_{cold} = T_{hot,out} - T_{cold,in} \; ; \quad R_R = \frac{recycle\ flow}{process\ exit\ flow} \; ; \quad \dot{n}_{i,feed} + \frac{R_R \dot{n}_{i,reactor\ out}}{1+R_R} - \dot{n}_{i,reactor\ in} = 0 \; ;$$

$$\sum_{\substack{i=all \\ species}} \dot{n}_{i,feed} \int_{T_{feed}}^{T_{reactor\ in}} \hat{C}_{p,i}\, dT + \sum_{\substack{i=all \\ species}} \dot{n}_{i,r} \int_{T_{reactor\ out}\left(=T_{recycle}\right)}^{T_{reactor\ in}} \hat{C}_{p,i}\, dT = 0$$

Short Answer Questions (5 points each)

1. True or false: During an exothermic reaction in an isothermal CSTR, the rate of heat transfer, $\dot{Q}$, will be positive.

2. If the same, typical reaction is taking place isothermally at the same temperature in a CSTR and in a PFR of equal volume, using the same feed temperature, composition and flow rate, will the rate of reaction at the inlet of the PFR be greater or less than the rate of reaction in the CSTR?

3. If a single, first-order, irreversible, liquid phase reaction takes place isothermally in a steady state plug flow reactor, will the conversion increase, decrease, or stay the same if the inlet volumetric flow rate is doubled?

4. A CSTR is going to be started up by first filling it with pure water and then, once it is full, the feed stream containing 10 moles per hour of A will be started. When solving the transient mole balance for species A in this problem, what initial condition is used for the molar flow rate of A?

5. True or false? When processing a typical single reaction isothermally, the volume of a CSTR required to achieve a specified conversion is larger than that of a PFR.

6. Which of the following might initiate a period of transient CSTR operation (select all that apply)
    a. The inlet flow rate is changed
    b. The flow leaving the reactor is directed to a new storage tank
    c. The flow of coolant through the reactor jacket is interrupted
    d. The spinning rate of the agitator is increased
    e. The inlet temperature changes

Problems (35 Points Each)

7. The irreversible, homogeneous, liquid-phase reaction A → R + S takes place in an adiabatic, steady-state CSTR. Pure A is fed to the reactor at a rate of 50 L min^{-1}, 4 mol/L, and at a temperature of 350 K. The reaction is second order in A with a rate coefficient given by equation (1).

$$k = (1.76 \times 10^{-2} \text{ L mol}^{-1} \text{ s}^{-1}) \exp\{-(17,300 \text{cal/mol})/(RT)\} \tag{1}$$

Heat capacities of the species, in cal mol^{-1} K^{-1}, are as follows: A = 11.3, R = 10.1, and S = 13.0; and the heat of reaction is constant and equal to -22 kcal/mol. What must the space velocity equal for the conversion to be 50%, and what will be the outlet temperature at this space velocity?

8. A perfectly insulated PFR with a diameter of 14 in. is being fed a total of 100 mol/s of a gas mixture containing 20% inerts, 60% A and 20% B at a temperature of 150 °C and a pressure of 2 atm. The rate expression for the gas phase reaction between A and B is $r = kC_A\sqrt{C_B}$, with the rate constant given by $k = 2 \times 10^{-3} \exp\{(-25,100 \text{ cal/mol})/RT\}$ L$^{0.5}$ mol$^{-0.5}$ s^{-1}. The reaction is A + B → C + D with ΔH(298K) = -10 kcal/mol. The heat capacities in cal/mol/K are as follows:

Species, i	Heat Capacity, $\hat{C}_p$
A	5
B	7
C	6.5
D	5.7
Inert, I	4.2

The heat capacities may be assumed to be constant with respect to temperature. The reaction can also be assumed to be irreversible and pressure drop in the reactor may be assumed to be negligible. If 95% of the limiting reagent must be converted, how long must the reactor be?