

CE 329, Fall 2015
Third 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 6 short answer questions, each worth 5 points and two problems worth 35 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, $0 = f_i(\text{unknowns list}) = \text{expression}$. 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, $(\text{derivative } i) = f_i(\text{independent variable, dependent variable list}) = \text{expression}$. 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

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

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

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

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

Thermodynamic Relationships

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

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

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

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

Rate, Composition and Reaction Progress Relationships

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

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

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

Elementary Reaction Relationships

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

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

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

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

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

Age Function Relationships

$$F(\lambda) = \frac{w_t - w_0}{w_f - w_0}; F(\lambda) = 1 - \exp\left\{-\frac{\lambda}{\bar{t}}\right\}; F(\lambda) = \frac{\dot{M} \int_0^t [w_{out}(t) - w_0] dt}{m_{tot} t_0}; F(\lambda) = 0 \text{ for } t < \bar{t}; F(\lambda) = 1 \text{ for } t \geq \bar{t};$$

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

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

Reactor Relationships

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

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

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

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

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

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

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

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

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

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

Other Relationships

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

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

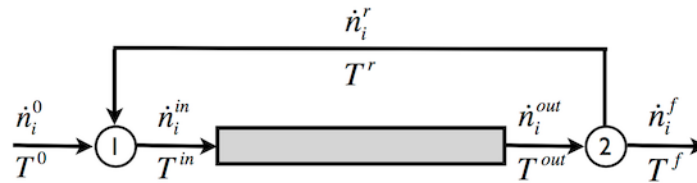
$$\Delta T_{\text{cold}} = T_{\text{hot},\text{out}} - T_{\text{cold},\text{in}}; \quad R_R = \frac{\text{recycle flow}}{\text{process exit flow}}; \quad \dot{n}_{i,\text{feed}} + \frac{R_R \dot{n}_{i,\text{reactor out}}}{1 + R_R} - \dot{n}_{i,\text{reactor in}} = 0;$$

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

Short Answer Questions (5 points each)

- If the rate expression for the liquid phase reaction $A \rightarrow P$ is $r = k[A]^2$ and the heat of reaction is small
 - three CSTRs in parallel would be a good reactor choice
 - a CSTR would be preferred over a PFR
 - a PFR would be preferred over a CSTR
 - a CSTR and a PFR would be equivalent in performance.
- In the energy balance for an ideal CSTR, \dot{Q}
 - is usually equal to $UA(T_e - T)$
 - is zero for an isothermal system
 - is the rate of heat input to the system
 - all the above (a-c)
 - (a) and (c), but not (b)
- True or false? When designing a parallel reactor network it is advantageous to mix a stream with low conversion together with a stream with high conversion.
- True or false? When the axial dispersion coefficient is equal to zero, the axial dispersion model becomes identical to the CSTR model.

Questions 5 and 6 refer to the following figure:



5. Which stream in the schematic above is used as the initial conditions when solving the PFR design equations

- 0
- in
- out
- f
- r

6. The recycle ratio is defined as the ratio of the volumetric flow rates of which two streams

- 0
- in
- out
- f
- r

Problems (35 Points Each)

7. Liquid phase reaction (1) obeys first order kinetics with a rate constant equal to 0.8 h^{-1} at $163 \text{ }^\circ\text{C}$ and an activation energy of $28960 \text{ cal mol}^{-1}$. The heat of reaction is equal to -83 cal g^{-1} and the molecular weights of A and B are equal to 250. The heat capacity of both A and B are equal to $0.5 \text{ cal g}^{-1} \text{ K}^{-1}$ and their densities are 0.9 g cm^{-3} . Pure A at $20 \text{ }^\circ\text{C}$ flows into an adiabatic 100 gal CSTR at a rate of 4 gal h^{-1} . The effluent from the CSTR is fed to an adiabatic PFR. What PFR volume will be required to attain 97% conversion, and what will be the outlet temperature of the PFR?



8. A semibatch reactor is initially charged with 1.5 L of a solution containing 0.01 mol/L of A. To start the process, 0.03 L/min of a solution containing 0.01 mol/L of B starts flowing into the reactor. The reaction $A + B \rightarrow S + T$ takes place isothermally with a rate given by the equation below. Assuming constant density, calculate the moles of A remaining in the reactor as a function of time until the reactor volume (5 L) becomes full.

$$r = (5 \text{ L/mol/min}) C_A C_B$$