

**CE 329, Fall 2015**  
**Assignment 31, Practice 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,  $0 = f_i(\text{unknowns list}) = \text{expression}$ . 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)

- True or false? Batch reactors are often suitable for the production of specialty chemicals.
- True or false? A cascade of CSTRs improves performance compared to a single CSTR by reducing the reactant concentration to its final level in multiple steps instead of one single step.
- True or false? Adding thermal backmixing to a PFR is usually advantageous if an endothermic reaction is taking place.
- When the recycle ratio becomes very large, the behavior of a recycle pfr approaches that of a
  - batch reactor
  - cstr
  - inverted pfr
  - recycle cstr
  - autothermal batch reactor
- What distinguishes semi-batch operation from batch operation?
  - In semi-batch operation the reactor is never more than half full.
  - In semi-batch operation the headspace is always hemispherical.
  - In semi-batch operation at least one reagent is added to or removed from the reactor while the reaction is taking place.
  - In semi-batch operation the reaction is only allowed to continue for half as long as in batch operation.
  - In semi-batch operation the number of reactor operators is half the number used during batch operation.
- True or false? The semibatch design equations include all the terms in the batch reactor design equations.

### Problems (35 Points Each)

7. The following liquid phase reactions are to be carried out in a series of two isothermal CSTRs with equal volumes:



The feed to the process is to be  $500 \text{ gal h}^{-1}$  and the concentration of A in the feed is to be  $6 \text{ moles gal}^{-1}$ . Neither V nor W is present in the feed. If the objective is to maximize the effluent concentration of V, what size should the reactors be, and what is the fraction of A converted to V?

8. Analyze the selectivity of a semibatch reactor where reactions (1) and (2) can take place. The reactor will operate isothermally at a temperature where the rate coefficients for reactions (1) and (2) are  $0.5 \text{ L/mol-h}$  and  $0.25 \text{ L/mol-h}$ , respectively. The  $10,000 \text{ L}$  reactor initially contains  $2000 \text{ L}$  of solution with  $2 \text{ mol/L}$  of A and  $0.25 \text{ mol/L}$  of B. The reactor will be fed  $1000 \text{ L}$  per h of a solution containing  $0.5 \text{ mol/L}$  of B for a period of  $7 \text{ h}$ . Determine the concentrations of all species at the end of the run and the overall selectivity ( $\text{mol C/mol B}$ ).

