AFCoKaRE Exam Information

These three pages will be included as part of every exam in this course. It is strongly recommended that you make a copy of these pages, and use them as your only reference when you solve in-class and homework problems. In that way, you will be better prepared for exams. If there is information not presented here that you feel you will need on an exam, you will have to memorize that information.

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

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

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

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

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

Thermodynamic Relationships

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

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

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

$$a_i = \frac{y_i\varphi_iP}{1\text{ atm}};\ a_i = \gamma_ix_i\,;\ a_i = x_i\,;\ a_i = h_ix_i$$

Rate, Composition and Reaction Progress Relationships

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

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

$$P_i = \frac{n_iRT}{V};P_i = \frac{\dot{n}_iRT}{\dot{V}};P_i = y_iP\,;\ \mu = \frac{r_g}{C_{cells}}$$

Elementary Reaction Relationships

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

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

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

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

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

Age Function Relationships

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

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

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

Reactor Relationships

$$\tau = \frac{V}{\dot{V}^0};\ SV = \frac{1}{\tau};\ \frac{dn_i}{dt} = V\left(\sum_{\substack{j=\text{all}\\\text{reactions}}}\nu_{i,j}r_j\right);\ \dot{Q}-\dot{W} = \left(\sum_{\substack{i=\text{all}\\\text{species}}}n_i\hat{C}_{p,i}\right)\frac{dT}{dt} + V\left(\sum_{\substack{j=\text{all}\\\text{reactions}}}r_j\Delta H_j\right) - V\frac{dP}{dt} - P\frac{dV}{dt};$$

$$\dot{n}_i^0 + V\sum_{\substack{j=\text{all}\\\text{reactions}}}\nu_{i,j}r_j = \dot{n}_i + \frac{d}{dt}\left(\frac{\dot{n}_iV}{\dot{V}}\right);$$

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

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

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

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

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

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

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

Other Relationships

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

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

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

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