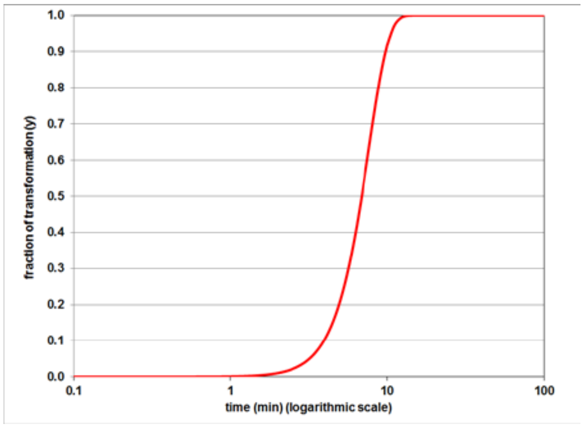
Final Exam
Administered: Friday, December 4, 2015
8:00 AM – 10:00 AM
22 points

Problem 1. (6 points)

"Most solid-state transformations do not occur instantaneously because obstacles impede the course of the reaction and make it dependent on time." [Callister, W.D., "Materials Science and Engineering: An Introduction, Wiley & Sons, New York, Fifth Ed., p. 296]. One expression used to describe the fraction of solid that has transformed is the Avrami equation, shown in the equation and Figure below, where *y* is the fraction of transformation, *t* is time (min), *k* is a rate constant (min^{-1}) and *n* is an exponent.

$$y = 1 - \exp\left(-kt^n\right)$$



(a) Linearize this equation so that it is linear in the unknown parameters, *k* and *n*.
(b) Using the table of data providing *y* and *t* in the file "xm4p01_f15.txt" on the exam portion of the course website, perform a linear regression to determine the mean values of *k* and *n* for this data.
(c) Also report the standard deviations of *k* and *n*.

Problem 2. (4 points)

Measurements of the elastic modulus, *E*, of large-particle composites, formed by particles (*p*) distributed in a matrix (*m*) at a particle volume fraction, V_p, ($V_m = 1 - V_p$) are known to fall between upper and lower limits, given by [Callister, W.D., "Materials Science and Engineering: An Introduction, Wiley & Sons, New York, Fifth Ed., pp. 523-524].

$$E_{upper} = E_m V_m + E_p V_p \qquad E_{lower} = \frac{E_m E_p}{E_m V_p + E_p V_m}.$$

Experiments are performed with tungsten particles dispersed in a copper matrix and the following results are obtained. For $V_p = 0.6$, $E_{upper} = 260$ GPa and $E_{lower} = 180$ GPa.

(a) Given this information, what numerical method can be used to determine the intrinsic elastic moduli of the matrix, E_m, and the particle, E_p.

(b) Determine E_m and E_p.

Problem 3. (4 points)

It has been observed that the relative weight gain, *W*, as a function of time, *t*, due to formation of oxides on metals follows the following functional form [Callister, W.D., "Materials Science and Engineering: An Introduction, Wiley & Sons, New York, Fifth Ed., p. 593]

$$W(t) = K_1 \ln\left(K_2 t + K_3\right)$$

where three empirically determined constants appear and time is measure in days. This expression arises from a weight gain rate equation of the form

$$\frac{dW(t)}{dt} = \frac{K_1 K_2}{K_2 t + K_3}$$

For a surface with a composition gradient, the constants become dependent on the local composition and are therefore functions of time. We propose a form

$$K_1(t) = c_1 \exp\left(-\frac{(t - t_{\max})^2}{s_1} \right).$$

such that the weight gain is now given by

$$W(t) = \int_{t=0}^{t} \frac{K_1(t) K_2}{K_2 t + K_3} dt$$

(a) What method could be used to evaluate the weight gain as a function of time?

(b) Determine the weight gain of such a model at t = 14 days with the following parameters: $c_1 = 0.2$, $s_1 = 3$, $t_{\max} = 4$, $K_2 = 5$, and $K_3 = 6$.

Problem 4. (8 points)

Consider the dimerization reaction:

$$2A \rightarrow B$$

The reaction rate is given by

$$rate = C_A^2 k_o e^{-\frac{E_a}{RT}} \qquad \text{[moles/m}^3\text{/sec]}$$

with the following variables defined: concentration of A, C_A [moles/m^3]; prefactor, k_o [m^3/(moles·sec)]; activation energy for reaction, E_a [Joules/mole]; constant, $R = 8.314$ [Joules/mole/K] and temperature, T [K]. If this reaction were to take place in a continuous stirred tank reactor, the mole balances on A and B would have the form

$$V\frac{dC_A}{dt} = C_{A,in}F - C_A F - 2rate \qquad (1)$$

$$V\frac{dC_B}{dt} = C_{B,in}F - C_B F + rate \qquad (2)$$

Equations (1) and (2) represent a set of two non-linear coupled ordinary differential equations. Assume the following parameter values: inlet concentration of A: $C_{A,in} = 2{,}000$ [moles/m^3]; inlet concentration of B: $C_{B,in} = 0$ [moles/m^3]; prefactor: $k_o = 0.90$ [m^3/(moles·sec)]; activation energy: $E_a = 56{,}000$ [Joules/mole]; temperature: $T = 500$ [K]; reactor volume: $V = 1$ [m^3] and flowrate: $F = 0.01$ [m^3/sec]. Also, assume that reactor initially has no A or B in it, so that the initial conditions are given by: $C_A(t=0) = 0$ [moles/m^3] and $C_B(t=0) = 0$ [moles/m^3].

Numerically solve the ordinary differential equations.

(a) Sketch the plot of the concentrations for A and B as a function of time.

(a) Report the steady state concentration of A.

(c) From this calculation, how do you know that the function is at steady state?

(d) From this calculation, verify that you have used a sufficiently fine temporal resolution.