Final Exam
Administered: Wednesday, December 7, 2016
36 points

For each problem part: 0 points if not attempted or no work shown,
1 point for partial credit, if work is shown,
2 points for correct numerical value of solution

Problem 1. (8 points)
For many polymers it has been observed that tensile strength (TS) increases with increasing molecular weight. Mathematically, TS is a function of the number-average molecular weight, $\overline{M}_n$, according to

$$TS = TS_\infty - \frac{A}{\overline{M}_n} \quad (1)$$

where TS_∞ is the hypothetical tensile strength at infinite molecular weight and A is a constant. [Materials Science and Engineering: An Introduction, 5th Edition, William D. Callister, John Wiley & Sons, Inc., New York, 2000, p. 480.]
For the TS vs $\overline{M}_n$ data given in the file, http://utkstair.org/clausius/docs/mse301/data/xm4p01_f16.txt, perform the following tasks.
(a) Identify all variables, $y = mx + b$, when equation (1) is linearized.
(b) Report the best value of A and TS_∞.
(c) Report the standard deviations of A and TS_∞.
(d) Report the measure of fit.

Problem 2. (12 points)
We are testing a polymer membrane designed to catalytically filter microbes. The concentration of microbe A, $C_{A,0}$, on one side of the membrane, located at $z = 0$, is $C_{A,0}$. The gradient of the microbe concentration on the same side of the membrane is $\left.\frac{dC_A}{dz}\right|_0$. Inside the polymer membrane, a chemical agent kills the microbe. The following equation describes the profile of the microbe concentration within the membrane,

$$0 = D\frac{d^2C_A}{dz^2} - k\sqrt{C_A}$$

Answer the following questions.
(a) Is this ODE problem linear or nonlinear?
(b) Is this ODE problem an initial value problem or a boundary value problem?
(c) Convert this second order ODE into a system of two first order ODEs.
(d) For a membrane of thickness, $L = 5$ cm, and the following numerical values, $D = 1.0 \cdot 10^{-6} \frac{cm^2}{s}$, $k = 2.8 \cdot 10^{-9} \frac{\left(\frac{mol}{\ell}\right)^{1/2}}{s}$, $C_{A,0} = 1.0 \cdot 10^{-2} \frac{mol}{\ell}$ and $\left.\frac{dC_A}{dz}\right|_0 = -2.5 \cdot 10^{-3} \frac{mol}{\ell \cdot cm}$, find the concentration of the microbe on the far side of the membrane.
(e) For the conditions in part (d) sketch the concentration profile.
(f) For the conditions in part (d), verify that your discretization resolution was sufficient.

Problem 3. (12 points)
Molecular simulations have shown that chitosan polymer films have shown that the diffusivity of oxygen in chitosan polymer films is enhanced under humid conditions. [McDonnell, M.T., Greeley, D.A., Kit, K.M., Keffer, D.J, "Molecular Dynamics Simulations of Hydration Effects on Solvation, Diffusivity, and Permeability in Chitosan/Chitin Films" J. Phys. Chem. B 120(34) 2016 pp. 8997-9010.] Consider the diffusivities of oxygen for several simulations at low (15%) and high (95%) relative humidity.

	15 % RH			95% Relative Humidity	
	D	D^2		D	D^2
sample	(m^2/s)	(m^2/s)^2	sample	(m^2/s)	(m^2/s)^2
1	2.66E-11	7.07E-22	1	1.91E-10	3.64E-20
2	4.46E-11	1.99E-21	2	1.14E-10	1.30E-20
3	2.60E-11	6.78E-22	3	1.31E-10	1.72E-20
4	3.61E-11	1.31E-21	4	1.12E-10	1.25E-20
5	4.73E-11	2.24E-21	5	1.26E-10	1.59E-20
6	3.39E-11	1.15E-21	6	1.15E-10	1.32E-20
7	1.60E-11	2.56E-22	7	1.30E-10	1.69E-20
sum	2.30638E-10	8.32801E-21	sum	9.187E-10	1.251E-19

(a) Compute the sample mean of the diffusivity for both RH.
(b) Compute the sample variance of the diffusivity for both RH.
(c) What PDF is appropriate for determining a confidence interval on the difference of means?
(d) Find the lower limit on a 98% confidence interval on the difference of means.
(e) Find the upper limit on a 98% confidence interval on the difference of means.
(f) Translate your result from (d) and (e) into a statement a non-statistician can understand.

Problem 4. (4 points)
The crystalline volume fraction, ϕ_c, of a polymer specimen (s) can be related to the densities of the specimen and the density of the polymer in perfectly amorphous (a) and perfectly crystalline (c) states, via

$$\phi_c = \frac{\rho_c(\rho_s - \rho_a)}{\rho_s(\rho_c - \rho_a)} \tag{2}$$

[Materials Science and Engineering: An Introduction, 5th Edition, William D. Callister, John Wiley & Sons, Inc., New York, 2000, p. 464.]
For a particular polymer the transparency, measured in terms of the fractional transmittance of light, f_t, is related to the crystalline volume fraction via

$$f_t(\phi_c) = c_0 + c_1\phi_c + c_2\phi_c^{\,2} \tag{3}$$

where the coefficients, c, are fit to a particular polymer.

(a) For the a polymer with f_t = 0.94 and ρ_c = 1.40 g/cm^3 and ρ_a = 1.20 g/cm^3, find the density of the polymer. The coefficients for this polymer in equation (2) are c_0 = 0.1, c_1 = 17.67 and c_2 = -17.32.
(b) What is the crystalline volume fraction?