10.491 Integrated Chemical Engineering Materials Design Module

Assignment #3: Additivity Calculations
Due Mon, 4/26/99, 10am

With this assignment, you should begin to think about how to modify a polymer to achieve a desired design objective. In particular, focus on issues which might relate to polymers which are for environmentally benign and sustainable. Additivity methods for property estimation provide a quick means for screening many possible structures in order to observe trends, and to test your own intuition regarding what affects material properties.

In preparation for this assignment, work through the following Biosym Polymer tutorials:

(i) QSPR Module/Lesson 5 “QSPR van Krevelen Methodology: Example Calculation for Polystyrene”

(ii) Synthia Module/Lesson 2 ”Example Calculation for a Copolymer” (for this tutorial, you will probably get an error message indicating an unknown “Designer_Correl”. Go ahead and run the tutorial up to this point, to get a feel for how the calculations are done. You can continue to step past the error and read the Pilot messages.)

For this assignment, you should use Biosym’s QSPR and Synthia modules and Chapter 18 from van Krevelen’s book (see course web pages).

1. Using both QSPR (with van Krevelen’s parameters) and Synthia, estimate the following properties for poly(ethylene terephthalate) [hint: repeat unit chemical formula=$C_{10}H_8O_4$] at room temperature. For the QSPR calculations, a chain with DP=5 suffices; Synthia requires only the repeat unit itself. Please report all numbers in the units indicated.

Glass transition temperature, Tg (K)
melting temperature, Tm (K)
“attainable” degree of crystallinity (%)
density of amorphous phase (g/cm^3)
density of crystalline phase (g/cm^3)
tensile modulus at 25 degrees C

Answer the following questions abou;t this polymer:

a) Would you expect this polymer to crystallize? Why or why not?
b) At room temperature, would the amorphous phase be glassy or liquid-like?
c) Assuming that the overall density can be calculated as the linear combination of the individual phase densities, what would be the density of this polymer?

2. Repeat part 1 for the following polymers:

isotactic poly(3-hydroxybutanoic acid)
atactic poly(3-hydroxybutanoic acid)

3. Answer the following questions and explain why you think the change you propose will have the desired effect.. Provide a QSPR or Synthia output for the new polymer to back up your response:

a) Starting from the polymer structure given in part 1, how might you modify its architecture in order to eliminate crystallization?

b) How might you modify the architecture of the polymer in part 1 in order to lower its Tg below room temperature (if the Tg of the polymer in part 1 is above room temperature) or raise Tg above room temperature (if the Tg in part 1 is below room temperature)?

4. For this part of the homework, refer to Chapter 18 of van Krevelen in addition to the software. Estimate the diffusivity and solubility of H_2O at 25 degrees C for each of the5 polymers created in parts 1-3, using both QSPR and Synthia wherever possible. For estimates of solubility and diffusivity from Synthia, use the estimate provided for permeability of nitrogen at 298 K and the relations discussed in class. [Note: permeability values in Synthia are reported in "Dow units": (cm^3 *10^{-3} in)/(day *100 in^2*atm) amd must be converted. 1 DU=4.5x10-16 (cc(STP)*cm)/(cm^2*Pa*s).]

For this assignment, turn in your QSPR and/or Synthia output for each polymer evaluated and label each output with the name of the polymer it refers to. However, you should compile all the results requested above on a separate sheet. In addition to your QSPR and Synthia results, hand in a printout showing each of the polymers you made in parts 1-3, with the chains sufficiently extended and each atom labeled by atom type so that the TA can see the correct architecture of the chain.