CHE5134
Polymer Physics
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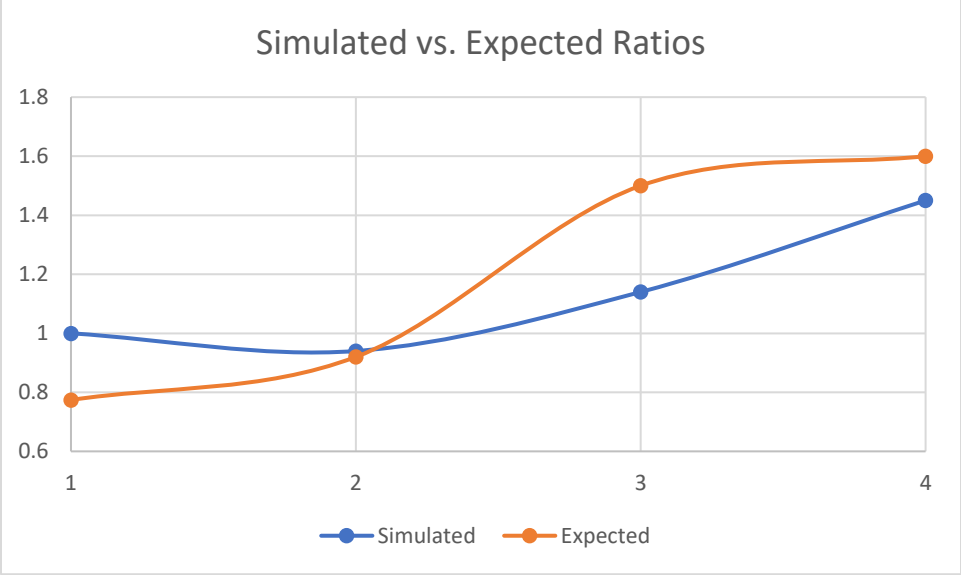
Quiz 7

a.) Grosberg's model uses the fact that $\alpha^2 = R^2/R_0^2$ while the Flory-Krigbaum model uses the fact that $\alpha = R^2/R_0^2$ which then affects the approximation of n. For the Grosberg model, $\alpha \sim n^{1/10}$ while the F-K model gives an approximation of $\alpha \sim n^{1/5}$. The time scales between the two are different as well. For the coarse-grained explanation, Grosberg will allow for analysis of larger molecules because of the differences in the n-value. This leads to a prediction of coil collapse because the value of α can be estimated. So, if $\alpha < 1$, then the coil will contract and eventually lead to collapse.

b.)

	$R_{g,max}$ @ N=5	$R_{g,max}$ @ N=18	$R_{g,max}$ @ N=30	$R_{g,max}$ @ N=100	d_f
Red (globule)	5	10.4	11	17	3
Black (coil)	5	11.9	16	16	2
Ratio (black/red)	1	1.14	1.45	0.94	

The plot for N=30 gives a ratio of 1.5 which is close to 1.5 indicating theta solvent, and the plot for N=100 gives a ratio of 0.94 which is close to 0.92 indicating a draining sphere. The following plot is a graph of the simulated and expected ratios plotted in numerical order:



c.) For the two distribution curves, e and f, there is a noticeable difference in the distribution of the smaller R_g, which indicates that the coil is more collapsed at that point, and the second peak in both have the higher R_g and means that it is more expanded. By starting the simulation in the different conformational states, there is the noticeable difference in both the R_g value and the differences in distribution between the two peaks. When the simulations are ran in the shorter time period, it is harder to see the measure in a more coarse-grained mode, while the larger

time period allows for a much longer measurement simulation time, giving a better coarse-grained picture.

d.) Plot d is a 5-mer chain, and because it is so small, there is barely any difference in the R_g value and the distribution. This is because the molecule is so small, there are only so many different conformations and ways that the chain can be affected.

e.) The plots of Rg versus temperature for different starting conformations shown exhibit a first order transition. A first order transition involves a change in volume, like how when a metal melts, the volume changes, but in a second order transition, there is not volume change but there is a noticeable change in the properties. The plots show a first order transition because the volume changes. This is thought of physically as a polymer of different conformations will have different volumes, and therefore will have different temperatures at which the chain to globule transition will occur. Theoretically, R_g, the radius of gyration, is related to the volume because it has to do with the cross-sectional area.