Modeling Reaction Dynamics

Navigate to your lab group's Dropbox folder and open the file "NetLogoLite.jar," which you will find in the NetLogo folder. When the "Open: NetLogo Model" window appears, select the file "ReactionDynamics.nlogo;" this will launch a mathematical model of the equilibrium reaction

$$A \leftrightarrows B$$

As the molecules zip around and collide, some molecules of A react to form B and some molecules of B react to form A. The reaction of A $\rightarrow$ B occurs twice as often as the reaction of B $\rightarrow$ A. The slider labeled "number-reactants" allows you to vary the initial number of As from 1 to 255; the number of Bs is always 256 – number of As. Adjust the slider so that the reaction begins with 255 molecules of A and one molecule of B.

Press the button labeled "Setup" and make note of the values in the boxes at the top left of the screen. Press the button labeled "Go" and watch the reaction take place. Note that the values in the boxes change and that two graphs appear showing the molecules of A and B as a function of time and the value of ΔG as a function of time (for the reaction A $\rightarrow$ B). Once you have a feeling for how the program works, press "Go" to end the model. You can readjust the slider and use the setup button to initiate a new model.

Using this program, investigate the following by running several simulations beginning each trial with a different initial amount of A:

1. How do the relative amounts of A and B change over time? Does your conclusion depend on the initial amount of A?

   Whether the amount of A or B increases or decreases depends on the initial amount of A; however, the amounts trend toward approximately 85 As and 171 Bs.

2. How does the ratio B/A change over time? Does your conclusion depend on the initial amount of A?

   Whether the ratio increases or decreases depends on the initial amount of A; however, the ratio trends toward a ratio of 2.

3. How does the value of ΔG change over time? Does your conclusion depend on the initial amount of A?

   Whether ΔG becomes more positive or more negative depends on the initial amount of A; however, the trend for ΔG is always towards a value of zero. Note that when ΔG is positive, the reaction B $\rightarrow$ A is favorable.

4. What is the value of ΔG when the initial amounts of A and B are identical? What are the values of A and B when ΔG is zero?

   When A and B are identical, the value of ΔG is approximately –1.7. When ΔG is zero, the values of A and B are approximately 85 and 171, respectively.

5. How does the initial value of ΔG depend on the relative amounts of A and B at the start of the reaction? Gather some data by adjusting the slider, pressing setup and reading the value for the initial ΔG. As we learned, ΔG is a function of the relative concentrations of reactants and products. For this reaction, the exact relationship is

$$\Delta G = \Delta G^{o} + RT\ln(B/A)$$

   Using Excel or another similar program, graph your results and verify that they are consistent with the equation provided above. Using your graph, find values for ΔG^{o} and RT and determine whether your results are reasonable.

   A plot of ΔG vs. ln(B/A) is a straight line. The y-intercept is–1.7, which is the value of ΔG^{o}. The slope of the line is 2.44, which is equivalent to RT when T is 298 K; that is

$$slope = (8.314\times10^{-3}\ kJ/mol\bullet K)\times 298\ K = 2.48\ kJ/mol$$

6. At equilibrium the value of ΔG is zero; thus

$$\Delta G^{o} = -RT\ln K_{eq}$$

   What is the value of the equilibrium constant, K_{eq} for the reaction A ⇆ B? Is this value consistent with the observation that the reaction A → B occurs twice as often as the reaction B → A? Explain.

   Taking ΔG^{o} as –1.7 kJ/mol and solving for K_{eq} gives the equilibrium constant as 1.98, which is consistent with an expected 2:1 ratio of B to A for this reaction.