

Modeling Reaction Dynamics

Open the “Public” folder in the class’s I-Drive account and open the file “NetLogoLite.” When the open file window appears, select the file “ReactionDynamics.” This will launch a mathematical model of the equilibrium reaction



Two constraints exist for this model: (1) the combined number of As and Bs is fixed to be 256; and, (2) the reaction $A \rightarrow B$ occurs twice as frequently as the reaction $B \rightarrow A$. As the molecules zip around and collide, some As react to form Bs and some Bs react to form As. The slider labeled “number-reactants” allows you to vary the initial number of As from 1 to 255. Adjust the slider so that the reaction begins with 255 As.

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 absolute numbers of As and Bs vs. time and the value of ΔG vs. time (for the reaction $A \rightarrow B$). Once you have a feeling for how the program works, press “Go” again 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 amounts of A and B change over time? Does your conclusion depend on the initial amount of A?
2. How does the ratio B/A change over time? Does your conclusion depend on the initial amount of A?
3. How does the value of ΔG change over time? Does your conclusion depend on the initial amount of A?

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?
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 recently, ΔG is a function of the relative concentrations of reactants and products. For this reaction, the exact relationship is

$$\Delta G = \Delta G^\circ + RT \ln(B/A)$$

Using LoggerPro or Excel, graph your results and verify that they are consistent with the equation provided above. Using your graph, find values for ΔG° and RT and determine whether your results are reasonable.

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

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

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