

Modeling Chemical Kinetics and Equilibrium with Stella

Background

In a previous experiment, you used volume change in a buret to illustrate the physical significance of reaction rate and to experimentally derive a rate law for the observed kinetic phenomena. The resultant conclusions were that the flow rate ($\Delta V/\Delta T$) through the buret setup followed a first-order rate law and was proportional to the amount of water remaining in the buret at any time; thus the differential rate law for a first order reaction was verified to be $-\Delta V/\Delta T = k \cdot V$. Today, you will apply your knowledge of rate laws in coordination with STELLA, a dynamic programming environment, in an effort to model the kinetic behavior of a chemical system.

Objectives

The objectives of this experiment are to examine the kinetics of chemical systems exhibiting first, second and zeroth-order behavior and to illustrate the principle of chemical equilibrium via experimentation with STELLA.

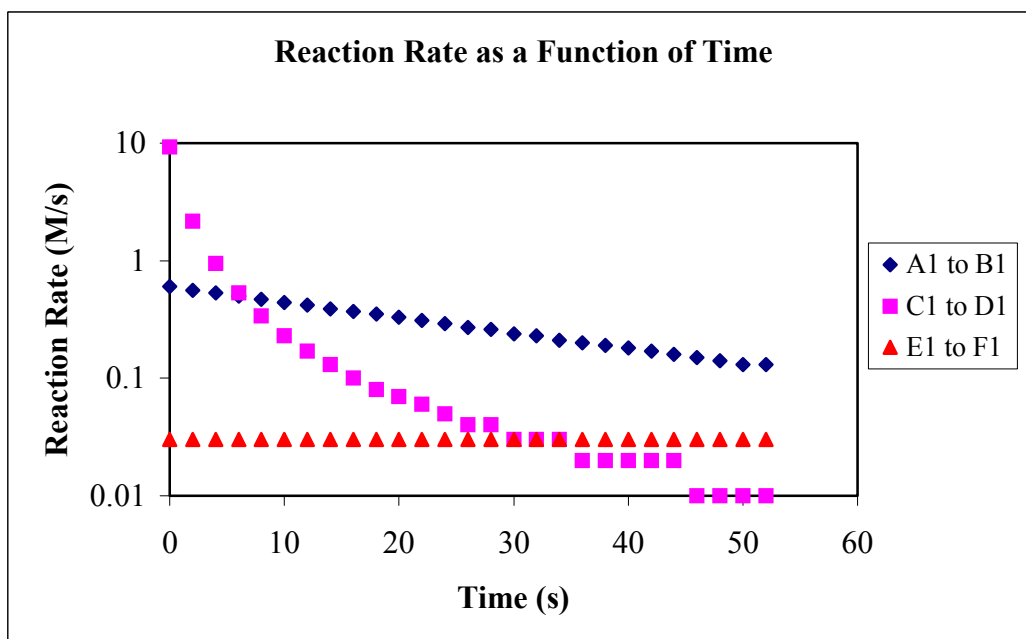
Experimentation

A few things before you jump into the program: jot down the differential rate laws for a first, second and zeroth order reaction below and correlate the equations that you obtain with the graph below. Try to remember your observations from the buret experiment and use the graph to help you match a rate law to the correct STELLA model.

First-Order

Second-Order

Zeroth Order



- Initialize stock concentrations A1, C1, E1 to a value of 20 moles by clicking on the appropriate box in STELLA and entering the value in the field. You must then use the run menu and select run (open apple-R)
- Obtain and record the half-life of the reaction (time to reach $\frac{1}{2}$ of the initialized concentration); this can be achieved either by moving the small hand across your graph while depressing and holding the click pad or by clicking on the table after having run the model.
- Hypothesize how the half-life would change if you doubled the magnitude of the initial stock concentration for each reaction. Important!! Record your hypothesis on the table before you change anything in STELLA, just as would during any chemical experiment.
- While leaving stocks A1, C1 and E1 alone, enter a value of 40 moles into each of the stocks labeled A2, C2 and E2. Run the model to test your hypothesis and record your result.
- Try entering other initial concentrations to observe how changes affect system behavior.
- Make a conclusion about your results and state whether they support your hypothesis. Also note any other results that you found interesting during the experiment.

| Order (Trial) | Hypothesis | Initial Half-Life | New Half-Life | Conclusions | kfor | krev | EQ prod Conc | EQ react Conc |
|-------------------------------|-------------------|--------------------------|----------------------|--------------------|-------------|-------------|---------------------|----------------------|
| <i>First (1)</i> | | | | | | | | |
| <i>Second (2)</i> | | | | | | | | |
| <i>Zeroth (3)</i> | | | | | | | | |
| <i>Additional Conclusions</i> | | | | | | | | |

- Examine the first-order equilibrium system and graph and record the values of k forward and k reverse by clicking on the appropriate converter (circle). Note the point at which the system reaches chemical equilibrium.
- What do kfor and krev signify in terms of equilibrium? Quantitatively, how do these two rate constants relate to each other? How does this relationship affect your final equilibrium result? Test your hypotheses with a few different guesses.