Computer Modeling of Equilibrium Systems

INTRO

Often computer systems are used to make predictions about everything from trends in economics, to weather patterns. We can study simple equilibrium systems by modeling what happens during a reaction. Today we will create a simple modeling system using the spreadsheet and graphing capabilities of ClarisWorks.

GOAL

Your goal is to create the following models to learn about equilibrium. Today we will be studying the simple equilibrium A<==>B.

Design of the Model

1) You are to design your model so that you have two columns of data, one showing the concentration of reactants and one for the concentration of products.
2) You should also have a column which calculates the ratio of products:reactants.
3) As part of this model you should have two cells in the spreadsheet, one of which describes the forward rate and one which describes the reverse rate. By adjusting these cells you should affect the data calculated in you concentration columns.
4) The concentration data will then be plotted on a graph.

Create the following equilibrium system:

1) Reactant A begins with a concentration of 100.
2) Reactant B begins with a concentration of 150.
3) The forward reaction rate is 0.65.
4) The reverse reaction rate is 0.25.
5) Graph your results by highlighting the data (including titles) from your concentration columns and choosing "**Make Chart**" from the "**Options**" menu. Then select the line graph option. You can label the axes by double clicking on them. Label the y-axis "Concentration" and the x-axis "Time".
6) Record this graph, all of the above starting conditions, and **equilibrium ratio** in your notebook. You will record this information for each new "experiment" that you create using this simulation.

(over)

Now create the following additional equilibrium systems: Record as above the below systems.

1) Same as above but reverse the starting concentrations.
2) Same as above but drastically change the starting concentrations for both A and B.
3) Now record two graphs in which you change the reaction rate. For reaction rates the range should be between 0 and 1.

Now it's time to use Le Chetalier's principle:

You can simulate the injection or reduction of substance A or substance B by typing a number into the place where you normally calculate the concentration. The example below illustrates how to do this.

	A	B	C	D
1		A Concentratio	B Concentratio	Ratio of B:A
2	Initial Conc.:	100.000	150.000	1.500
3		72.500	177.500	2.448
4		69.750	180.250	2.584
5	--> reaction rate	69.475	180.525	2.598
6	0.65	69.448	180.553	2.600
7	<-- reaction rate	69.445	180.555	2.600
8	0.25	69.444	180.556	2.600
9		69.444	180.556	2.600
10		69.444	180.556	2.600
11		69.444	180.556	2.600
12		200.000	180.556	0.903
13		115.139	265.417	2.305
14		106.653	273.903	2.568
15		105.804	274.751	2.597
16		105.719	274.836	2.600
17		105.711	274.845	2.600
18		105.710	274.846	2.600
19		105.710	274.846	2.600
20		105.710	50.000	0.473
21		49.498	106.211	2.146
22		43.877	111.833	2.549
23		43.315	112.395	2.595
24		43.259	112.451	2.599
25		43.253	112.457	2.600
26		43.253	112.457	2.600
27		43.253	112.457	2.600
28		43.253	112.457	2.600
29		43.253	112.457	2.600
30		43.253	112.457	2.600

After the system came to equilibrium, the number 200 was typed into cell B12. This simulates the injection of substance A into the system. Notice how the system quickly regains equilibrium.

Here is a simulation of the removal of a substantial quantity of substance B from the equilibrium system. The number 50 was typed into cell C20.

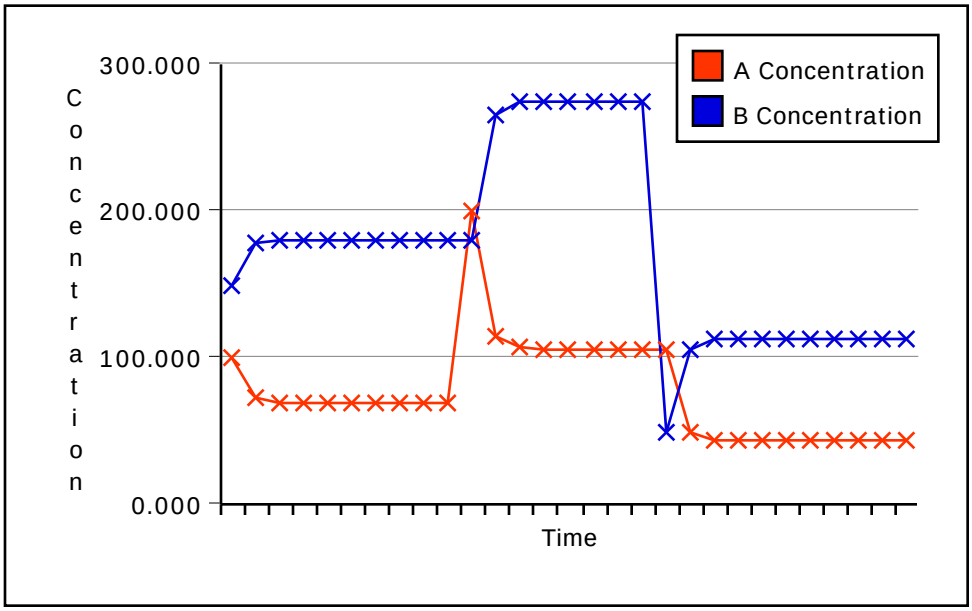
1) Before doing the following, try to predict how the shape of the graph will change as a result of injecting or removing various substances to this equilibrium system.
2) Predict what will happen to the graph if you inject more B into the system, by sketching what you think will happen. Try this by typing a large number into the B column to simulate injection of B.
3) Predict what will happen to the graph if you remove A from the system. Sketch what you think will happen to the graph.
4) Try experimenting with various scenarios until you feel comfortable with how and why the graph changes as it does.

Equilibrium Simulation Questions:

1) After studying the data (rates of reaction, initial concentrations, injection or removal of various substances) what factors seem to affect the final value for the equilibrium ratio?

2) What relationship do you see between the reaction rates and the equilibrium ratio?

Given the following graph answer the questions below:



3) The first part of this graph shows an equilibrium being reached between substance A and substance B. Then a large quantity of substance A is injected. Explain how the graph depicts the Le Chetalier response to this stress of increased substance A.

4) What happens in the last third of the graph?

5) What remains constant throughout this experiment and what changed?