Chemical Kinetics Using Spreadsheets

For the first order reaction

$$A \rightarrow B$$

the differential rate law is

$$\frac{dA}{dt} = -k\ A$$

and the integrated rate law is

$$A = A_0\ e^{-kt}$$

In this exercise we will calculate the concentrations of A and B as a function of time using both the analytically integrated rate law and by numerical integration of the differential rate law using Euler's method given by $x_2 = x_1 + f(x_1,t_1)\ (t_2 - t_1)$. Recall, for a first order reaction, a plot of ln A against time t is linear. General directions for Excel are given below–please ask for assistance as needed.

We will also construct a 'slider bar' in the Integral method sheet that will allow us to vary the rate constant k and interactively see the changes on the concentration vs time graphs. This is a useful tool to show students how changing a parameter affects the behavior of the system. It is also much easier to do than have students change numbers in cells to experiment with a model. Note that the Developer tab must appear on the Ribbon in Excel 2007.

1) Integral Method

Open Excel
A1 First Order Reaction A - -> B Integral Method
A3 a =
A4 k =
B3 1000
B4 1
A6 t
B6 A
C6 B
D6 ln A

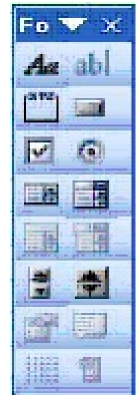
A7 0.0
A8 0.1
A9 0.2
Fill cells A10 to A107 so that A107 will contain 10.0
B7 =$B$3*EXP(-$B$4*A7)
C7 =$B$3*(1-EXP(-$B$4*A7))
D7 =LN(B7)
Fill down B7, C7, D7 through B107, C107, D107
Plot A and B against *t*
Plot ln A against *t*
Save and Close

2) Differential Method

Open Excel
A1 First Order Reaction A - -> B Differential Method Using Euler Integration
A3 a =
A4 k =
B3 1000
B4 1
B6 dA = -k A dt
C6 A = a - dA
D6 B = a - A
A7 t
B7 dA
C7 A
D7 B
E7 ln A
A8 0.0
A9 0.1
A10 0.2
Fill cells A11 to A108 so that A108 will contain 10.0
B8 0
C8 1000
D8 0
B9 =-B$4*C8*(A9-A8)
C9 =C8+B9
D9 =1000-C9
Fill down B9, C9, D9 through B108, C108, D108
E8 =LN(C8)
Fill down Copy E8 through E108
Plot A and B against *t*

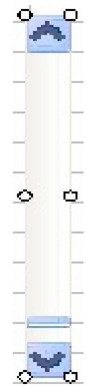
Plot ln A against *t*
Save and Close

(You might like to change the values in Column A to intervals of 0.5 to see the effect that the choice of dt *has on the accuracy of the Euler method.)*

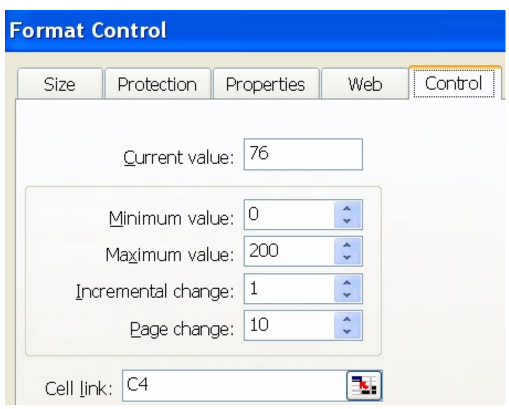


3) Building a Slider Bar

Open the Integral method sheet in Excel that you saved earlier.
Choose View > Toolbars > Forms from the pull down menu. Excel 2007 users should choose Developers > Insert Form Control > Scroll Bar.
You should see the forms menu shown at the right.
Click the slider bar icon (6th down on left), then click on an empty space in the worksheet. You should see a very large slider bar appear as shown at the right.



Adjust the size of the slider bar (narrower and longer) by dragging on a highlighted corner. Note that if the slider is not selected, clicking on it will *move* the entire slider rather than selecting it. To select it, right click on it so that it appears as shown.
Make sure the slider is selected, then double click the slider bar to bring up the Format Control window.



Change the maximum value to 200. In the Cell link: window, type in C4. This will be the cell that our slider bar will control.
Click OK to close the Format Control window.
In cell B4 (where the value for *k* is located)
B4 =C4/100
Our Slider bar controls cell C4 which drives cell B4 (the rate constant) to change values between 0 and 2 in increments of 0.01.
Click and drag the slider and observe the changes in the spreadsheet values and graphs.
Save and Close.