Chemistry 4000/5000/7000 Fall 2010 Assignment 1

Due: Friday, Sept. 17, 4:00 p.m.

Marks: 8 marks

Note that you must type up your assignment. You can either submit in print or by email. This will apply to all assignments this term.

In this assignment, you will learn to do a few basic things with `xppaut`.

If you don't already have access to a computer with `xppaut`, install it on your computer. Then, start up a text editor (e.g. Notepad in Windows) and create a file containing the following lines:

```
dx/dt=-k*x
param k=1
x(0)=1
done
```

Your file should have a `.ode` extension (e.g. `assignment1.ode`). Note that some Windows and Mac editors are very stubborn about giving text files a `.txt` extension, and that the file browsers on these systems sometimes hide the extension from you (so you may end up creating a file with a `.ode.txt` extension that looks like it has a `.ode` extension in Windows Explorer or in the Mac Finder). If this happens, you may find it difficult to load your input file into `xppaut`. In a terminal window, the `ls` command (in Cygwin or on a Mac) will always show you the correct file name. You can then use the `mv` command to rename a file, as follows:

```
mv file.ode.txt file.ode
```

You may be able to guess the meaning of the lines in this file, but for the record, here is a line by line explanation:

1. This line defines the differential equation we want to study, in this case linear (first-order) decay.

2. Our equation contains a parameter, the decay (rate) constant k. We have to provide default values for all parameters in an `xppaut` input file.

3. By default, all initial conditions are set to zero. In this case, that would be a bad idea, so we set the initial value of x to 1.

4. All `xppaut` input files must end with the keyword `done`.

Run this model in `xppaut`: Start up `xppaut` using this file as the input file, then click on `Initialconds` and `Go`. Then click on `Window/zoom` and `Fit`. To label the axes, click on `Viewaxes` and `2D`, then put in t as the `Xlabel` and x as the `Ylabel`.

Now we want to get our graph out of `xppaut` so that you can include it in your report. You can export the graph directly from `xppaut`: Click on `Graphic stuff` and `Postscript`. Accept all the defaults in the pop-up window and click on the `Ok` button. This will bring up a window that will let you set a name for your output file. Pick a name with a `.eps` extension and click on `Ok`. If you're writing your report with Microsoft Word, be aware that Word handles Encapsulated PostScript (eps) files very badly, and often crashes when including them in a document. There are two options for dealing with this problem:

Option 1: Convert your eps file to another format. The png format tends to work well in Word.

Windows with Cygwin: Run the Cygwin installer (`setup.exe`) and install `ImageMagick`. ImageMagick is a set of utilities for manipulating graphic files. Once it is installed, you can convert your eps file to a png, which Word handles much better, with the following command:

```
convert -rotate 90 file.eps file.png
```

You would of course replace `file` by the actual name of your file. The `-rotate 90` option takes `xppaut`'s landscape orientation graphic and puts it in the correct orientation for import into Word.

Windows without Cygwin: Install Ghostscript and GSview from this web site: `http://pages.cs.wisc.edu/~ghost`. Ghostscript is a PostScript interpreter, and `GSview` is a program that uses Ghostscript to display PostScript files and to convert them to other formats. The `File` menu contains a `Convert` option that you can use to generate a png file.

Mac: Preview can display PostScript files and convert them to the png format.

Option 2: The other option is to get your data out of `xppaut` and to use another program to plot it (e.g. Excel, if that's what you're comfortable with). You will see a row of buttons at the top of the `xppaut` window. One of them says `Data`. Click on this button, which will pop up a window showing the data generated by running the model. This window has several buttons of its own. Click on `Write`, which will pop up a dialog box for saving your data to a file. `Xppaut` saves your data as a text file with the columns separated by spaces. The first column is always the time, t. Each additional column contains one of the variables of the model. In this case, there is only one, x. These files are easily loaded into graphing programs and spreadsheets.

Once you have made one graph, go back to `xppaut`. Look at the row of buttons at the top of the main window. In particular, locate the two buttons marked `ICs` and `Param`. These will pop up windows that will let you change, respectively, the initial conditions (in this case, $x(0)$) and parameters (k) of your model. Pick new values for *both* of these quantities (any values that strike your fancy that are different from the default values, except $x(0) = 0$) and run the model again. Make sure to click on `Ok` in each of these windows after typing in a new parameter value or IC, or else `xppaut` won't use the new value. Note that both the ICs and parameter windows have a `Go` button, so once you have changed these quantities, you can run the model by clicking on one of these buttons (either one). Generate a graph of x vs t for your new parameters.

Your report for this assignment should consist of

(a) the graph obtained for the default parameters, and

(b) the graph obtained for the values of k and $x(0)$ you selected. Be sure to provide these values in your report.