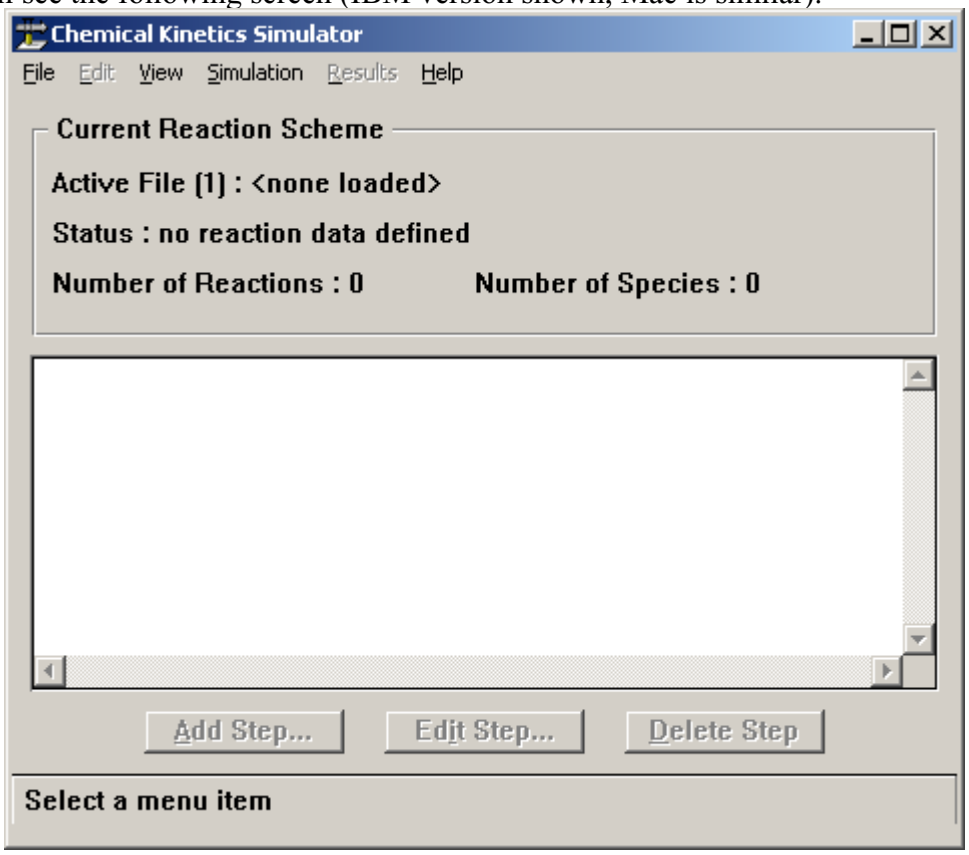
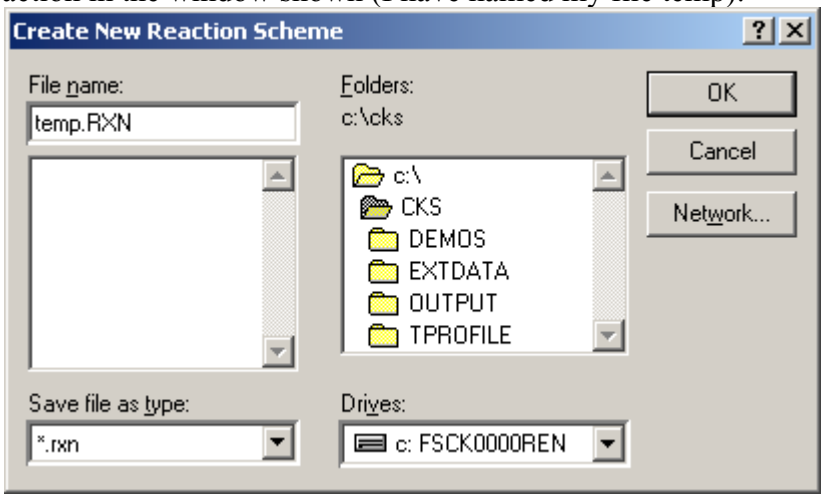
# CKS

CKS is the program that you use to simulate reactions. It can be found in the 7.51 folder on the Desktop of all Pit computers (Macs and PCs). When you start up the simulator, you will see the following screen (IBM version shown, Mac is similar).

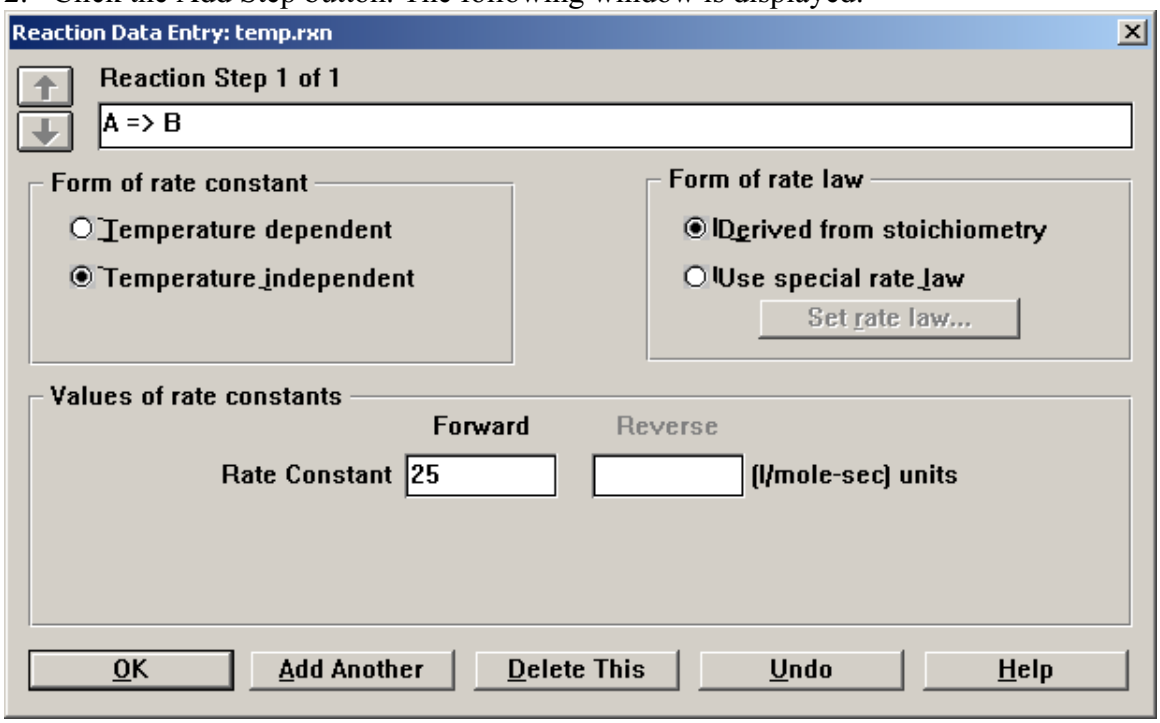



1. Create a new simulation by selecting Create from the File menu. Type in any name for the reaction in the window shown (I have named my file temp):



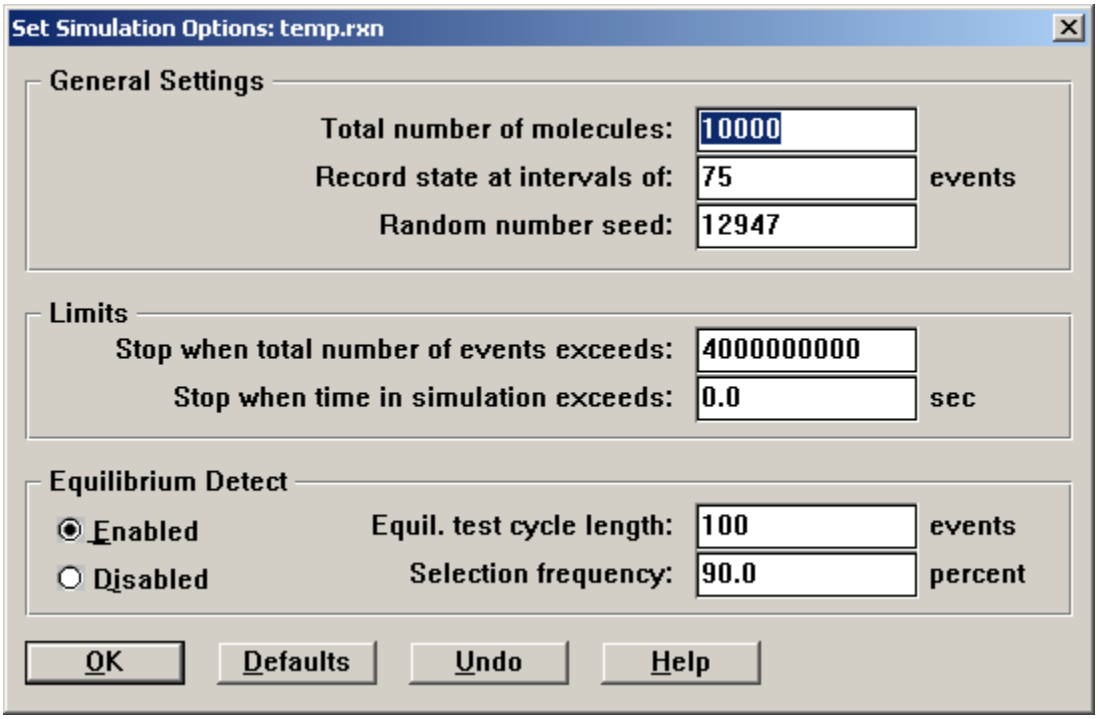

Click OK. You will be returned to the main window.

2. Click the Add Step button. The following window is displayed:



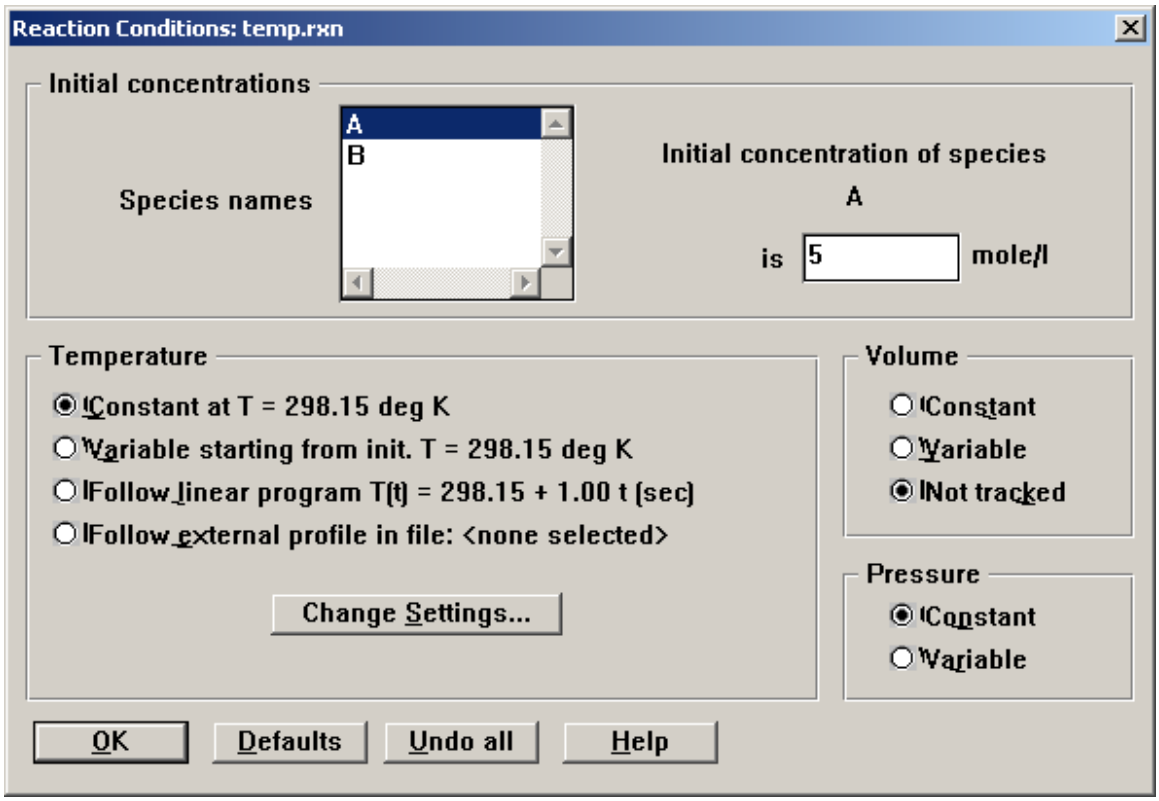

Enter the chemical equation you are simulating. **Note that a space is required between the species and the arrows, and that => is used for a unidirectional reaction, and that <=> is used for a bi-directional reaction**.
Also enter a rate constant for the reaction. Hit OK to close the window. For a multistep reaction, click on Add Another , and enter the next equation in the window shown.
You will be returned to the main window.

3. Select the Simulation Settings option from the Simulation menu. You will be presented with the following window:



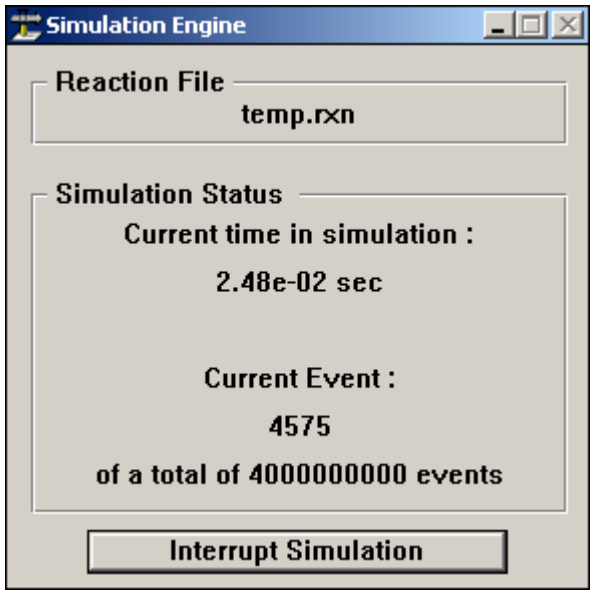

Enter the number of molecules that you want to simulate, as well as other parameters that you want to change, and click on OK. You will be returned to the main window.

4. Select Reaction Conditions from the Edit Menu.



Enter the concentration of all the species, by first selecting the species from the list shown, and then entering the concentration in M in the initial concentration box. When you are finished, click on OK. You will be returned to the main window.

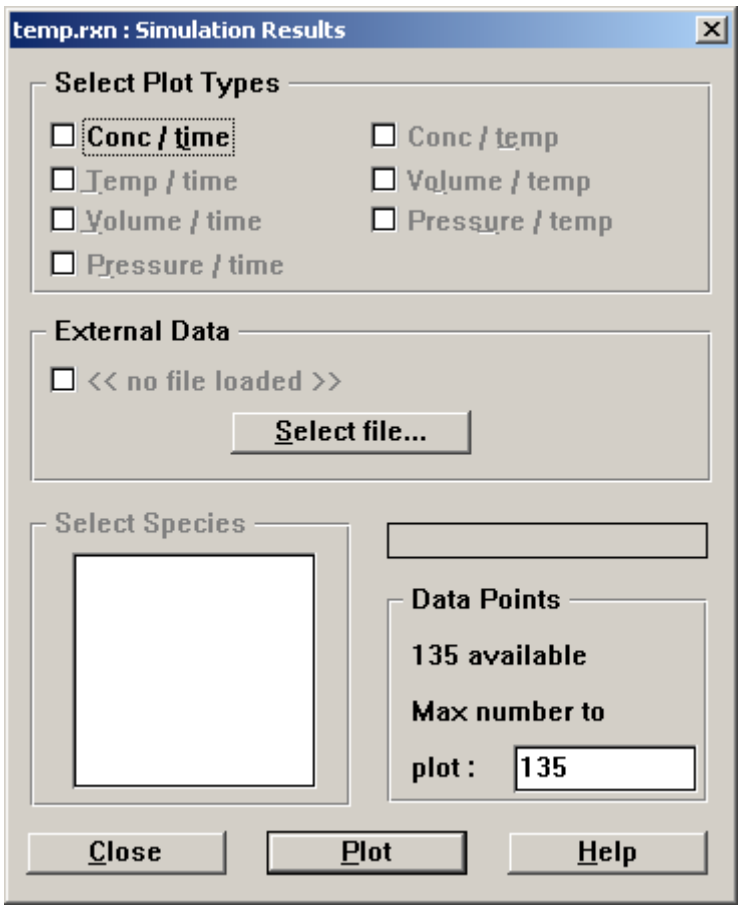
5. Select Start from the Simulation menu. A window will appear with a display of the progress:




Click on Interrupt Simulation if you don t want to continue. Otherwise, wait till the end when the following window is shown:


Click OK. You will be returned to the main window.

6. Plot the results, by selecting Plot Results from the Results menu. You will see the following window:




Select Conc/time, the species from the Select Species box, and click on the Plot button. The data will be plotted as shown below: