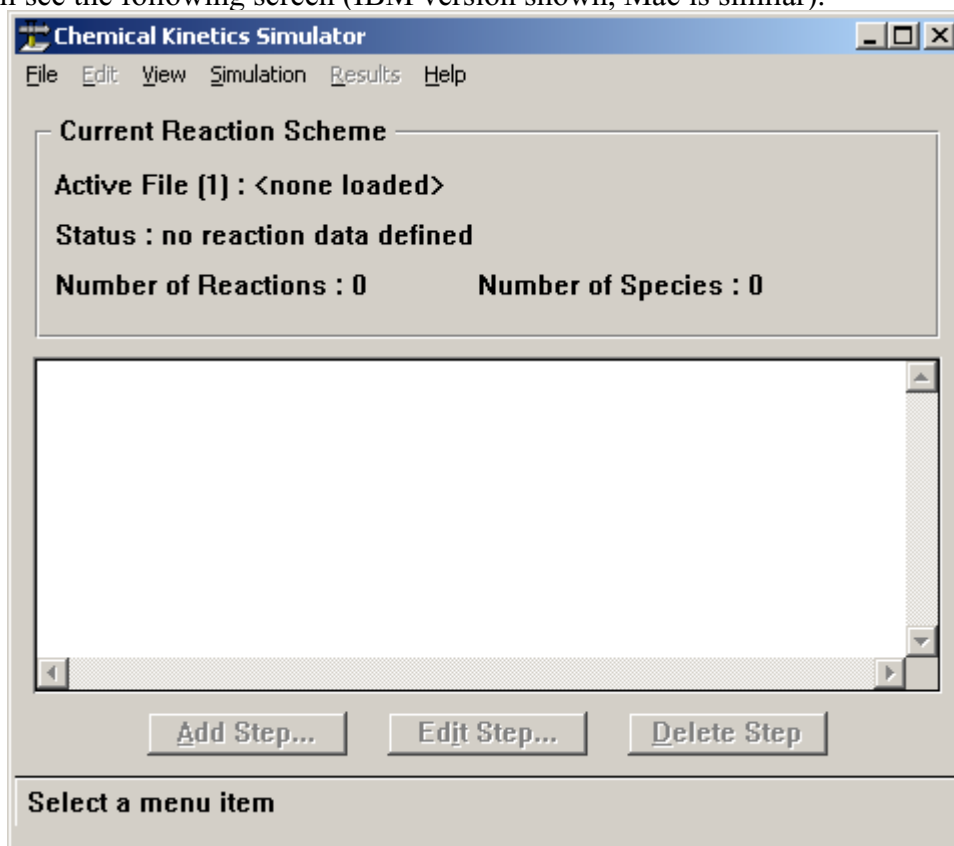
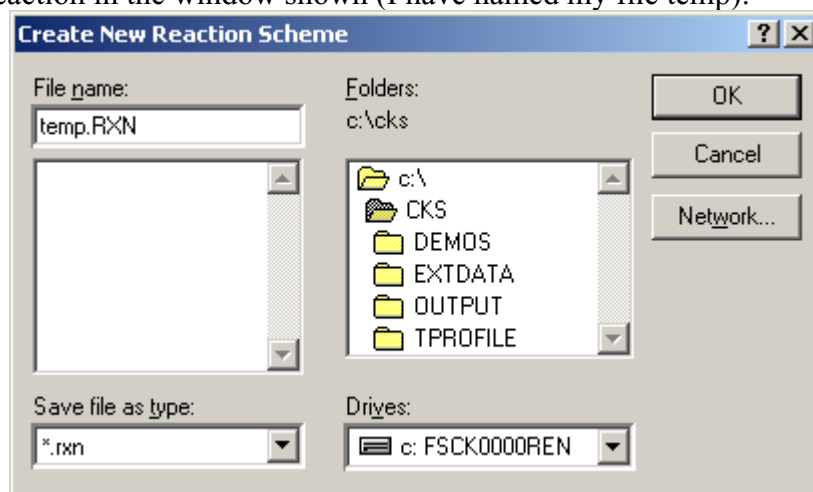


CKS

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:

Reaction Data Entry: temp.rxn

Reaction Step 1 of 1

A => B

Form of rate constant

Temperature dependent

Temperature independent

Form of rate law

Derived from stoichiometry

Use special rate law

Set rate law...

Values of rate constants

	Forward	Reverse	
Rate Constant	25		(l/mole-sec) units

OK Add Another Delete This Undo Help

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:

Set Simulation Options: temp.rxn

General Settings

Total number of molecules:

Record state at intervals of: events

Random number seed:

Limits

Stop when total number of events exceeds:

Stop when time in simulation exceeds: sec

Equilibrium Detect

Enabled Equil. test cycle length: events

Disabled Selection frequency: percent

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.

Reaction Conditions: temp.rxn

Initial concentrations

Species names:

Initial concentration of species A is mole/l

Temperature

Constant at T = 298.15 deg K

Variable starting from init. T = 298.15 deg K

Follow linear program $T(t) = 298.15 + 1.00 t$ (sec)

Follow external profile in file: <none selected>

Volume

Constant

Variable

Not tracked

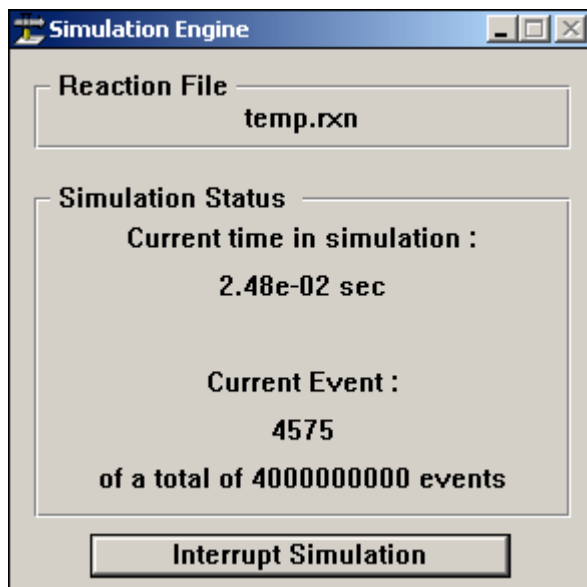
Pressure

Constant

Variable

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:

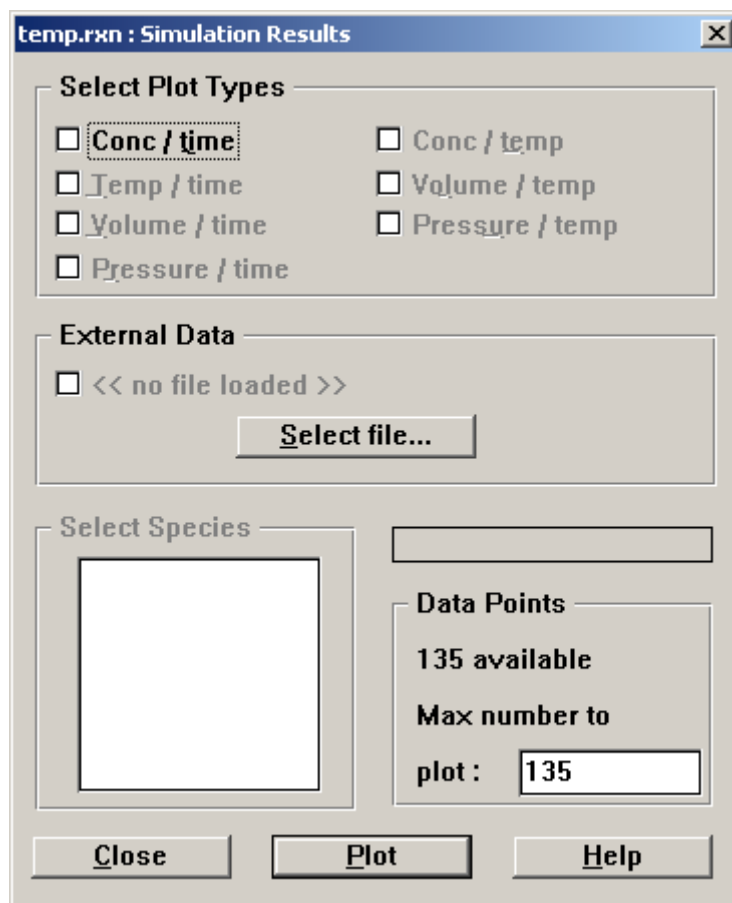


Click on Interrupt Simulation if you don't want to continue. Otherwise, wait till the end when the following window is shown:



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:

