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).

| 🐮 Chemical Kinetics Simulator | | | | |
|--|----------|--|--|--|
| <u>File Edit View Simulation R</u> esults <u>H</u> elp | | | | |
| Current Reaction Scheme | | | | |
| Active File (1) : <none loaded=""></none> | | | | |
| Status : no reaction data defined | | | | |
| Number of Reactions : 0 Number of Species : 0 | | | | |
| | | | | |
| | ^ | | | |
| | | | | |
| | | | | |
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| | | | | |
| | | | | |
| त | | | | |
| Add Step Edit Step Delete Step | | | | |
| Select a menu item | | | | |

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):

| | | - | |
|------------------------------------|---|---|------------------|
| Create New Reaction Schem | e | | ? × |
| File <u>n</u> ame: temp.RXN | Eolders: c:\cks | | OK Cancel |
| | CKS DEMOS EXTDATA OUTPUT TPROFILE | • | Net <u>w</u> ork |
| Save file as <u>type:</u> *.rxn | Drives: | • | |

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 | X | | |
|---|-----------------------------|--|--|
| Reaction Step 1 of 1 | | | |
| A => B | | | |
| Form of rate constant | - Form of rate law | | |
| O Temperature dependent | IDgrived from stoichiometry | | |
| • Temperature_independent | O Use special rate_law | | |
| | Set rate law | | |
| Values of rate constants Forward Reverse | | | |
| Rate Constant 25 | (l/mole-sec) units | | |
| <u>QK</u> <u>A</u> dd Another <u>D</u> elete This <u>U</u> ndo <u>H</u> elp | | | |

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: 10000 | | | |
| Record state at intervals of: 75 event | s | | |
| Random number seed: 12947 | | | |
| | | | |
| Limits | | | |
| Stop when total number of events exceeds: 400000000 | | | |
| Stop when time in simulation exceeds: 0.0 sec | | | |
| – Equilibrium Detect | | | |
| | | | |
| Enabled Equil. test cycle length: 100 event | S | | |
| O Disabled Selection frequency: 90.0 perce | nt | | |
| | | | |
| <u>O</u> K <u>D</u> efaults <u>U</u> ndo <u>H</u> elp | | | |

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 | ncentration of species A s 5 mole/l |
| Temperature | Volume |
| ● <u>©</u> onstant at T = 298.15 deg K | O Constant |
| O. Va riable starting from init. T = 298.15 deg K | O⊻ariable |
| O Follow_linear program T(t) = 298.15 + 1.00 t (sec) | ● INot tracked |
| O Follow_external profile in file: <none selected=""></none> | |
| | Pressure |
| Change <u>S</u> ettings | ● Co <u>n</u> stant |
| | O Va riable |
| <u>O</u> K <u>D</u> efaults <u>U</u> ndo all <u>H</u> elp | |

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:

| temp.rxn : Simulation Results | × | |
|-------------------------------|-----------------|--|
| C Select Plot Types | | |
| Conc / time | Conc / temp | |
| | Volume / temp | |
| Uolume / time | Pressure / temp | |
| Pressure / time | | |
| – External Data | | |
| << no file loaded >> | | |
| Select file | | |
| | | |
| - Select Species | | |
| | | |
| | Data Points | |
| | 135 available | |
| | Max number to | |
| | plot : 135 | |
| | plot : 135 | |
| <u>C</u> lose <u>P</u> lo | t <u>H</u> elp | |
| | | |

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

