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				
	^			
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:

