Matlab interactive kinetics visualization package developed by: Phalgun Lolur, <u>plnp6@mst.edu</u> Missouri University of Science and Technology

User Instructions

The reaction kinetics package is an educational tool to visualize different types of reaction kinetics. The execution is fairly straightforward. The package is to be downloaded and saved in some chosen folder. The following four reactions can be explored using the package:

Reaction 1 (r1)

$$A \frac{k_1}{k_2} I \frac{k_3}{k_4} B$$

Reaction 2 (r2)

$$A \frac{k_1}{k_2} B + C$$

Reaction 3 (r3)

$$A \frac{\frac{k_1}{k_2}}{k_2} I_1 \frac{\frac{k_3}{k_4}}{k_4} I_2 \frac{\frac{k_5}{k_6}}{k_6} B$$





After setting the home directory of MATLAB to the folder containing the provided Matlab files, simply enter r1, r2, r3 or r4 in the command window to run the Graphical User Interface (GUI) for the corresponding reaction.

Command Window					
fx	>> r1				

This is how the GUI should look once it is initialized.





Set the values of rate constants, initial concentrations and the time range. To begin, hit "Start", a calculation of the species concentrations will appear and should look similar to –

After running the calculation, to further explore the reaction behavior, the rate constants can be varied using the sliders to produce dynamically updated results. The user can input the minimum and maximum values of each rate constant in their respective boxes. Hitting the left and right arrow on the slider will vary the value by 20% of the specified range. To obtain finer increments, the user can click on the gray area of the slider to vary the value of the rate constant by only 1%. This process is dynamic, i.e. the plot is updated as the slider is moved. The final concentrations are displayed in the "Concentration" section. Time and concentration data are saved in the working directory under the names of "time" and "concentration" respectively as ASCII values. They can be opened and exported using any text editing programs like Notepad, WordPad etc.