NumKinFit is a python-based (Python 3.7) program created to numerically calculate time resolved concentrations of reacting species. Moreover, it can also fit initial concentration and rate coefficient parameters of a reaction model to experimental measurements. Along with standard modules in Python 3.7 (default install with Anaconda) such as numpy, scipy, matplotlib and tkinter, a fitting module based on scipy, lmfit, are required to run this program. Listed here are the various inputs that should be provided by the user for kinetic modelling and fitting using the GUI version of this program:

1) The reactions should be entered in the 'Reaction Model' box. Each reaction is entered in a different line. An example of the reaction entry is provided as the default input. The reactants and products are separated by a '=' symbol. Each reaction needs a variable for rate coefficient separated from the reaction by a ':' symbol. All the letters and symbols are separated by a space key.

2) All the molecules involved in the model should be entered in the 'Reaction Species' entry. The species labels should be consistent with the 'Reaction Model' entry and should be separated by a ':' symbol.

3) Concentration of all the species should be provided in the 'Initial Concentrations, C0' entry. All the values should be entered in the same order as the 'Reaction Species' entries and each value are separated by a ':' symbol. The unit of concentrations should match the unit for 'Initial Rate Coefficient, k' entry which is described later. [Be aware that the gas phase and condensed phase units are generally different]

4) The 'Time Start' and 'Time Stop' entries for the simulation should be in the units of seconds. The 'Number of Steps' specified determines the step size of the simulation time.

5) Any species involved in the model can be selected to be plotted after numerical integrations. These are specified in the 'Species to Plot' entry which should be consistent with the species label in 'Reaction Species' entry. Each species label should be separated by a ':' symbol.

6) Initial value of the rate coefficients for each reaction should be provided in the 'Initial Rate Coefficients, k' entry. The rate coefficients are entered in the order that the reaction appear in the model and separated by a ':' symbol.

7) Pressing the 'Model' button will result in numerical simulation of the 'Reaction Model' based on the values given for 'Initial Concentrations, C0', 'Time Start', 'Time Stop', 'Number of Steps' and the 'Initial Rate Coefficients, k' entries. A plot window will appear with concentrations of species specified in the 'Species to Plot' entry.

8) The default 'Measured Species' entry is 'None' which results in a plot of modelled concentrations. However, if any reaction species label is provided in the 'Measured Species' entry, hitting the 'Model' button will open a dialog box which allows user to enter a measurement text file. The measurement text file should be tab separated and the first column should be time. The order of species label in the 'Measured Species' entry should match the order of the measurement columns after the time column. The simulated and experimental concentrations are then plotted in the same graph and this feature can be useful in initial refinement of the reaction model.

9) The 'Fit' button will result in fitting of the model to the experimental concentration of the species provided in the 'Measured Species' Entry. The parameters varied during the fitting process depends on the values for 'k min -Fit', 'k max -Fit', 'C0 min -Fit' and 'C0 max -Fit' entries. The values for each of these entries should be provided in the same order as the 'Initial Rate Coefficient, k' and 'Initial Concentrations, C0' entries. If the minimum and maximum values are equal, these parameters are fixed during the fitting process.

10) An example dataset (example_1.txt) has also been uploaded in the repository which contains three-tab separated columns for time, Species A and B. This dataset can be used by the user, as an example, to optimize the default reaction model parameters provided in the GUI.