Functional Specifications

Background:

Programming is a skill that not everyone in the science community has, especially young learners who have not had the opportunity to learn yet. This makes many analysis tools difficult to use because they are based so heavily on using the terminal or having previous knowledge of functional programming. We would seek to create a tool that would allow users to create their own reactions and model their reaction kinetics, viewing them on a graph. Similar packages such as COPASI do similar work by allowing their user to create their model from equations. What our package would offer is a more simplistic version of this to make modeling more accessible. In COPASI, the user must create the graph themselves which is a lot of work and requires knowledge of the system to begin with in order to make the axes and other components of the graph. Our package would take care of the simulation and plotting behind the scenes and would provide the graph to the user after they had inputted their equations and parameters. Another package that interacts with the user to create a model is JigCell. While JigCell allows the user to make a model through a drag and drop system, it does not run any simulations or create any output in the form of visualization. While our package does not allow for drag and drop visualization, it would be an easy way for users to create a model from equations and immediately see the steady state graphs. Another package that offers a similar experience is SBMLWebApp. This app only allows the user to analyze SMBL models, so our package would instead allow not just analysis of SMBL models, but also antimony.txt files and user created models. Finally the package that is most similar is EasyModels. This is a java based application that has the same functionality as our package but has a few added features such as viewing the model as you make it. While this app has higher functionality, one trade off with this is that the interface is confusing and not straightforward. For our package we have traded this functionality for a very simple design with a very straightforward process.

User Profile:

This tool would be useful for many different types of people, but it is built for those who have knowledge of the chemistry of reactions but do not have the programming knowledge to computationally model the kinetics. This includes but is not limited to students in chemistry classes or scientists without programming backgrounds. The user would have to be able to follow directions to download the package through their terminal, using pip install. Then they follow the readme file instructions which will produce a python file they execute, launching our app package.

Desired Information from the System:

Plots of computational system models. Users will want to be able to create concentration plots for the species in their systems as a final product.

Steady State Values: Users will want to learn what the steady state values are for their system.

Use Cases:

a) The user would build a reaction, input kinetic variables, and then output a steady state plot

b) The user would submit an antimony model and then view the resulting steady state plot

c) The user would submit an SMBL file and then view the resulting steady state plot