Quick Introduction into Modeler

Justin Womack, PhD Candidate
Medical College of Wisconsin
Biomedical Engineering
Jwomack@mcw.edu

Note to Readers

This program is meant to make modeling simple. This documentation will go over each aspect of the program, as well as present an example problem at the end.

Best of luck,

Justin Womack

Contents

1 Inputting Variables

This section will cover the basics of entering variables into the model (not that there is much to say)

1.1 UI

This section will cover step by step walkthrough of using the variable enter page.

2 Equation Builder

Cover basic info on how to use equation builder.

2.1 Chemical Equation

This section will cover the law of mass action and the UI of how to use it.

Chemical reactions are derived using the law of mass action. Using the following equation as a base:

$$aA + bB \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} cC + dD$$

The law is as follows:

$$-\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{c}\frac{d[C]}{dt} = \frac{1}{d}\frac{d[D]}{dt} = k_1[A]^a[B]^b - k_{-1}[C]^c[D]^d$$

From the above law, each individual term can is derived below:

$$\begin{aligned}
\frac{d[A]}{dt} &= -a * k_1[A]^a[B]^b + a * k_2[C]^c[D]^d \\
\frac{d[B]}{dt} &= -b * k_1[A]^a[B]^b + b * k_2[C]^c[D]^d \\
\frac{d[C]}{dt} &= c * k_1[A]^a[B]^b - c * k_2[C]^c[D]^d \\
\frac{d[D]}{dt} &= d * k_1[A]^a[B]^b - d * k_2[C]^c[D]^d
\end{aligned}$$

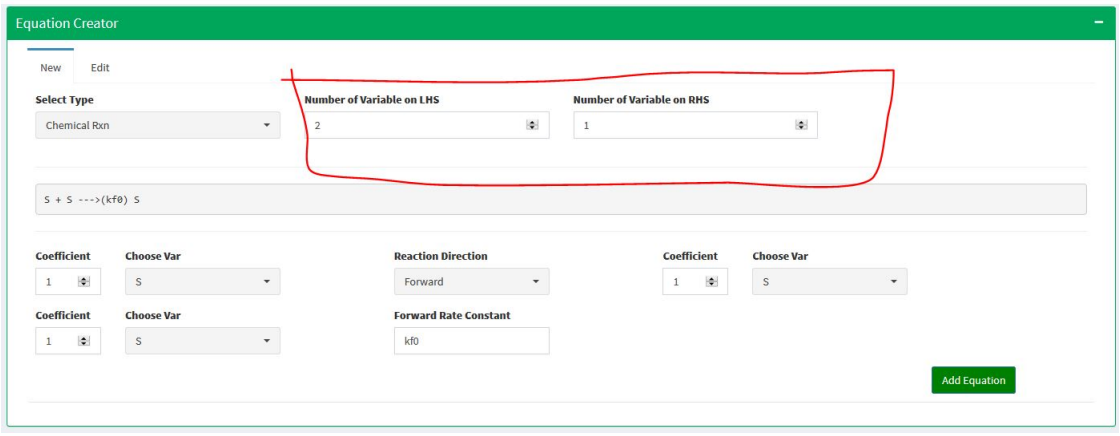
Each individual equation will be added to their overall flux differential equation in the differential equation solver section.

2.1.1 Chemical Equation UI

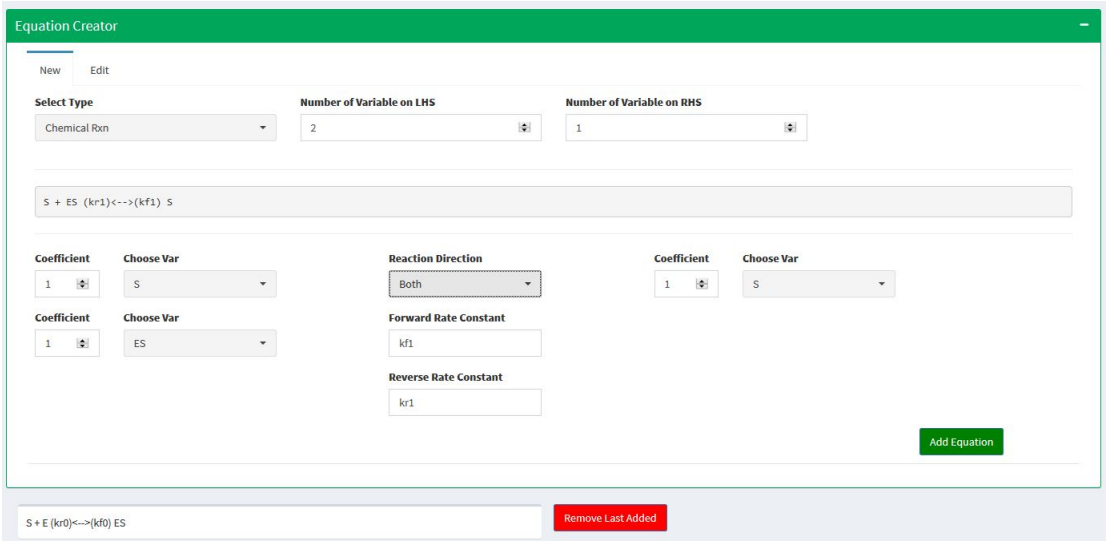
Chemical equation input currently has dropdowns and number selections to easily input your chemical reactions. For this section we will use a simple reaction of Substrate(S) reacting with an Enzyme (E) to from a substrate-Enzyme complex (ES).

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \tag{1}$$

To Start, simply select the number of variables you want to have on each side of your equation:



Then input the reaction variables, whether the reaction is in one direction or both directions, the variable coefficients, and press Add Equation. Note that the equation is currently shown in text form below the UI used to enter it. There is also a delete last equation button in the event of a quick error.



2.2 Passive Diffusion

This section will cover the basics of passive diffusion and Ficks Law.

3 Adding Input/Outputs to Your System

3.1 Simple Rate

A simple rate input(r_{in}) or output(r_{out}) will take in a rate constant to multiply by the targeted species (S). It is simply saying "I want this species entering or leaving at this rate". Input rate is give by the following flux J:

$$J = r_{in} * S$$

Output rate is given by:

$$J = -r_{out} * S$$

3.1.1 UI Walkthrough

Here we will place a picture by picture walk through of how to use rate in/out.

3.2 Passive Diffusion In/Out

This section will cover the flux equation of the passive diffusion input/output

3.3 Synthesis/Degradation Through Enzyme

Enzyme (E) degradation/synthesis in this application will use Michaelis-Menten (MM) kinetics for its equation solving. The Michaelis-Menten equation makes use of V_{max} (the maximum velocity of the reaction) and K_m (the MM constant). The following is the equation for synthesis of a substrate (S) by an enzyme:

$$J = \frac{V_{max} * S}{K_m + S} = \frac{k_{cat} * E * S}{K_m + S}$$

The following is the equation for the flux used to generate the degradation of a substrate by an enzyme:

$$J = -\frac{V_{max} * S * E}{K_m + S} = -\frac{k_{cat} * E * S}{K_m + S}$$

3.3.1 UI Walkthrough