Table 1| Bistable Network

Opened Network	Kinetic Constants
Y --> 2X 2X --> X+Y X+Y --> Y X --> 0 0 --> X	$k_1 = 35$ $k_2 = 1$ $k_3 = 1$ $k_4 = 9.74$ $k_5 = 33$
Refernce: Thomas Wilhelm. 2009 The smallest chemical reaction system with bistability https://bmcsystbiol.biomedcentral.com/articles/10.1186/1752-0509-3-90	

The original network considered consists of five reactions and four components. Component S is only seen as a reactant in reaction one and is thus eliminated from the system. Component P is also eliminated from the system, because it is only seen as a product. From eliminating these components, the modified reaction network can be considered opened. This leaves the kinetic constants the same as the original network. From this opened network, steady state mass balances on components X and Y is derived.

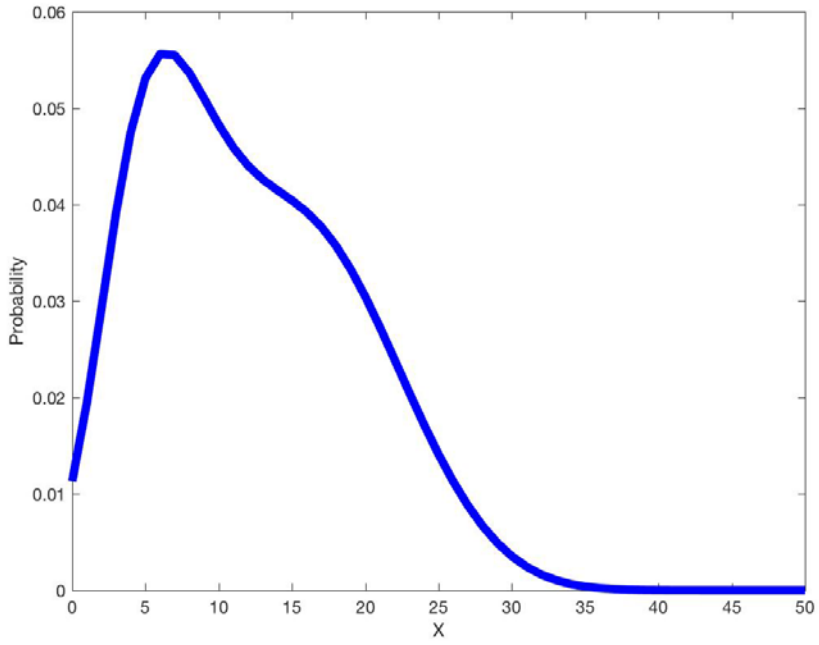
$$\frac{dX}{dt} = 0 = 2k_1Y - k_2X^2 - k_3XY - k_4X + k_5 \quad (1)$$

$$\frac{dY}{dt} = 0 = k_1Y + k_2X^2 \quad (2)$$

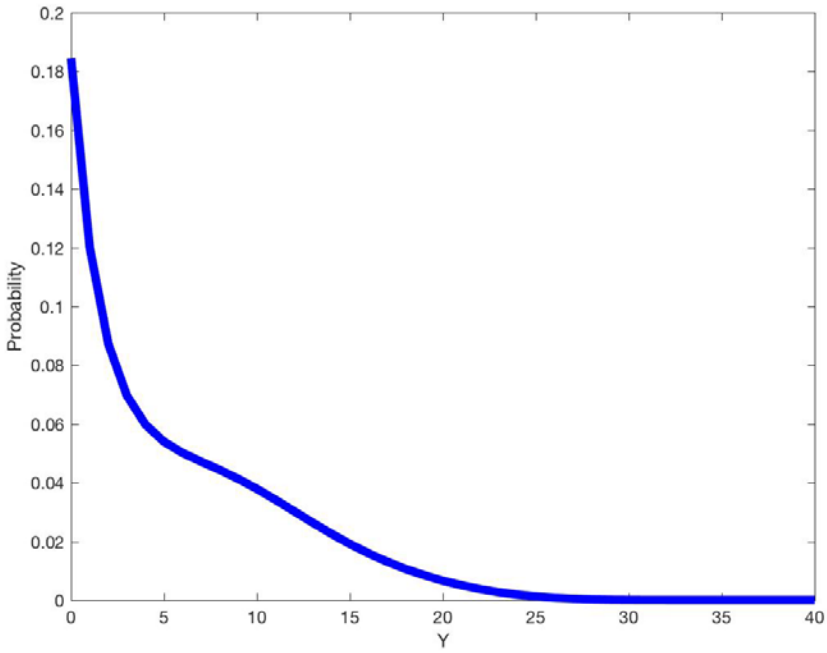
From the steady state balances there are two equations and eight unknowns, this leaves five variables to be specified. The kinetic constants, k_1, k_2, k_3, k_4, and k_5 are specified as 35, 1, 1, 9.74 and 33 respectively. To run the simulation the minimum value for both components is set to zero, and the maximum value for component X is set to 50 and the maximum value for Y is set to 40. The maximum number of moments is set to 4, and all of the initial guesses for the Lagrange Multipliers are set to zero. Table 2 summarizes the parameters required for the simulation, and Figure 1 displays the results.

Table 2| Simulation Parameters

Minimum Values (X,Y)	Maximum Value (X)	Maximum Value (Y)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	50	40	4	0



(A)



(B)

Figure 1| Results from Simulation. A. Component X **B.** Component Y