

Table 1| Reversible Reaction

Reaction Network	Kinetic Constants	Opened Network	Kinetic Constants
$2A \rightarrow B$ $B \rightarrow 2A$	$k_1 = 4$ $k_2 = 1$ $C = 20$	$2A \rightarrow 0$ $0 \rightarrow 2A$ $\frac{1}{2} A \rightarrow 2 \frac{1}{2} A$	$k_1 = 4$ $\frac{1}{2} k_2 * C = 10$ $-\frac{1}{2} k_2 = 0.5$

The original network is a two component, two reaction system. This system can be opened up by eliminating one of the two components, in this case component B is substituted for. The mass on the system is:

$$C = A + 2B \quad (1)$$

C is used to represent the total concentration of the system. When the mass balance is solved for component B the opened network system can be applied. This is displayed in Table 1. With the updated network the kinetic constants for reactions two and three have to be altered as well. The kinetic constant for reaction two is $\frac{1}{2} k_2 * C$ and the reaction constant for equation three is $-k_2$. From the opened network scheme the state mass balance for component A is derived.

$$\frac{dA}{dt} = 0 = -k_1 A^2 + \frac{1}{2} k_2 * C - \frac{1}{2} k_2 A^2 \quad (2)$$

Since there is one steady state balance and four unknown variables, three of the variables must be specified. In this case k_1 is specified as 4, k_2 is specified as 1, and C is specified as 20 molecules. The average concentration of A is then solved as positive and negative square root of twenty divided by nine or numerically approximately positive or negative 1.491. The negative solution is trivial and thus ignored, so the solution is 1.491 molecules. To run the simulation the minimum value for component A is set to zero, and the maximum value is set to 20. The maximum number of moments is set to 2, 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. The plot properly depicts the same steady state calculated from the component balance.

Table 2| Simulation Parameters

Minimum Value (A)	Maximum Value (A)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	20	2	0

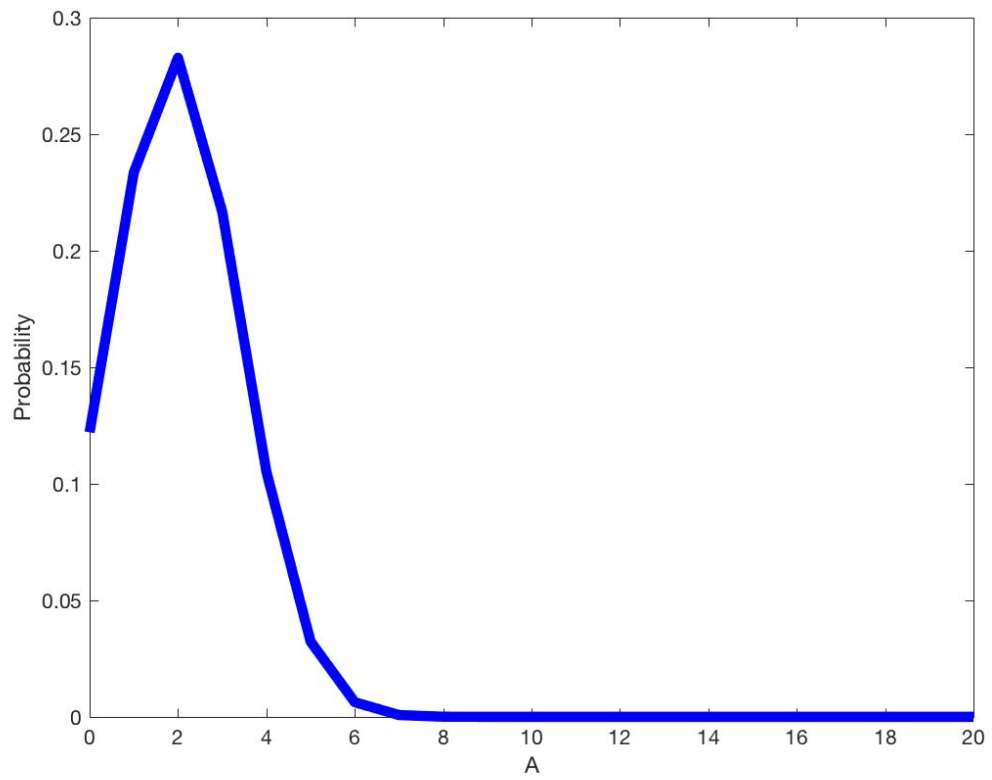


Figure 1| Results from Simulation. Component A results are displayed.