Table 1| Two Component Network

Reaction Network	Kinetic Constants
0 --> A A --> B B --> 0	$k_1 = 10$ $k_2 = 1$ $k_3 = 2$

The original network is a two component and three reaction network. By design this network is opened up. From this reaction network a steady state mass balance is derived for component A and B.

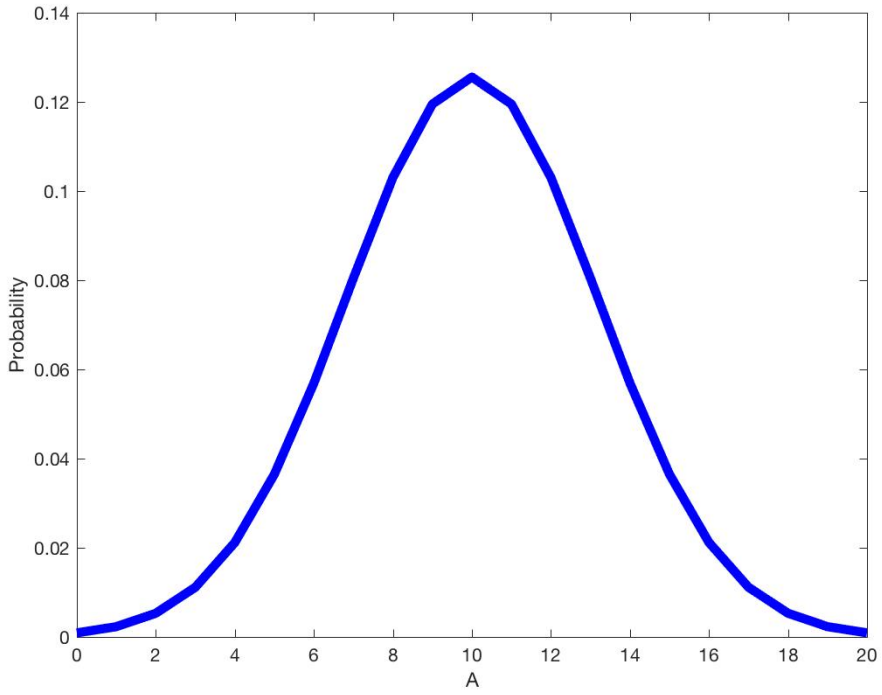
$$\frac{dA}{dt} = 0 = k_1 - k_2 A \tag{1}$$

$$\frac{dB}{dt} = 0 = k_2 A - k_3 B \tag{2}$$

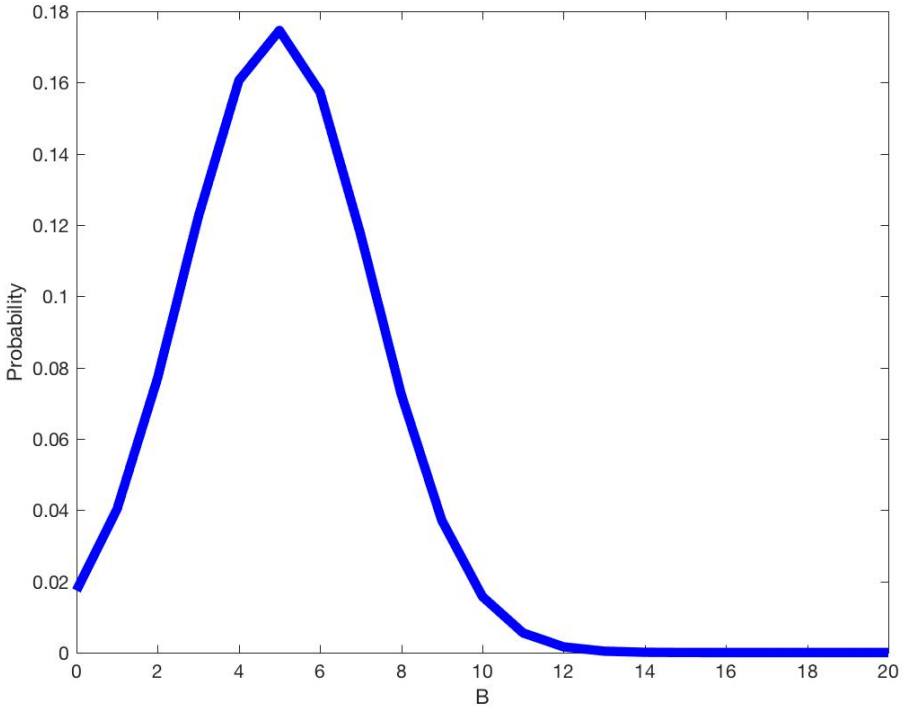
From the steady state balances there are two equations and five unknowns, this leaves three variables to be specified. The kinetic constants, k_1, k_2, and k_3 are specified as 10, 1, and 2 respectively. The average concentration of component A is solved as 10 molecules and the average concentration of component B is 5 molecules. To run the simulation the minimum value for both components is set to zero, and the maximum value for both components 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 plots properly depict the same steady states calculated from the component balances.

Table 2| Simulation Parameters

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



(A)



(B)

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