Table 1| Three Component Network

Reaction Network	Kinetic Constants
0 --> A	$k_1 = 60$
A --> B	$k_2 = 4$
B --> C	$k_3 = 3$
C --> 0	$k_4 = 1$

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

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

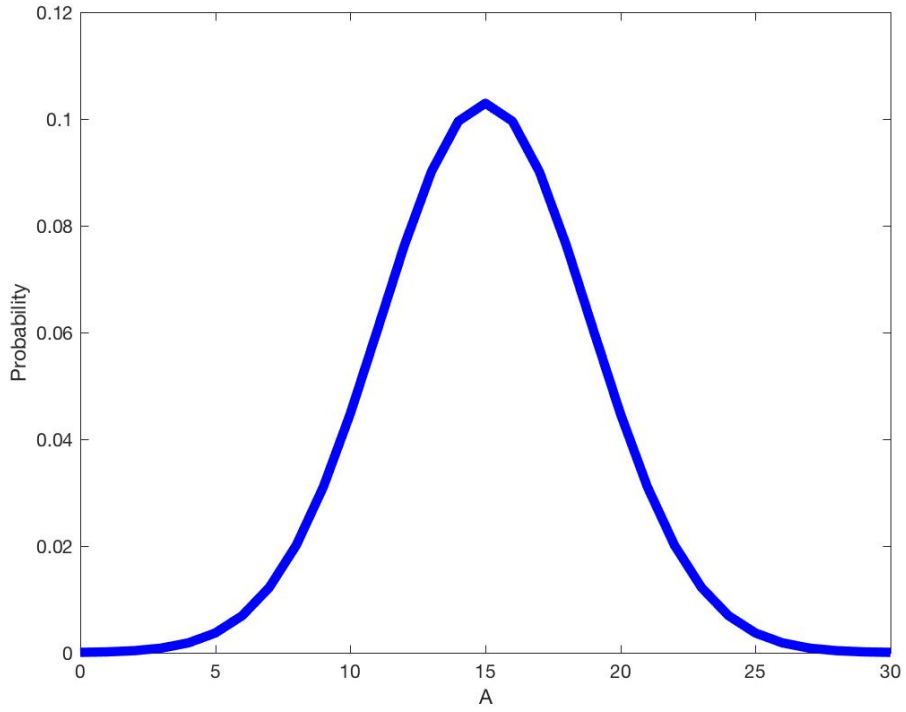
$$\frac{dB}{dt} = 0 = k_2 A - k_3 B \tag{2}$$

$$\frac{dC}{dt} = 0 = k_3 B - k_4 C \tag{3}$$

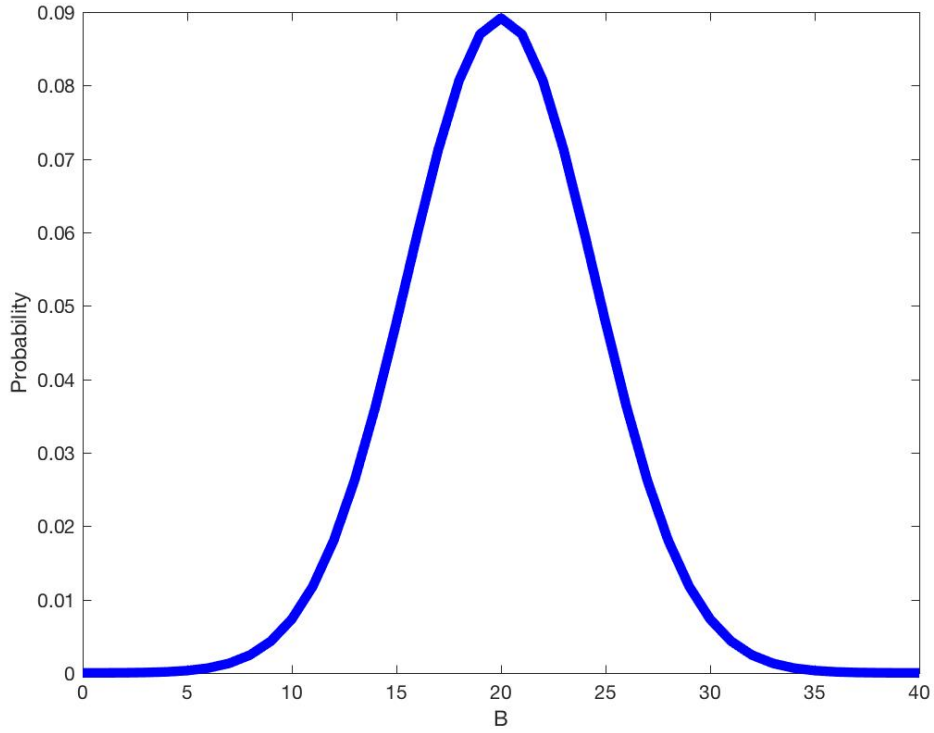
From the steady state balances there are three equations and seven unknowns, this leaves four variables to be specified. The kinetic constants, k_1, k_2, k_3, and k_4 are specified as 60, 4, 3, and 1 respectively. The average concentration of component A is solved as 15 molecules, the average concentration of component B is 15 molecules, and the average concentration of component C is 60 molecules. To run the simulation the minimum value for all components is set to zero, and the maximum values for components A, B, and C are 30, 40, and 120. These values are chosen to roughly center the steady states graphically. 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

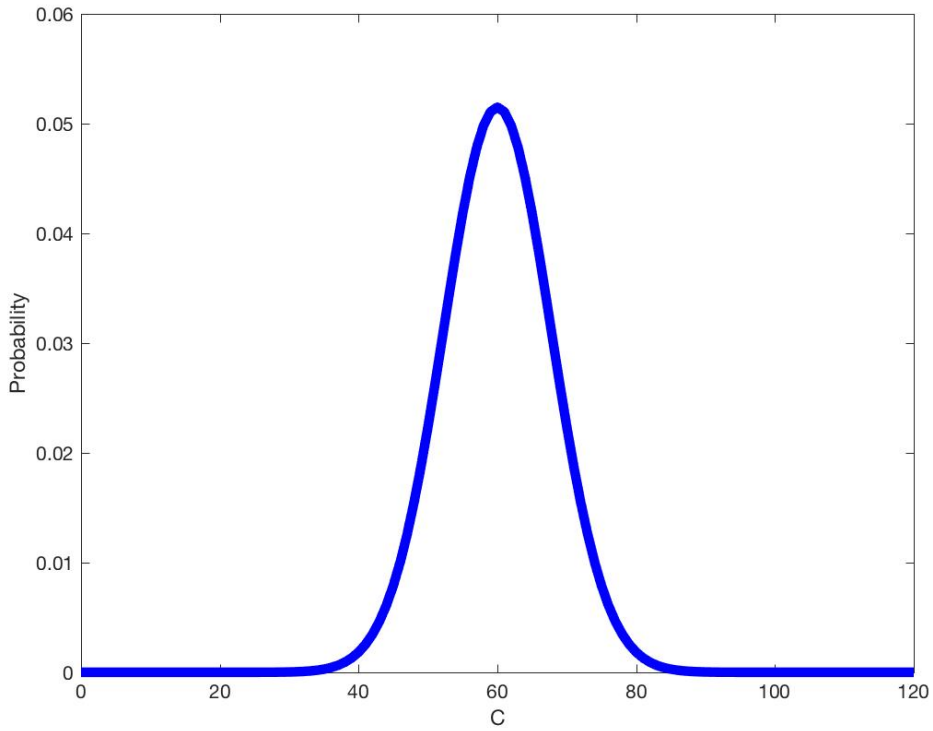
Minimum Values (A,B,C)	Maximum Value (A)	Maximum Value (B)	Maximum Value (C)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	30	40	120	2	0


0.12
0.1
0.08
0.06
0.04
0.02
0
Probability
0
5
10
15
20
25
30
A

(A)


0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
Probability
0
5
10
15
20
25
30
35
40
B

(B)



(C)

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