

Table 1| Four Component Network

Reaction Network	Kinetic Constants
0 --> A	$k_1 = 42$
A --> B	$k_2 = 7$
B --> C	$k_3 = 3$
C --> D	$k_4 = 2$
D --> 0	$k_5 = 1$

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

$$\frac{dA}{dt} = 0 = k_1 - k_2 A \quad (1)$$

$$\frac{dB}{dt} = 0 = k_2 A - k_3 B \quad (2)$$

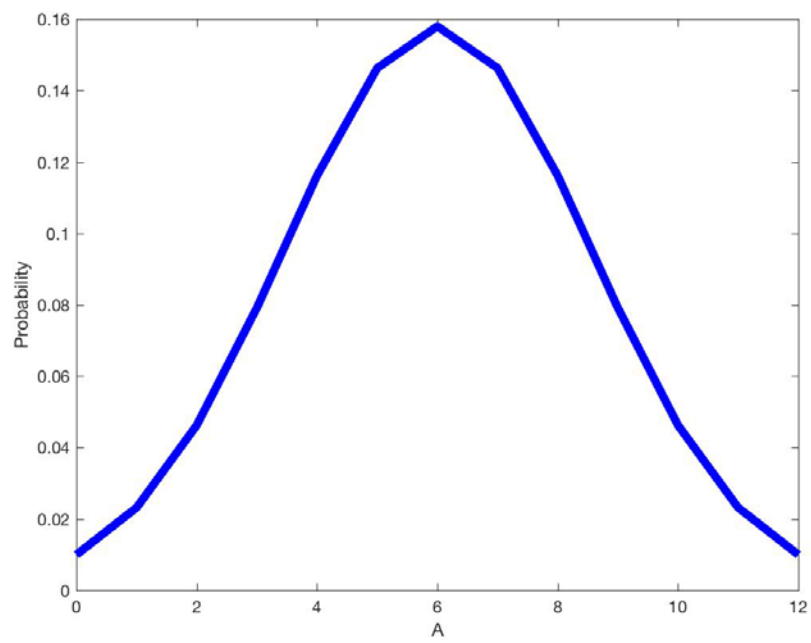
$$\frac{dC}{dt} = 0 = k_3 B - k_4 C \quad (3)$$

$$\frac{dD}{dt} = 0 = k_4 C - k_5 D \quad (4)$$

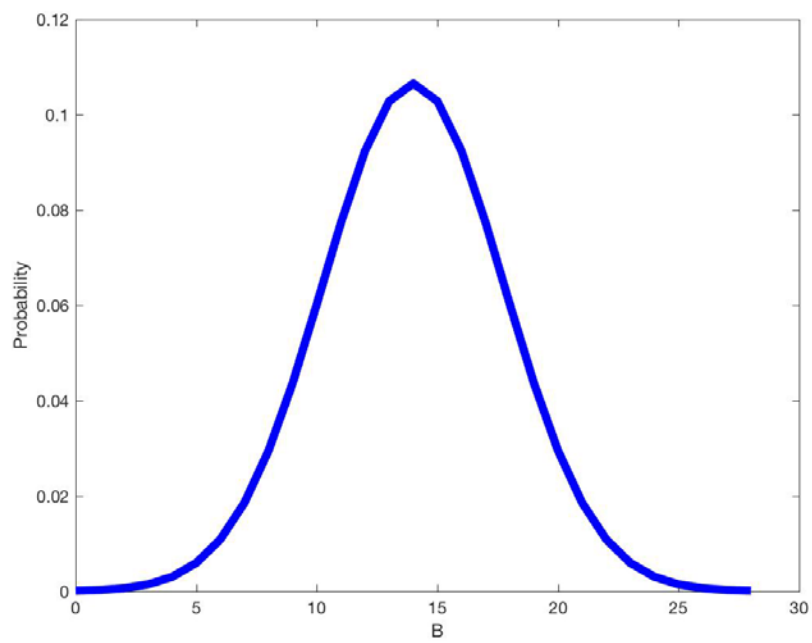
From the steady state balances there are four equations and nine unknowns, this leaves five variables to be specified. The kinetic constants, k_1 , k_2 , k_3 , k_4 , and k_5 are specified as 42, 7, 3, 2, and 1 respectively. The average concentration of components A, B, C, and D are solved for as 6, 14, 21, and 42 molecules respectively. To run the simulation the minimum value for all components is set to zero, and the maximum values for components A, B, C, and D are 12, 28, 42, and 84. 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

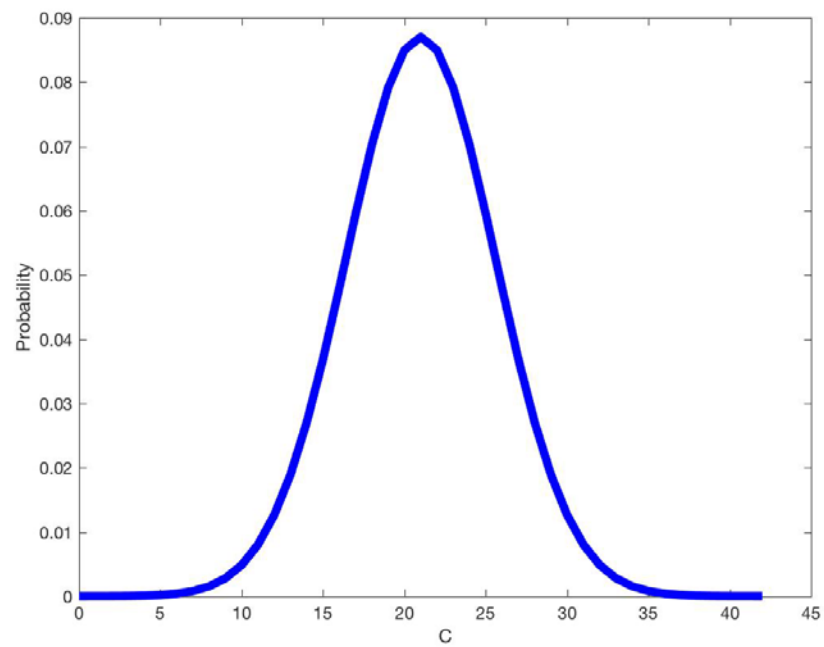
Minimum Values (A, B, C, D)	Maximum Value (A)	Maximum Value (B)	Maximum Value (C)	Maximum Value (D)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	12	28	42	84	2	0



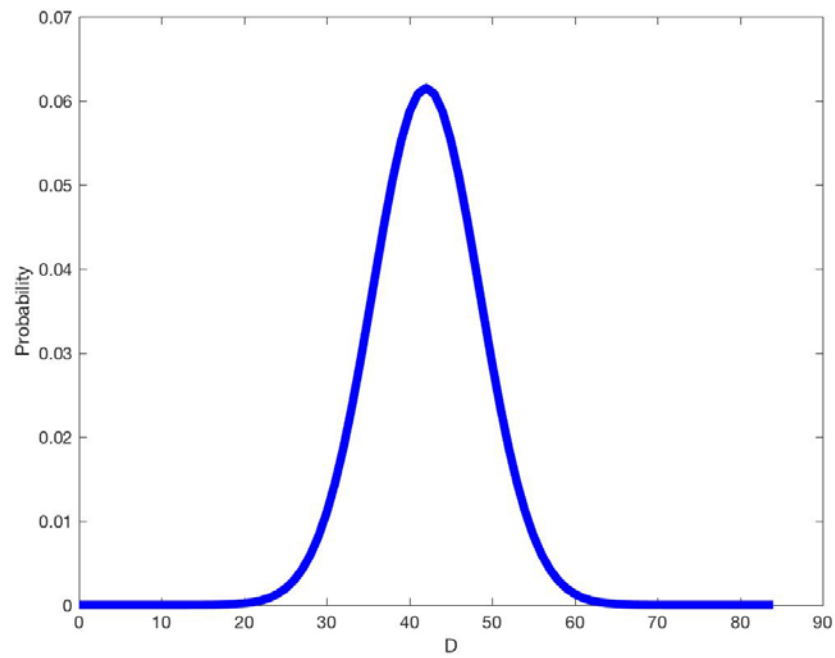
(A)



(B)



(C)



(D)

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