Table 1| Reversible Reaction

Reaction Network	Kinetic Constants	Opened Network	Kinetic Constants
S + E --> S : E S : E --> S + E S : E --> P + E P --> S	$k_1 = 0.1$ $k_2 = 0.1$ $k_3 = 1$ $k_4 = 1$ $E_T = 50$ $S_T = 100$	S + E --> 0 0 --> S + E E --> S + 2E 0 --> E E --> 2E 0 --> S E --> S + E S --> 2S	$k_1 = 0.1$ $E_T*k_2 = 5$ $-½\ k_2 = -0.1$ $E_T*k_3 = 50$ $-k_3 = -1$ $(S_T - E_T)*k_4 = 50$ $k_4 = 1$ $-k_4 = -1$
Reference: M. Vlysidis, Y.N. Kaznessis, 2018 A linearization method for probability moment equations https://doi.org/10.1016/j.compchemeng.2018.01.015			

The original network is a four component, four reaction system. This system can be opened up by eliminating the S:E and P components. To do this mass balances on components S and E are done:

$$E_T = S{:}E + E \tag{1}$$

$$S_T = S{:}E + S + P \tag{2}$$

E_T and S_T are used to represent the total concentration of E and S respectively. When the mass balances are solved for S:E and P the network can be opened up as displayed in Table. The adjusted kinetic constants for the opened network are also displayed in Table 1. From the opened network steady mass balances are derived for components E and S.

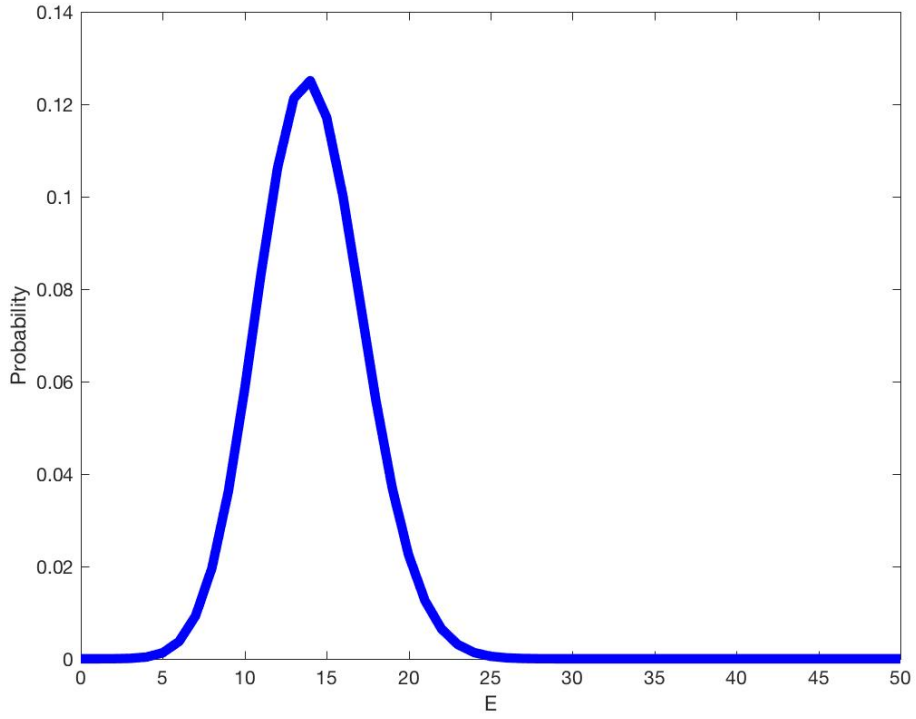
$$\frac{dE}{dt} = 0 = -k_1 SE + E_T k_2 - \frac{1}{2}k_2 E + E_T k_3 - k_3 E \tag{3}$$

$$\frac{dS}{dt} = 0 = -k_1 SE + E_T k_2 - \frac{1}{2}k_2 E + (S_T - E_T)k_4 + k_4 E - k_4 S \tag{4}$$

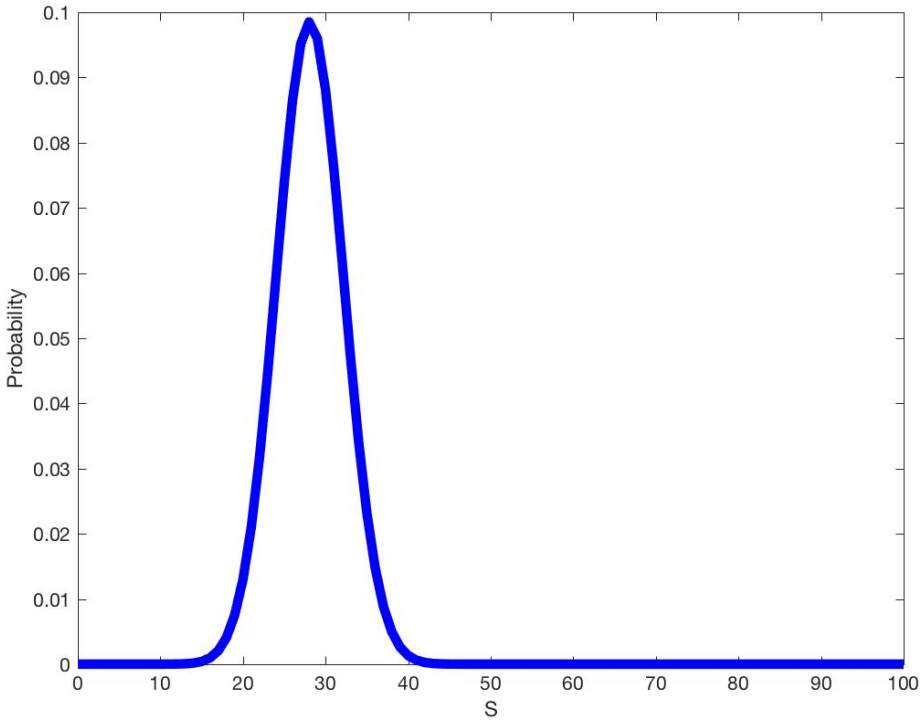
Since there are two steady state balances and eight unknown variables, six of the variables must be specified. In this case the kinetic constants k_1, k_2, k_3, and k_4 are specified as 0.1, 0.1, 1, and 1 respectively. The total concentrations of E and S are also specified as 50 and 100 molecules. To run the simulation the minimum value for both components is set to zero and the maximum values for components E and S are 50 and 100 respectively. 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. The plots properly depict the same steady state calculated from the component balances.

Table 2| Simulation Parameters

Minimum Values (E,S)	Maximum Value (E)	Maximum Value (S)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	50	100	2	0



(A)



(B)

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