Table 1| Autocatalator Network

Reaction Network	Kinetic Constants	Opened Network	Kinetic Constants
0 --> P D + P --> D + 2P P + P --> P + Q P + Q --> 2Q P --> 0 Q --> 0	k_1 = 20 k_2 = 10 k_3 = 50 k_4 = 40 k_5 = 20 k_6 = 500 P_T = 50	0 --> P P --> 2P 2P --> 3P P + Q --> 2P + Q P + P --> P + Q P + Q --> 2Q P --> 0 Q --> 0	k_1 = 20 k_2*P_T=500 -k_2=-1 -k_2=-1 k_3 = 50 k_4 = 40 k_5 = 20 k_6 = 500
Refernce: John Goutsias. 2007 Classical versus Stochastic Kinetics Modeling of Biochemical Reaction Systems https://www.sciencedirect.com			

The original autocatalator network consists of three components and six reactions. The reaction network is opened up by expressing a mass balance on the system and eliminating component D. The mass balance on the system is:

$$P_T = D + P + Q \tag{1}$$

After the mass balance is solved for component D, the reaction network can be opened up as displayed in Table 1. Reaction two from the original network is updated to reflect the elimination of component D. The reaction is now represented by reactions two, three, and four in the opened network column. Kinetic constants for the three new reactions are k_2P_T, -k_2, and -k_2 respectively. From the opened network scheme, steady state mass balances on components P and Q are derived.

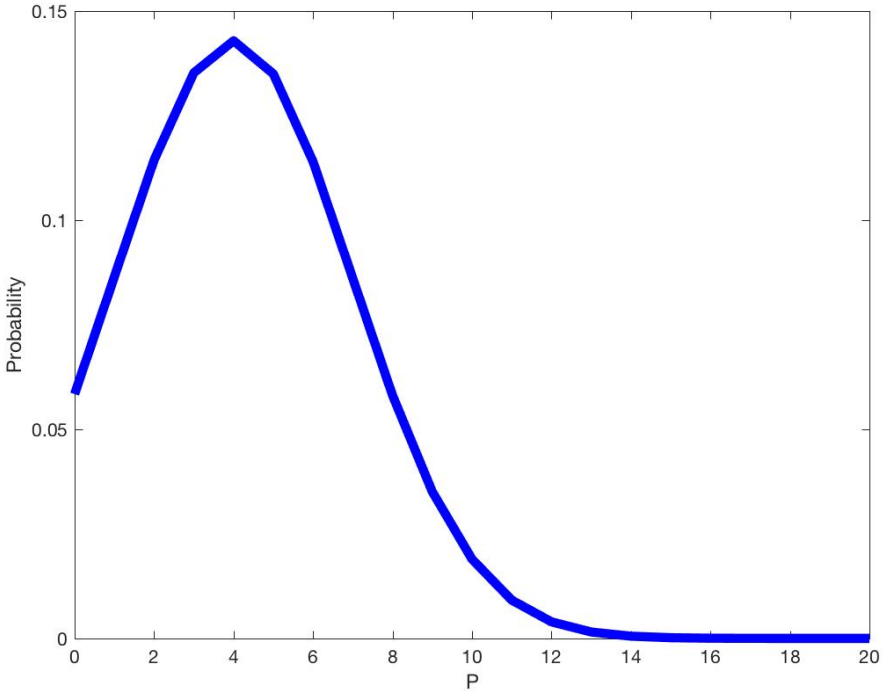
$$\frac{dP}{dt} = 0 = k_1 + k_2P_TP - k_2P - k_2PQ - k_3P - k_4PQ - k_5P \tag{2}$$

$$\frac{dQ}{dt} = 0 = 2k_3P + k_4PQ - k_6Q \tag{3}$$

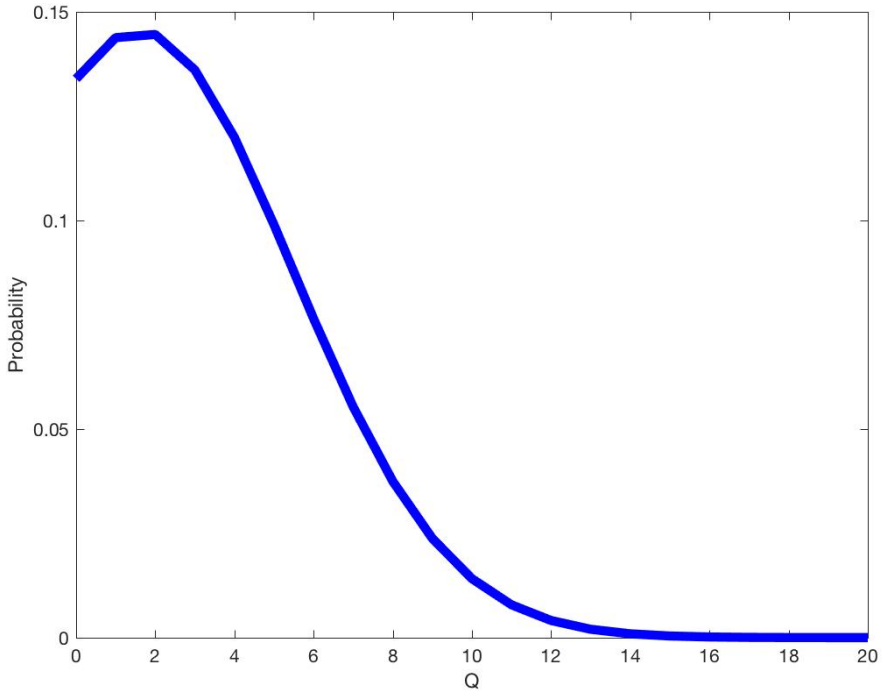
There are two equations from the steady state balances and eight unknowns, so the kinetic constants are specified and the total concentration was specified. The kinetic constants are 20, 10, 50, 40, 20, and 500 respectively, and the total concentration is 50 molecules. Average concentrations for each component are then calculated as 4.4 and 3.5 molecules for P and Q respectively. To run the simulation the minimum values for both components are 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. 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 (P,Q)	Maximum Value (P,Q)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	20	2	0



(A)



(B)

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