

Table 1| Schögl Network

Opened Network	Kinetic Constants
$3X \rightarrow 2X$ $2X \rightarrow 3X$ $X \rightarrow 0$ $0 \rightarrow X$	$k_1 = 0.0015$ $k_2 = 0.15$ $k_3 = 3.5$ $k_4 = 22$
Reference: Schlogl, F , 1971. On thermodynamics near a steady state. Z. Physik 458, 446–458	

The original network is a single component and four reaction network, that is already opened up. From the opened network a steady state mass balance on component X is derived.

$$\frac{dX}{dt} = 0 = -k_1X^3 + k_2X^2 - k_3X + k_4X \quad (1)$$

From the steady state balance there is one equation and five unknowns, this leaves four variables to be specified. The kinetic constants, k_1 , k_2 , k_3 , and k_4 are specified as 0.0015, 0.15, 3.5, and 22 respectively. To run the simulation the minimum value for component X is set to zero, and the maximum value for component X is set to 120. The maximum number of moments is set to 8, 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| Simulation Parameters

Minimum Value (X)	Maximum Value (X)	Maximum Number of Moments	LaGrange Multipliers (Initial Guess)
0	120	8	0

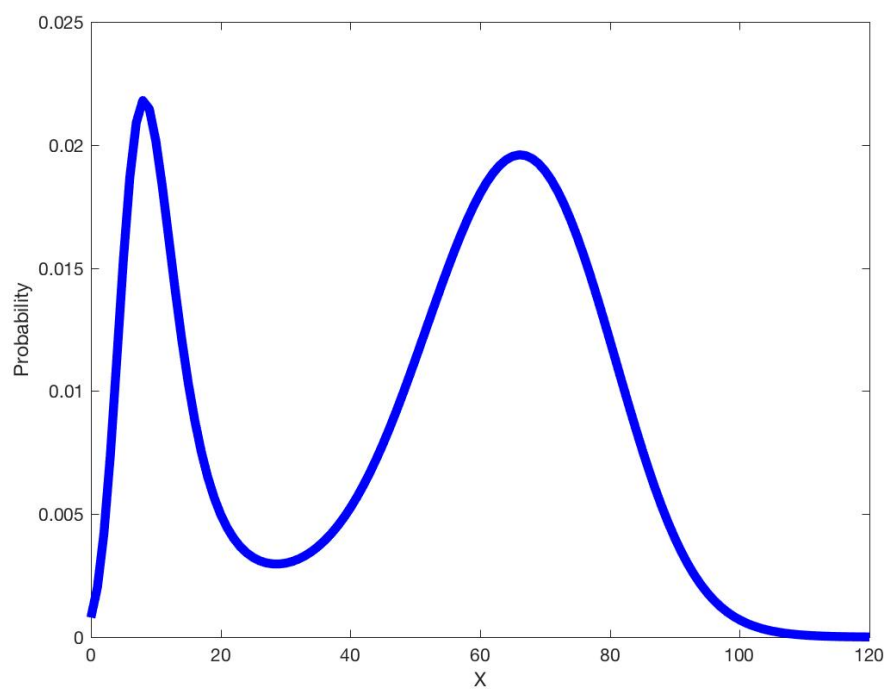


Figure 1| Results from Simulation. Component X