Modeling Reactions

This homework summarizes our material on modeling reactions using ODE, stochastic models, and master equations. It focuses on chemical reactions that admit periodic solutions.

1. For each of the reactions below, construct:
   - ODE model
   - A stochastic model for the evolution of the number of molecules of each type
   - A master equation
   - Use a MATLAB program to solve these equations. Draw phase diagrams for each case. (you should choose parameters that give rise to periodic solution). Such solutions correspond to closed curves in the phase space.

The reactions: (1) Brusselator

\[
\begin{align*}
A & \rightarrow X \\
B + X & \rightarrow D + Y \\
Y + 2X & \rightarrow 3X \\
X & \rightarrow E
\end{align*}
\]

Here assume that the \( A, B, D, E \) molecules are kept at constant values. We are interested in two cases (i) \( b < 1 + a^2 \), and (ii) \( b > 1 + a^2 \), where \( a, b, d, e, x, y \) are the concentration (or number) of molecules of type \( A, B, D, E, X, Y \).

(2) Oregonator

\[
\begin{align*}
A + Y & \rightarrow X + P \\
X + Y & \rightarrow 2P \\
A + X & \rightarrow 2X + 2Z \\
2X & \rightarrow A + P \\
B + Z & \rightarrow \frac{1}{2}fY
\end{align*}
\]
Here we take the number of the $A$ and $B$ type molecules to be constant, and let $f = 1$.

(iii) *Heterogeneous catalysis*

\[
\begin{align*}
P + S &\leftrightarrow X \\
X + 2S &\rightarrow 3S + C \\
Q + S &\leftrightarrow Y
\end{align*}
\]

(3)

Also this system admits periodic solutions. Can you find them.