Math 430 Mathematical Biology – Homework 5

Due: Tuesday, April 18, 2023.   NAME: ________________________

1) [5] Use Law of Mass Action to write out the (molar) concentration differential equations for the following reactions.

$$3X + Y \underset{k_2}{\overset{k_1}{\rightleftarrows}} X + Z$$

$$X + Y \xrightarrow{k_3} Z$$

2) [10] Let S=substrate, B=buffer and C=complex. A slightly different form of buffering is given by the reaction equations:

$$2S + B \underset{k_-}{\overset{k_+}{\rightleftarrows}} C$$

Using the Law of Mass Action the differential equations governing the molar concentrations is given by:

$$\frac{dS}{dt} = -2k_+BS^2 + 2k_-C \quad , \quad S(0) = S_0 \tag{1}$$

$$\frac{dB}{dt} = -k_+BS^2 + k_-C \quad , \quad B(0) = B_0 \tag{2}$$

$$\frac{dC}{dt} = k_+BS^2 - k_-C \quad , \quad C(0) = C_0 \tag{3}$$

a) Find the function $f(S, B)$ such that the above system can be reduced to

$$S' = 2f(B, S)$$
$$B' = f(B, S)$$

b) Find the function $g(S)$ such that $f = 0$ only if

$$B = g(S) = \frac{\bar{V}}{K_E + S^2}$$

for certain parameters $\bar{V}$ and K_E (write these out in terms of the original model parameters : k_-, k_+, S_0, B_0)

c) Use Matlab or any other plotting program to make a phase plane portrait like that done in my lecture notes for the regular buffering problem. It should be in the (S,B)-plane, be first quadrant only, have an accurate plot of $f = 0$ and several trajectories. Use the parameter values $k_+ = k_- = S_0 = B_0 = 1$ and S values in $[0, 2]$

3) [10] A variation of Michaelis-Menten kinetics is n-site cooperativity where n substrate molecules S must bind in order for the product P to be made. The reaction equations are:

$$nS + E \underset{k_2}{\overset{k_1}{\rightleftarrows}} C \overset{k_2}{\longrightarrow} P + E$$

The subsequent dimensional differential equations for the reaction are

$$\begin{aligned}
\frac{dS}{dt} &= f_1 = -nk_1 S^n E + nk_{-1} C \quad , \quad S(0) = S_0 \\
\frac{dE}{dt} &= f_2 = -k_1 S^n E + (k_{-1} + k_2) C \quad , \quad E(0) = E_0 \\
\frac{dC}{dt} &= -f_2 = k_1 S^n E - (k_{-1} + k_2) C \quad , \quad C(0) = 0 \\
\frac{dP}{dt} &= k_2 C
\end{aligned}$$

a) Without nondimensionalizing the equations, use conservation of receptors to find the quasi-steady state approximation of the production rate

$$\frac{dP}{dt} = V(S)$$

that only depends on S (and not E, C). This is the ubiquitous "Hille" function.

b) According to the fast-subsystem analysis (in class and notes), the complex concentration very quickly rises from 0 to a maximum value C_{max}. Find a formula for C_{max}