Biol 398/Math 388, Assignment 3

Terminology

- Look up the following terms and provide definitions. For each definition, three elements are required: you must quote a source, reference the source, and interpret the definition in your own words.

1. dynamical system "A means of describing how one state develops into another state over the course of time." A dynamical system comprises a set, the state space, of possible states the system can take, together with a time-dependent function that maps a given state (the initial state) to another state (the state later in time). Mathematical dynamical systems are models of real-world phenomena that change over time. Definition in quotes is from mathworld.wolfram.com
2. law of mass action "The law stating that the rate of any given chemical reaction is proportional to the product of the activities (or concentrations) of the reactants." The product of the concentrations of the reactants is, roughly speaking, the number of interactions of reactants that can produce the product. E.g., if we have 10 molecules of A and 20 molecules of B there are 10*20 = 200 pairs AB. The law of mass action says that the rate of reaction is proportional to the number of possible interactions of the molecules involved. Definition in quotes is from http://groups.molbiosci.northwestern.edu/holmgren/Glossary/Definitions/Def-L/law_of_mass_action.html
3. homeostasis "The ability or tendency of an organism or cell to maintain internal equilibrium by adjusting its physiological processes." Homeostatis involves more than the mathematical concept of equilibrium, in that the biological system usually employs a feedback mechanism to maintain an equilibrium and often moves from one equilibrium state to another depending on external conditions. For example, your heart rate at rest is typically maintained within a narrow range (60-80 beats/min is "normal") while during vigorous exercise a much higher rate is typically maintained (120-150 beats/min or more). Both of these conditions would be considered homeostasis. http://www.answers.com/topic/homeostasis
4. equilibrium "A condition in which all acting influences are canceled by others, resulting in a stable, balanced, or unchanging system." In a dynamical system, an equilibrium is a state that does not change over time: the time dependent mapping that takes an initial state to the future state does not move an equilibrium point. http://www.answers.com/topic/dynamic-equilibrium
5. oscillation. "the repetitive variation, typically in time, of some measure about a central value (often a point of equilibrium) or between two or more different states." An oscillation in a dynamical system has a rate of change that flips back and forth between positive and negative values (infinitely often over infinite time into the future).
6. autocatalysis "a state of chemical reaction in which a reaction product is also a catalyst for the reaction." In this type of reaction, one of the reaction products (and often also a reactant) plays the role of an enzyme to accelerate the formation of more product.

Applying the Law of Mass Action

- Construct differential equations that model the following reactions. Be sure to define your state variables and rate constants.

1. $A + B \rightarrow C$
2. $A + B \leftrightarrow C$
3. $A + B \leftrightarrow 2C$
4. $2A + 3B \leftrightarrow C{+}D$

Please note that the symbol ↔ is used to denote arrows (reactions) in both directions.

(1) [A],[B], [C] denote the concentrations of A, B, and C, respectively. The reaction has one rate constant, *k*. C is formed through mass action by combining A and B.

$$\frac{d[C]}{dt} = k[A][B]$$
$$\frac{d[A]}{dt} = -k[A][B]$$
$$\frac{d[B]}{dt} = -k[A][B]$$

(2) [A],[B], [C] denote the concentrations of A, B, and C, respectively. The reaction has two rate constants, k_1, k_{-1}. C is formed through mass action by combining A and B, and C breaks apart (the reverse arrow) into A and B constituents.

$$\frac{d[C]}{dt} = k_1[A][B] - k_{-1}[C]$$
$$\frac{d[A]}{dt} = -k_{-1}[A][B] + k_{-1}[C]$$
$$\frac{d[B]}{dt} = -k_{-1}[A][B] + k_{-1}[C]$$

(3) [A],[B], [C] denote the concentrations of A, B, and C, respectively. The reaction has two rate constants, k_1, k_{-1}. C is formed through mass action by combining A and B, and C breaks apart (the reverse arrow) into A and B constituents. The difference here is that A and B combine to make 2C's. The two C's lead to a $[C]^2$ term, and the rate of change is the rate of change of 2[C].

$$\frac{d(2[C])}{dt} = k_1[A][B] - k_{-1}[C]^2 \text{, or}$$

$$\frac{d[C]}{dt} = \frac{1}{2}\left(k_1[A][B] - k_{-1}[C]^2\right)$$

$$\frac{d[A]}{dt} = -k_{-1}[A][B] + k_{-1}[C]^2$$

$$\frac{d[B]}{dt} = -k_{-1}[A][B] + k_{-1}[C]^2$$

(4) [A],[B], [C],[D] denote the concentrations of A, B, C, and D, respectively. The reaction has two rate constants, k_1, k_{-1}. C and D are formed through mass action by combining 2A's and 3 B's, and C and D break apart (the reverse arrow) into 2A and 3B constituents. The 2 A's lead to a squared term, and the 3 B's lead to a cubed term. As in the previous system, the rate equations are the rate of change of 2A and of 3B.

$$\frac{d[C]}{dt} = k_1[A]^2[B]^3 - k_{-1}[C][D]$$

$$\frac{d[D]}{dt} = k_1[A]^2[B]^3 - k_{-1}[C][D]$$

$$\frac{d[A]}{dt} = \frac{1}{2}\left(-k_{-1}[A]^2[B]^3 + k_{-1}[C][D]\right)$$

$$\frac{d[B]}{dt} = \frac{1}{3}\left(-k_{-1}[A]^2[B]^3 + k_{-1}[C][D]\right)$$

Simulating Reaction Kinetics

- Use the matlab code provided at my lionshare folder to study the simple reaction $E + S \leftrightarrow ES \rightarrow E + P$ that we have studied in class. Set the parameters as follows:

- $[S_0] = 1.0$
- $[E_0] = 0.2$
- $[ES_0] = 0.0$
- $[P_0] = 0.0$
- $k_1 = 2.0$
- $k_{-1} = 0.0$
- $k_2 = 10$

Plot the output, and save the plot as an image. Post the image on the wiki as the answer to the question.