NATIONAL TAIWAN UNIVERSITY,
GRADUATE INSTITUTE OF BIOMEDICAL ENGINEERING AND BIOINFORMATICS

Mathematical Modeling of System Biology
Homework 1

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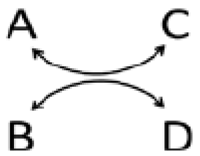
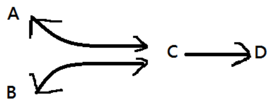
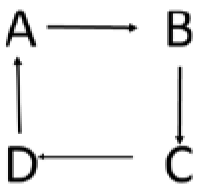
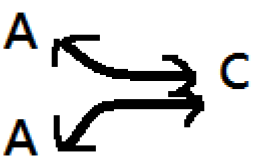
Complete the following table. Assume mass action kinetics for all reaction mechanisms.

	Interaction graph	Rate equation scheme	ODE
a)	$\to A \to$	$\xrightarrow{k_1} A$ $A \xrightarrow{k_2}$	$\frac{d[A]}{dt} = k_1 - k_2\,[A]$
b)		$A + B \underset{k_{-1}}{\overset{k_1}{\longleftrightarrow}} C + D$	$\frac{d[A]}{dt} = -k_1\,[A]\,[B] + k_{-1}\,[C]\,[D]$, $\frac{d[B]}{dt} = -k_1\,[A]\,[B] + k_{-1}\,[C]\,[D]$, $\frac{d[C]}{dt} = k_1\,[A]\,[B] - k_{-1}\,[C]\,[D]$, $\frac{d[D]}{dt} = k_1\,[A]\,[B] - k_{-1}\,[C]\,[D]$
c)		$A + B \underset{k_{-1}}{\overset{k_1}{\longleftrightarrow}} C \xrightarrow{k_2} D$	$\frac{d[A]}{dt} = -k_1[A][B]+k_{-1}[C]$ $\frac{d[B]}{dt} = -k_1[A][B]+k_{-1}[C]$ $\frac{d[C]}{dt} = k_1[A][B] - (k_{-1}+k_2)[C]$ $\frac{d[D]}{dt} = k_2[C]$
d)		$A \xrightarrow{k_1} B$ $B \xrightarrow{k_2} C$ $C \xrightarrow{k_3} D$ $D \xrightarrow{k_4} A$	$\frac{d[A]}{dt} = -k_1\,[A] + k_4\,[D]$ $\frac{d[B]}{dt} = -k_2\,[B] + k_1\,[A]$ $\frac{d[C]}{dt} = -k_3\,[C] + k_2\,[B]$ $\frac{d[D]}{dt} = -k_4\,[D] + k_3\,[C]$
e)		$A + A \xrightarrow{k_1} C$	$\frac{d[A]}{dt} = -2k_1\,[A]^2$, $\frac{d[C]}{dt} = k_1\,[A]^2$

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2.1 Problem Set 2.4.7

a) Consider the closed reaction network in Figure 2.16 with reaction rates v_i as indicated. Suppose that the reaction rates are given by mass action as $v_1 = k_1 [A][B]$, $v_2 = k_2 [D]$ and $v_3 = k_3 [C]$.

   i) Construct a differential equation model for the network. Use moiety conservations to reduce your model to three differential equations and three algebraic equations.

   Initially, we can construct a set of differential equations of every species.

$$\frac{d[A]}{dt} = -v_1, \qquad \frac{d[B]}{dt} = -v_1 + v_2, \qquad \frac{d[C]}{dt} = v_1 - v_3,$$
$$\frac{d[D]}{dt} = v_1 - v_2, \qquad \frac{d[E]}{dt} = v_3, \qquad \frac{d[F]}{dt} = v_3$$

   Then, we can further combine many differential equation to make this set of equations smaller, because there are only three independent variables. Actually, we only need three linearly independent equations. That is, the three differential equations can be derived by moiety conservations:

$$\frac{d[A]}{dt} + \frac{d[C]}{dt} + \frac{d[E]}{dt} = 0, \qquad \frac{d[A]}{dt} + \frac{d[C]}{dt} + \frac{d[F]}{dt} = 0, \qquad \frac{d[B]}{dt} + \frac{d[D]}{dt} = 0,$$

   where the three algebraic equations are

$$v_1 = k_1 [A][B], \qquad v_2 = k_2 [D], \qquad v_3 = k_3 [C]$$

   ii) Solve for the steady-state concentrations as functions of the rate constants and the initial concentrations. (Note, because the system is closed, some of the steady-state concentrations are zero.)

   iii) Verify your result in part (ii) by running a simulation of the system from initial conditions (in mM) of ([A], [B], [C], [D], [E], [F]) = (1, 1, 1 , 0, 0, 0). Take rate constants k1 = 3/mM/sec, k2 = 1/sec, k3 = 4/sec.

b) Next consider the open system in Figure 2.17 with reaction rates vi as indicated. Suppose that the reaction rates are given by mass action as v0 = k0, v1 = k1[A][B], v2 = k2[D], v3 = k3[C], v4 = k4[E], and v5 = k5[F].

2.2 Problem Set 2.4.8

2.3 Problem Set 2.4.9