1.2 Homework # 2 (Due Wednesday, Oct. 17)

1. Consider the following chemical reaction system:

\[ A \xrightarrow{\alpha} X, \quad X + Y \xrightarrow{\beta} 2Y, \quad Y \xrightarrow{\phi} X, \quad Y \xrightarrow{\psi} B. \]

We again follow the convention as in Homework 1, Problem 1.

(a) According to the Law of Mass Action, write the ordinary differential equations for the chemical reaction system.

(b) Find all the steady states of the ODE system.

(c) Carry out linear stability analysis for all the fixed points.

(d) Using internet resource to learn more about SIR model in epidemiology. In terms of the language of epidemiological dynamics, what is the system of ODEs in (a) called?

2. Consider a single, reversible reaction

\[ \nu_1 X_1 + \nu_2 X_2 + \cdots + \nu_N X_N \xrightarrow{R^+(x)} \kappa_1 X_1 + \kappa_2 X_2 + \cdots + \kappa_N X_N, \quad (1.2) \]

with general rate laws \( R^+(x) \) and \( R^-(x) \).

(a) Show that for a single reversible reaction, there always exists a Gibbs potential function \( G(x) \) such that

\[ \ln \left( \frac{R^+(x)}{R^-(x)} \right) = \sum_{\ell=1}^N (\nu_\ell - \kappa_\ell) \mu_\ell(x), \quad \mu_\ell(x) = \frac{\partial G(x)}{\partial x_\ell}. \]

Is the potential function \( G(x) \) unique for the given \( R^\pm(x) \)?

(b) We now consider the Law of Mass Action (LMA):

\[ R^+(x) = k_+ \prod_{j=1}^N x_j^{\nu_j}, \quad R^-(x) = k_- \prod_{j=1}^N x_j^{\kappa_j}, \quad (1.3) \]
in which \( k_+ \) and \( k_- \) are the rate constants in the LMA. Show that the chemical potential of the species \( X_k \) is defined as

\[
\mu_{X_k} = \frac{\partial G(x)}{\partial x_k} = \mu_{X_k}^o + k_B T \ln x_k, \tag{1.4}
\]

in which \( \mu_{X_k}^o \) is a constant specific to the chemical species \( X_k \), independent of its concentration. \( k_B \) is the Boltzmann constant and \( T \) is temperature in Kelvin. \( k_B T \) enters our discussion as the “unit” for Gibbs potential function \( G(x) \).

(c) Prove one of the most important properties of the chemical potentials: When the reaction reaches its chemical equilibrium according to

\[
\frac{dx_k}{dt} = (\kappa_k - \nu_k) \left( R^+(x) - R^-(x) \right) = 0, \; k = 1, 2, \ldots, N;
\]

\[
\sum_{k=1}^{N} \nu_k \mu_{X_k} = \sum_{k=1}^{N} \kappa_k \mu_{X_k}.
\]

That is, the chemical potential difference

\[
\Delta \mu \equiv \sum_{k=1}^{N} (\nu_k - \kappa_k) \mu_{X_k} = k_B T \ln \left( \frac{R^+(x)}{R^-(x)} \right) = 0.
\]

(d) Find a relationship between the “constant term”

\[
\sum_{k=1}^{N} (\nu_k - \kappa_k) \mu_{X_k}^o
\]

in Eq. 1.4 and the rate constants \( k_+ \) and \( k_- \) in Eq. 1.3.

3. Consider the Lotka-Volterra system with all reactions reversible:

\[
A \xrightarrow{k_1} X, \quad X + Y \xrightarrow{k_2} 2Y, \quad Y \xrightarrow{k_3} B. \tag{1.5}
\]

We again follow the notations as in Problem 1. However, we assume all \( A, B, X \) and \( Y \) are in a closed system, which means \( A \) and \( B \), as well as \( X \) and \( Y \), are all changing with time following the Law of Mass Action.
(a) Write the *four* ordinary differential equations for the chemical reaction system.

(b) Let the chemical potentials for species \( A \), \( X \), \( Y \), and \( B \) be:

\[
\mu_A = \mu_A^0 + k_B T \ln a, \quad \mu_X = \mu_X^0 + k_B T \ln x, \quad \mu_Y = \mu_Y^0 + k_B T \ln y, \quad \mu_B = \mu_B^0 + k_B T \ln b.
\]

Find the relationship between difference \( \mu_A^0 - \mu_X^0, \mu_X^0 - \mu_Y^0, \mu_Y^0 - \mu_B^0 \), and the kinetic parameters \( k \)'s in (1.5).

(c) Consider the Gibbs potential function:

\[
G(a, x, y, b) = a(t) \mu_A + x(t) \mu_X + y(t) \mu_Y + b(t) \mu_B
\]

\[
= a(t) \left( \mu_A^0 + k_B T \ln a(t) \right) + x(t) \left( \mu_X^0 + k_B T \ln x(t) \right) + y(t) \left( \mu_Y^0 + k_B T \ln y(t) \right) + b(t) \left( \mu_B^0 + k_B T \ln b(t) \right).
\]

\( G \) is a function of time \( t \) since \( a, x, y \), and \( b \) are all changing with time according to the system of differential equations from part (a). Show that

\[
\frac{dG(a(t), x(t), y(t), b(t))}{dt} = \sum_{\sigma = a, x, y, b} \left( \frac{\partial G}{\partial \sigma} \right) \frac{d\sigma}{dt} \leq 0. \quad (1.6)
\]

(d) Based on Eq. 1.6, what can you say about the kinetics of this reversible Lotka-Volterra system?