BEBI5009 Homework2
Due 04/05/2018(Thur) before midnight

1. **2.4.8 Rapid equilibrium approximation.**

Consider the closed system:

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} C.$$

with mass-action rate constants as shown. Suppose the rate constants are (in min−1) k1 = 0.05, k2 = 0.7, k−1 = 0.005, and k−2 = 0.4.

(a) Construct a differential equation model of the system. Simulate your model with initial conditions (in mM) of A(0) = 1.5, B(0) = 3, C(0) = 2. Plot the transient and steady-state behaviour of the system. You may need to make two plots to capture all of the dynamics (i.e. two different window sizes).

(b) It should be clear from your simulation in part (a) that the system dynamics occur on two different time-scales. This is also apparent in the widely separated rate constants. Use a rapid equilibrium assumption to reduce your description of the system to two differential equations (describing one of the original species and one combined species pool) and two algebraic equations (describing the contents of the combined pool).

(c) Run a simulation of your reduced model in part (b) to compare with the simulation in part (a). Verify that the simulation of the reduced system is in good agreement with the original, except for a short initial transient. (Note, you will have to select initial conditions for the reduced system so that the initial total concentration is in agreement with part (a), and the rapid equilibrium condition is satisfied at time t = 0.)

2. **2.4.9 Quasi-steady-state approximation.**

Consider the reaction network:

$$\xrightarrow{k_0} A \xrightarrow{k_2} \qquad\qquad A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B$$

Suppose the mass-action rate constants are (in min−1) k0 = 1, k1 = 11, k−1 = 8, and k2 = 0.2.

(a) Construct a differential equation model of the system. Simulate your model with initial conditions A(0) = 6 mM, B(0) = 0 mM. Plot the transient and steady-state behavior of the system. You may need to make two plots to capture all of the dynamics (i.e. two different window sizes).

(b) It should be clear from your simulation in part (a) that the system dynamics occur on two different time-scales. This is also apparent in the widely separated rate constants. Use a quasi steady-state assumption to reduce your description of the system by replacing a differential equation with an algebraic equation.

(c) Run a simulation of your reduced model in part (b) to compare with the simulation in part (a).

Verify that the simulation of the reduced system is a good approximation to the original at steady state, but not over the initial transient. (Note, you will have to select initial conditions for the reduced system so that the total concentration is in agreement with part (a), and the quasi-steady state condition is satisfied at time $t = 0$, as in Exercise 2.2.4.)