Understanding the Comp2ExchangeReaction Model

This is a two compartment model for two substances, A and B. Both substances can passively move from one compartment to the other. A is irreversibly converted to B in either or both compartments.
The governing ordinary differential equations are

$$dA_1/dt = (PS_a/V_1)\cdot(A_2 - A_1) - (G_1/V_1)\cdot A_1 \quad ,$$

$$dB_1/dt = (PS_b/V_1)\cdot(B_2 - B_1) + (G_1/V_1)\cdot A_1 \quad ,$$

$$dA_2/dt = (PS_a/V_2)\cdot(A_1 - A_2) - (G_2/V_2)\cdot A_2 \quad ,$$

$$dB_2/dt = (PS_b/V_2)\cdot(B_1 - B_2) + (G_2/V_2)\cdot A_2$$

The initial conditions are given as

$$A_1(0)=A_1 0,\ A_2(0)=A_2 0,\ B_1(0)=B_1 0, \text{ and } B_2(0)=B_2 0.$$

Analytic solutions exist, but are very long.

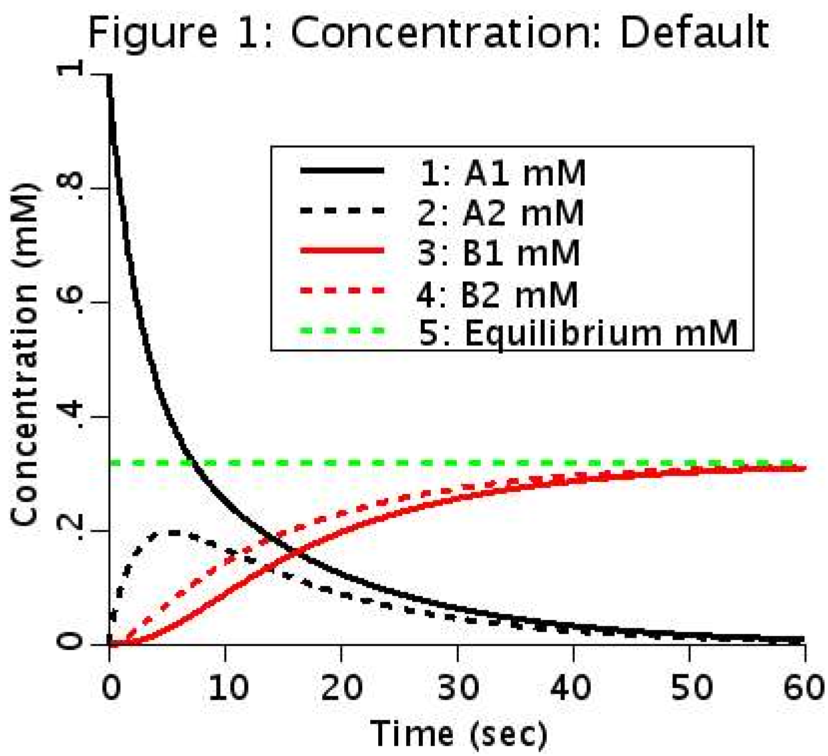
Questions:

(1) What are the equilibrium concentrations if Psa and Psb are non-zero, and at least one of G1 or G2 is non-zero?

(2) Set any parameters except the rate parameters so that B2(0) = B2(long time). Show analytically that this result is correct.
(Answers at the end.)

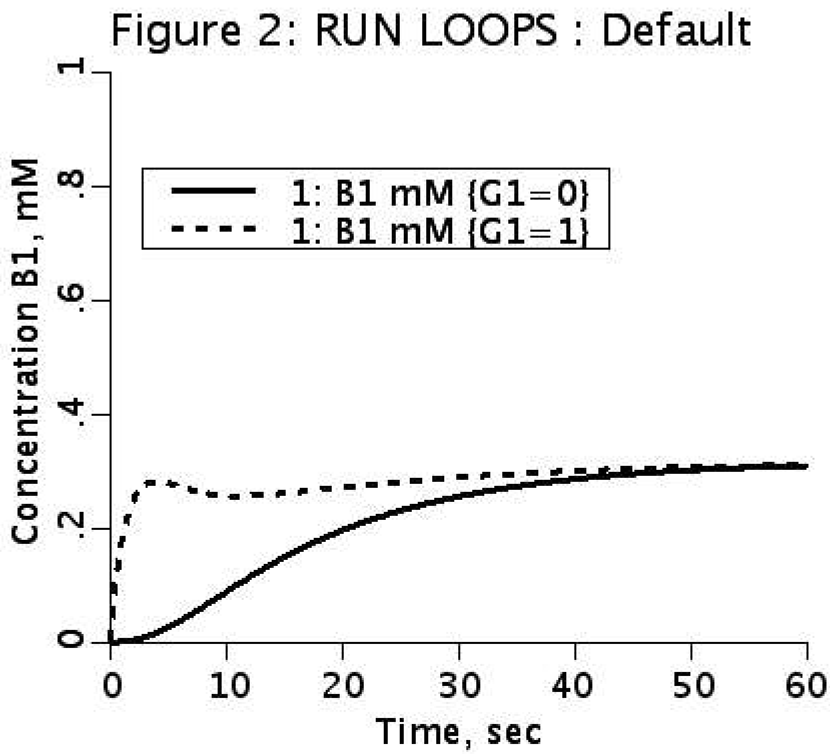
Figures and Explanations

Figure 1: Concentrations: Default parameter set



Concentration of A1 (black solid line), A2 (black dashed line), B1 (red solid line), and B2 (red dashed line) are plotted as a function of time. The equilibrium concentration for either B (G1 and G2 not both 0) or for A (G1 and G2 both 0)is plotted (green dashed line).

Figure 2: RUN LOOPS : Default



The B1 concentration is plotted as a function of time when G1=0 and G2=1 (solid black line), and when G1=1 and G2=0 (dashed line) as a function of time.

Case 1: G1=0, G2=1. B1 rises slowly because A1 must first cross the barrier (A1->A2), then be converted to B2 (A2->B2) and then cross the barrier again (B2->B1).

Case 2: G1=1, G2=0. B1 rises quickly because A is directly converted to B (A1->B1), and A1 is initially set to a high value.

Where the reaction takes place usually makes a big difference in the shapes of the concentration curves in multi-compartment problems when a substance reacts to become a different substance.

Answers:

(1) The equilibrium concentrations for B1 and B2 are equal and given by

$$(V1*(A10+B10)+V2*(A20+B20))/(V1 + V2).$$

(2) To have B2(initial) = B2(infinity), solve

$$V1*(A10+B10)+V2*(A20+B20) = (V1+V2)*B20$$

i.e. the total amount of material in the system initially (RHS) is the total amount of material in the system finally (LHS). For this problem, at equilibrium, B1=B2, that is the final amount of material is

$$\begin{aligned} V1*B1+V2*B2 &= V1*B2+V2*B2 \\ &= (V1+V2)*B2 \\ &= (V1+V2)*B20. \end{aligned}$$

Therefore

$$B20 = \frac{V1\ A10 + V1\ B10 + V2\ A20}{V1}$$

Set A10=1 mM, B10=0.5 mM, A20=2.0 mM. Set B20 to 5.7857143, and run model for 600 seconds and check final value for B2.