Understanding the Comp1Reaction Model

In a single compartment, C is converted to D with rate constant Gc2d, and D is converted back to C with rate constant Gd2c. The governing equations are:

$$dC/dt = -(G_{c2d}/V)\cdot C + (G_{d2c}/V)\cdot D$$

$$dD/dt = +(G_{c2d}/V)\cdot C - (G_{d2c}/V)\cdot D \quad ,$$

with initial conditions

$$C(0) = C_0 \text{ and } D(0) = D_0 \quad .$$

The analytic solutions are given by

$$C_{analytic} = \frac{(G_{d2c}\cdot(C_0 + D_0) - (G_{c2d}\cdot C_0 - G_{d2c}\cdot D_0)\cdot \exp(-(G_{c2d}+G_{d2c})\cdot t/V))}{(G_{c2d}+G_{d2c})}$$

$$D_{analytic} = \frac{(G_{c2d}\cdot(C_0 + D_0) - (G_{c2d}\cdot C_0 - G_{d2c}\cdot D_0)\cdot \exp(-(G_{c2d}+G_{d2c})\cdot t/V))}{(G_{c2d}+G_{d2c})} \quad .$$

Figures and Explanations

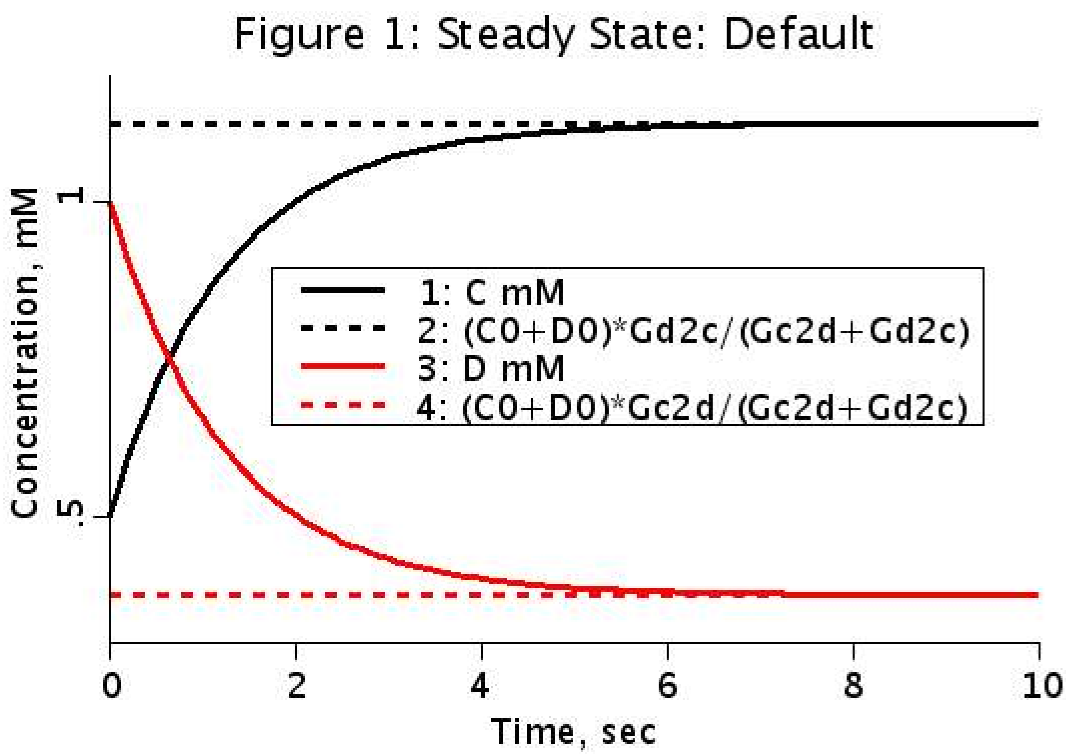
Questions:

(1) What are the concentrations of C and D at long time?

(2) If the volume is increased, does the time when concentration C equals D increase, stay the same, or decrease?

(3) At steady state what is the flux of C to D in units of micromoles/sec?

Figure 1: Steady State: Default parameter set



Concentration of C (black solid line) and D (red solid line) are plotted as functions of time. The asymptotic limits at long time are plotted as dashed lines. The rate constants and compartmental volume are given as

Gc2d = 0.01 ml/sec
Gd2c = 0.03 ml/sec
V = 0.05 ml.

Substance	Initial Concentration	Asymptotic Concentration
C	0.5 mM	1.125 mM
D	1.0 mM	0.375 mM

The sum of the concentrations is 1.5 mM.
Since C is produced 3 times faster than D, the concentration of C is 3/4*1.5 mM, and D=1/4*1.5 mM.

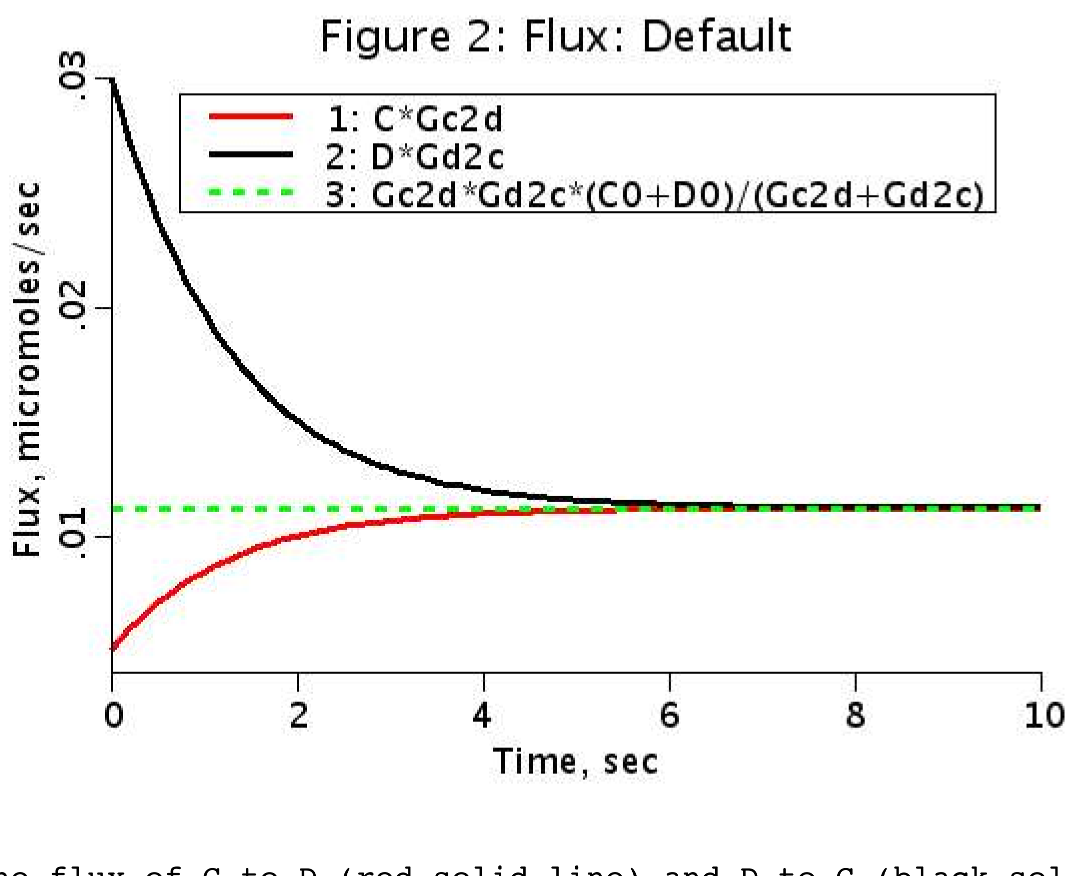
This can also be shown by solving the combination of the steady state equation and the mass conservation statement for C and D.

Steady State Equation:
   dC/dt = 0 = -(Gc2d/V)*C + (Gd2c/V)*D.
Mass Conservation:
   C + D = C0 + D0, yield

$$C = \frac{Gd2c\ (C0 + D0)}{Gc2d + Gd2c}, \quad D = \frac{Gc2d\ (C0 + D0)}{Gc2d + Gd2c}.$$

Use Run LOOPS, increasing the volume. What happens to the time when concentration C equals D? Why?

Figure 2: Flux: Default parameter set



The flux of C to D (red solid line) and D to C (black solid line) is plotted as a function of time. The two fluxes are not zero at large time, they are equal. The flux for C to D is given as

$$\text{Flux} = Gc2d * C(t = \text{long time}).$$

$$\text{Flux} = \frac{Gc2d\ Gd2c\ (C0 + D0)}{Gc2d + Gd2c} = 0.01125\ \text{umol/sec}.$$

This value is plotted as the horizontal dashed green line.