Understanding the Comp1FlowReactions2 Model

A Flow, F, carries an inflow concentration, Cin, into a one compartment model with a given volume, V. Cin is constantly and instantaneously well mixed becoming C, the concentration of C in the compartment. C is irreversibly converted to become D with rate constant Gc2d. D is irreversibly converted to become E with rate constant Gd2e.

The governing ordinary differential equations are given as

$$dC/dt=(F/V)\cdot(C_{\mathrm{in}}-C)-(G_{c2d}/V)\cdot C \quad ,$$

$$dD/dt=(F/V)\cdot(-D)+(G_{c2d}/V)\cdot C-(G_{d2e}/V)\cdot D \quad ,$$

$$dE/dt=(F/V)*(-E)+(G_{d2e}/V)\cdot D \quad .$$

with initial conditions

$$C(0)=C_0 \quad , \quad D(0)=D_0 \quad , \text{ and } \quad E(0)=E_0 \quad .$$

Figures and Explanations

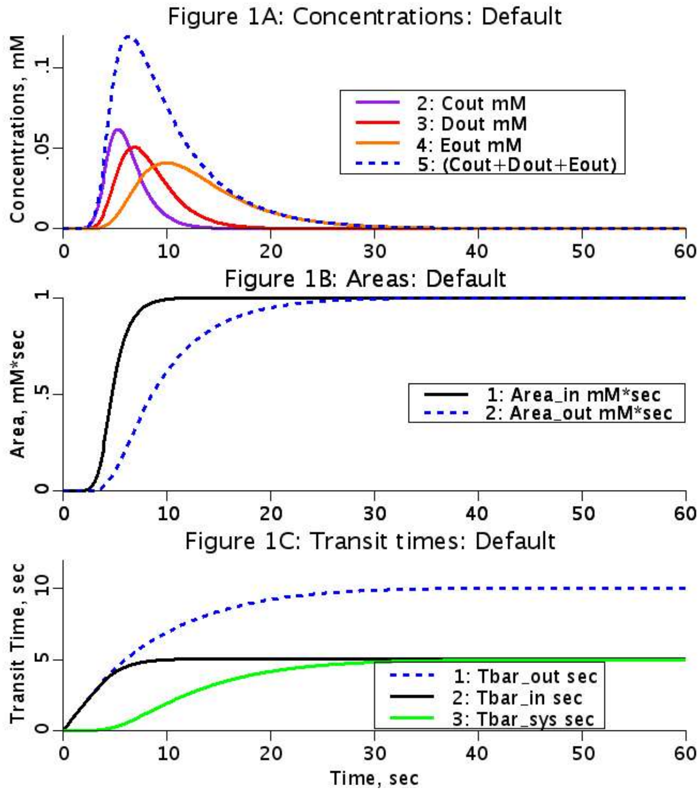
Questions:

(1) Does the integrated output area (Area_out) for C+D+E and the transit time depend on the conversion rates?

(2) How does the output area for each curve depend on the model parameters?

(3) What are the steady state concentrations when Cin is a constant?

Figure 1A: Concentrations: Default parameter set.



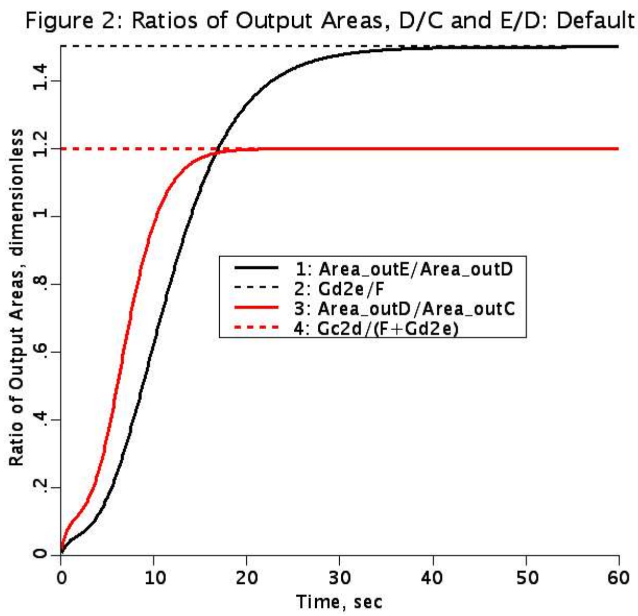
Cout (purple), Dout (red), Eout (orange), and their sum (blue dashed) are plotted as functions of time.

Figure 1B: Areas: Default parameter set
The integrated inflow and outflow concentrations with respect to time are plotted as functions of time. Note That the Area of the sum of the outputs eventually equals the area of the inflow concentration.

Figure 1C: Transit times: Default parameter set
The transit time calculation reaches a final value after the transient concentrations have washed out.
Tbar_sys is also given as

Tbar_sys=V/F.

Figure 2: Ratio of Output Areas, D/C and E/D, Default parameter set



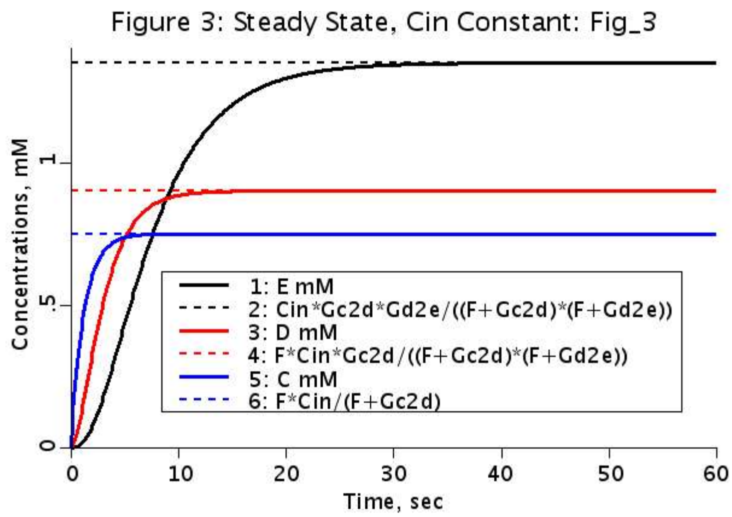
Determine the functional relationship for the ratio of the area of Dout divided by the area of Cout, and the ratio of the area Eout divided by the area of Dout.

$$\frac{\text{Area\_out(D)}}{\text{Area\_out(C)}} = \frac{\text{Gc2d}}{\text{F + Gd2e}},$$

$$\frac{\text{Area\_out(E)}}{\text{Area\_out(D)}} = \frac{\text{Gd2e}}{\text{F}}.$$

Does this relationship hold when Cin is a constant?

Figure 3: Steady State, Cin Constant: Fig_3 parameter set



The steady state concentrations for Cin = 3 are calculated numerically and compared with solving the ordinary differential equations when the rate of change is 0, i.e. solving

$$\frac{F\,(Cin - C)}{V} - \frac{Gc2d\;C}{V} = 0,$$

$$-\frac{F\,D}{V} + \frac{Gc2d\;C}{V} - \frac{Gd2e\;D}{V} = 0,$$

$$-\frac{F\,E}{V} + \frac{Gd2e\;D}{V} = 0,$$

for C, D, and E, yielding

$$C = \frac{F\;Cin}{F + Gc2d},$$

$$D = \frac{F\;Cin\;Gc2d}{(F + Gc2d)\;(F + Gd2e)}, \text{ and}$$

$$E = \frac{Cin\ Gc2d\ Gd2e}{(F + Gc2d)\ (F + Gd2e)}.$$

Prove: C+D+E=Cin.