# Understanding the Comp1FlowPlus Model

This is a one compartment model with flow. The flow rates for inflow and outflow are equal and the compartment volume remains a constant. The governing ordinary differential equation for the concentration is given as

$$dC/dt=(Flow/Volume)\cdot(C_{\mathrm{in}}-C_{out}) \quad .$$

Since the compartment is instantaneously well mixed, the equation becomes

$$dC/dt=(Flow/Volume)\cdot(C_{\mathrm{in}}-C) \quad ,$$

since $C_{out}=C$, with initial condition

$$C(0)=C_0 \quad .$$

Various checks can be done on the model. If an closed analytic solution exists, it can be compared with the numeric result. The Comp1Flow model has a closed analytic solution for constant inflow concentration:

$$C_{analytic}(t)=C_0+(C_{\mathrm{in}}-C_0)\cdot(1-\exp(-Flow*t/Volume)).$$

The quantity of material that enters the compartment can be calculated in two different ways:

$$Q(t)=C(t)*Volume$$

and also as

$$Q_{integral}(t)=\int_0^t Flow\cdot(C_{\mathrm{in}}(t')-C_{out}(t'))\,dt' \quad .$$

Checks can be done on the model inflow and outflow concentrations. After a long time, the integrals of $C_{\mathrm{in}}$ and $C_{out}$ with respect to time, known as Area_in and Area_out, must become equal (input quantity=output quantity).

Another check performed is transit time. The transit time of an curve is defined by the integral of its first moment divided by its zeroth moment (the area). Transit time is known as $\bar{t}$ , usually pronounced as “Teebar”, but spelled as “Tbar”.

$$\bar{t}=\frac{\int_0^\infty C(t)\cdot t\,dt}{\int_0^\infty C(t)\,dt} \quad .$$

Tbar can also be given as a function of time, in which case

$$\bar{t}(t)=\frac{\int_0^t C(t')\cdot t'\,dt'}{\int_0^t C(t')\,dt'} \quad .$$

In this model the areas and transit times are given as functions of time. Elsewhere, they are given as the values after long time. The transit time of the system is given as

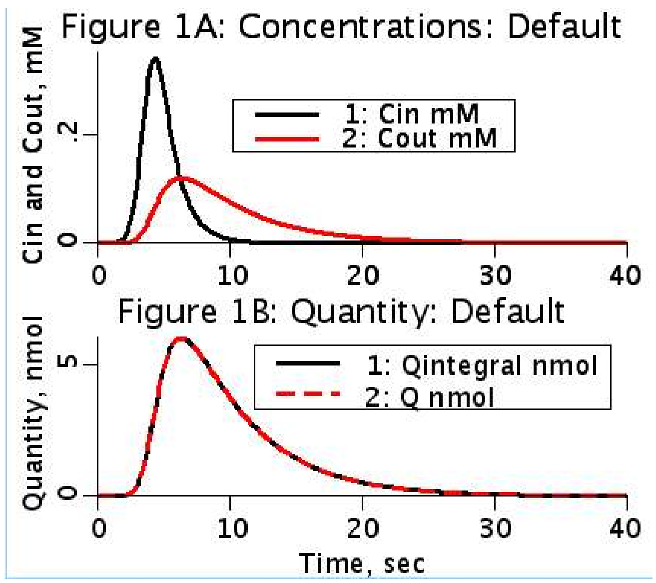
$$\bar{t}_{sys}=\bar{t}_{out}-\bar{t}_{\text{in}} \quad .$$

Tbar_sys is also given as

$$\bar{t}_{sys}=Volume/Flow \quad .$$

## Figures and Explanations

Figure 1A: Concentrations: Default parameter set and
Figure 1B: Quantity: Default parameter set




The inflow and outflow concentrations are graphed as functions of time. The inflow concentration, Cin, is given by a function generator, fgen_1. Note that the outflow concentration, Cout, has reduced amplitude and is more spread out. Cout equals C, the concentration in the compartment, because the compartment is instantaneously well mixed.

The quantity of C, given in nanomoles, is calculated by two different methods.

Q(t)=Volume*C(t), and

Qintegral(t) = integral from 0 to t [Flow*(Cin-Cout)] dt.

Figure 2A: Area of Cin and Cout: Default Parameter set

The running integral of Cin and Cout with respect to time is plotted. Eventually the areas are equal after a "long" time, in this case 40 seconds.

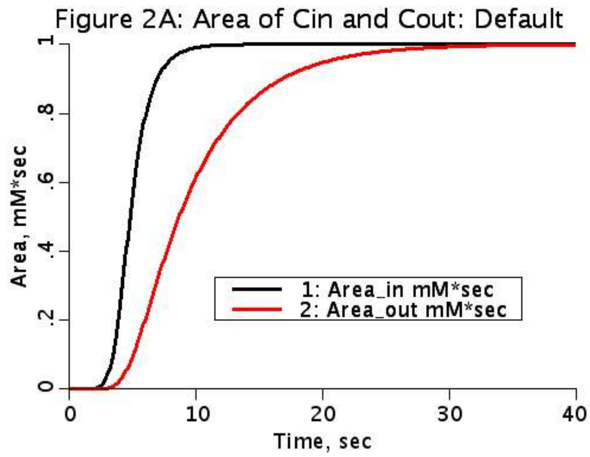



Figure 2B: Transit Time: Default parameter set

The running calculation of Tbar_in, Tbar_out, and Tbar_sys is plotted along with the calculation of Tbar_sys equal to Volume/Flow (green dashed line). It is seen that after 40 seconds when the area of the output concentration curve matches the area of the input concentration curve, Tbar_sys (orange line) approaches the value given by the system transit time (green dashed line).

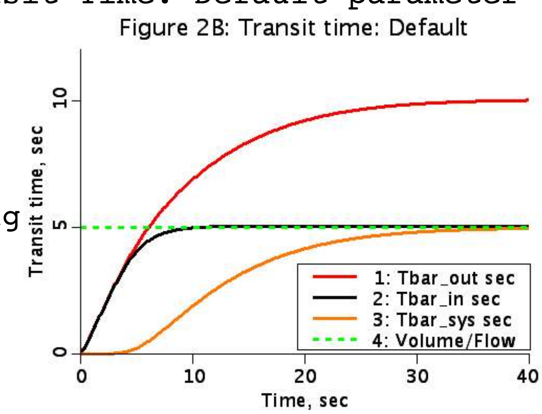
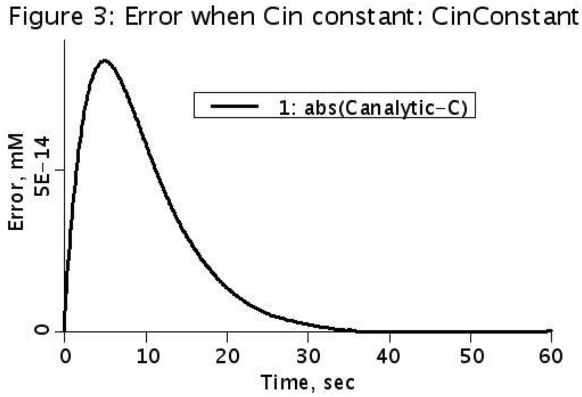


Figure 3: Error when Cin constant: CinConstant parameter set




It is necessary to change parameter sets to the CinConstant parameter set and rerun the model. The error in the numeric solution given by

Error(t) = Canalytic(t)-C(t) is plotted.

The amount of error in a solution usually depends on the model step size, the particular solver used, and the parameters given to the solver. The solvers can be found on the Run Time graphical user interface (GUI) under the Pages button. Compare the error from the solver, Auto (used here) with the Euler solver with 1 step.