Comp1DecayPlus: One compartment model with decay of substance

This is a one compartment model with a substance, C, that decays. The governing equation is

$$dC/dt = -(G/V) * C \ ,$$

with initial condition

$$C(0) = C_0 \ ,$$

where C(t) is the concentration at time t, G is the consumption rate, V is the volume of the compartment and C_0 is the initial concentration. The analytic solution is

$$C_{analytic}(t) = C_0 \cdot \exp\left(\frac{-G \cdot t}{V}\right) \ .$$

Numeric and analytic solutions are plotted.

Results:

Figure 1A: Numeric and Analytic Solutions: Default parameter set

Figure shows numeric and analytic Solutions as functions of time. The rate of change of the solution also decays.

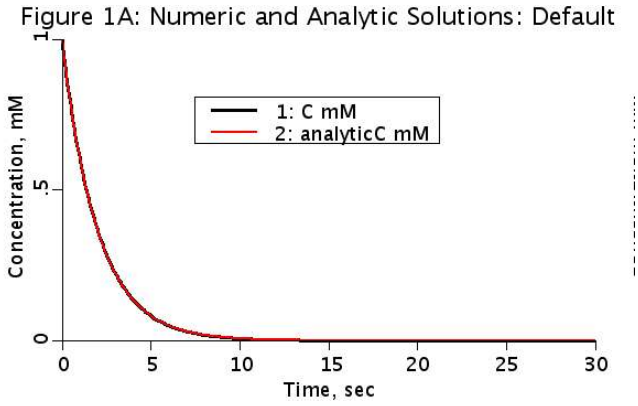

Figure 1B: Numeric and Analytic Solutions: Default parameter set

On a semi-logarithm plot, the numeric and analytic solutions appear as straight lines.

Figure 1B: Numeric and Analytic Solutions: Default

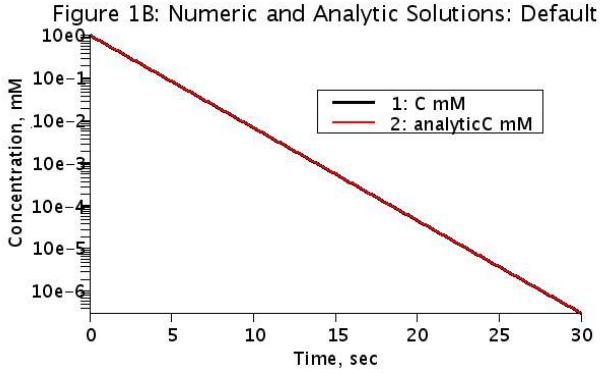

Figure 1C:
Absolute Error: Default parameter set

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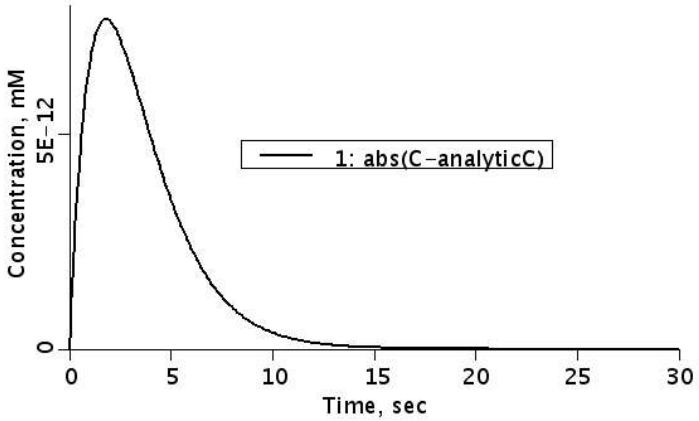

The absolute error is plotted as a function of time. The ordinary differential solvers can be accessed from the Run Time GUI under the Pages button by selecting Solvers. Change the solver to Euler with one step and run again and note the maximum error. Change the Euler to 10 steps and run again. How does the error change. Do the same with RK4 (Runge-Kutta 4th order). You should rerun these numeric experiments by first making t.delta ten times smaller.

Figure 2: Amount of C remaining: Default

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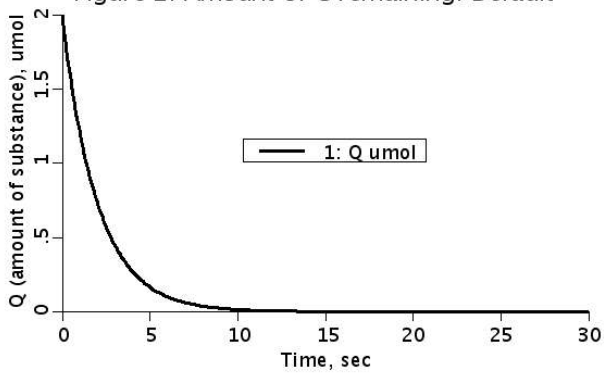
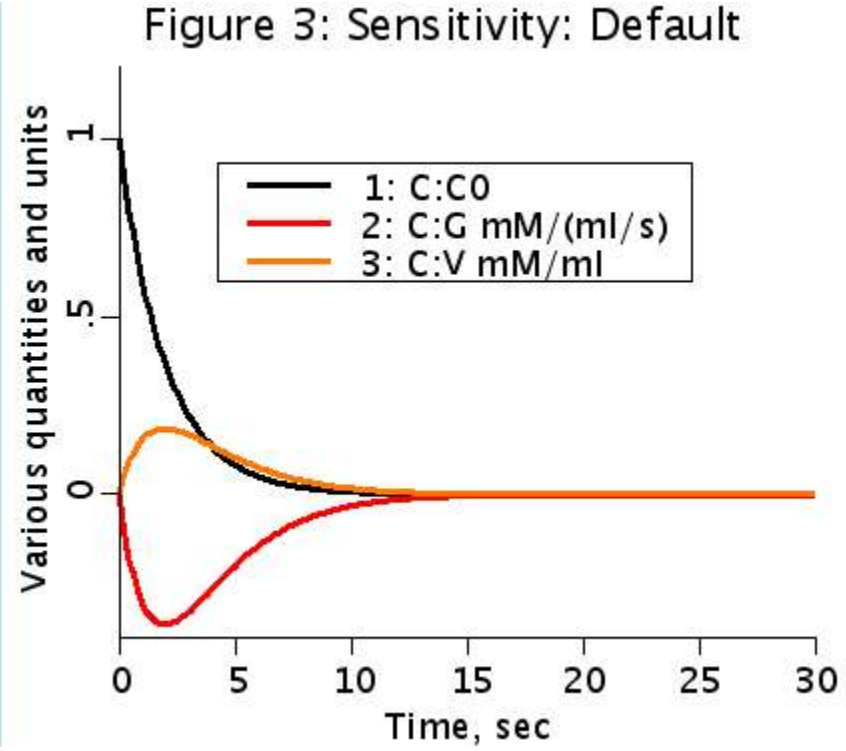


The amount of C remaining in micromoles is plotted as a function of time.

Figure 3: Sensitivity: Default parameter set



Do a sensitivity run (Sensitivity button at bottom of the Run Time GUI.) Three curves are displayed.

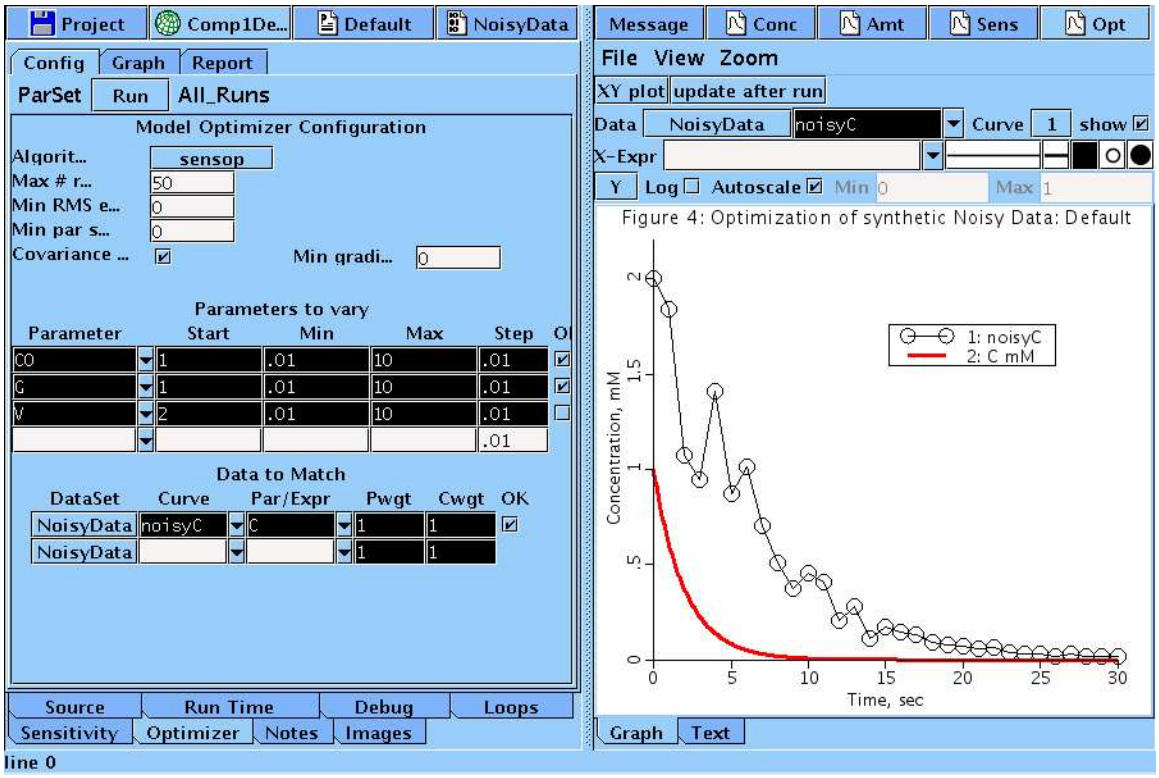
The black curve is dC/dC0, the change in C with respect to C0. This is coded in JSim as C:C0 in the plot variable window. The curve is every where positive. This means that making C0 larger will have the effect of raising the solution. The solution will change the most at time=0, but will hardly make any change after 10 seconds.

The red curve is dC/dG, the change in C with respect to G. This is coded in JSim as C:G in the plot variable window. Increasing G will the effect of lowering the solution after time equals 0. It will have its greatest effect around 2 seconds.

The orange curve is dC/dV. It has the opposite effect as G. Go to the plot variable window for curve 3 and change it from C:V to -2*C:V. What you are see is that the two parameters covary with each other. The governing equation

for this system is dC/dt = -(G/V)*C. The ratio of G/V is the "real" parameter. This will have consequences for optimizing data.

Figure 4: Optimization of synthetic Noisy Data: Default parameter set



(1) Try to fit the data by first varying C0 and G using what you have learned from the sensitivity analysis.

(2) After you have a "good" fit, change the Y axis to Log scaling and see if you can improve your manual fit.

(3) Finally use the Optimizer (Optimizer button at bottom of Run Time GUI). The optimizer has been set up for you. There are three separate areas for viewing the optimization: Config Graph and Report.

(a) Config allows the user to change how the optimization will be done--which parameters to use, their limits, which data sets matched with what variables, etc.
(b) Selecting Graph brings up the View button to view different graphs related to the optimization.

(c) Report gives details about the optimization results including confidence limits for the estimates and covariance between parameters.

(4) After running the optimizer, check the Report. See what information it contains. Note the confidence limits on the parameters.

(5) Return to the Config GUI. Add the volume, V, to the parameters being optimized (check box to left of parameter). Run the optimizer again and check the confidence limits now. Do the confidence limits expand or shrink? Check the covariance between G and V.

If two parameters have a covariance whose absolute value is greater than 0.95 in magnitude, one of them should probably be omitted from the optimization. High covariance between two or more parameters in an optimization leads to great uncertainty in both of them.