Solving Continuous Stirred Tank Reactor (CSTR) equations with Comsol Multiphysics[1]

Outline
1. Problem from Figure 8.14, p. 162, steady CSTR
2. Problem from Table 8.1, p. 163, steady CSTR with multiple solutions
3. Problem from Eq. (8.58), p. 165, transient CSTRs, Figures 8.15-8.18.

Problem from Figure 8.14, p. 162

Equation 8.56 is to be solved for c, with the parameters in Figure 8.14 and shown below in the variables.

$$\frac{Q}{V}(1-c) = c\,\exp\{\gamma * [1 - 1/(1+\beta-\beta c)]\}$$

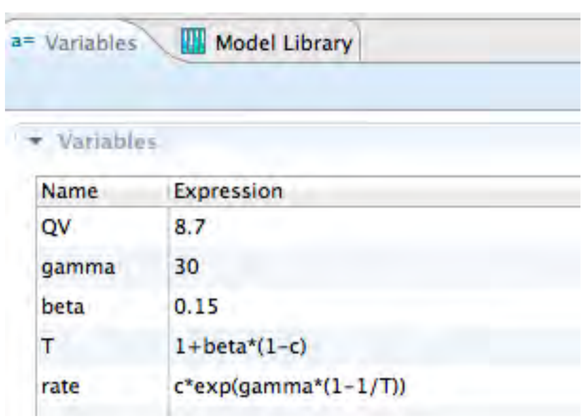
Step 1, Begin: Open Comsol Multiphysics and choose the 0D option, right arrow; then Global ODEs and DAEs (ge) (under Mathematics/ODE and DAE Interfaces); then right arrow and finally Stationary and the Finish flag.

Step 2, Prepare the Model: Model 1 opens, with Global ODEs and DAEs (ge). Click on Global Equations. Type in 'c' for the name and

$$QV*(1-c) - rate$$

for the f. (The window uses u, but you can think in terms of your variable, *c*.)

Step 3, Insert the Variables and their values:



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[1] Bruce A. Finlayson, Introduction to Chemical Engineering Computing, 2nd ed., Wiley (2012); ChemEComp.com for info, Buy Now .

Step 4, Solve the Problem: Right click on Solve and choose =. The answer (under Derived Values, c, click the =) is 0.0.731092. This is what was obtained in Excel and MATLAB.

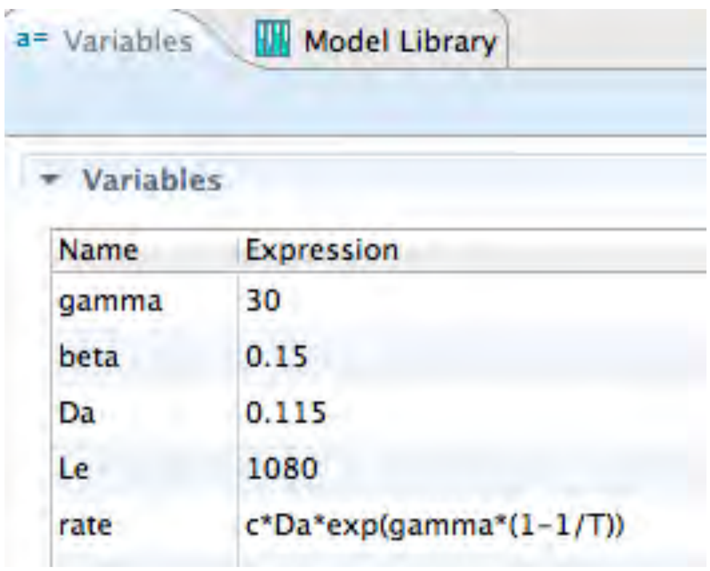
Problem from Table 8.1, p. 163

Change the QV to 25 and β to 0.25 and redo the calculations. The answer is 0.0863. When there are multiple steady states you have to look for them all. Change the initial guess from the default value of 0.0 to 0.5 and recalculate. The answer is 0.5577. With an initial guess of 1.0 the answer is 0.9422. All of these are the same as achieved in MATLAB, Table 8.1.

Summary: A nonlinear algebraic may have more than one solution, and the one you get depends upon your initial guess. In addition, the tolerance may be important for achieving good accuracy.

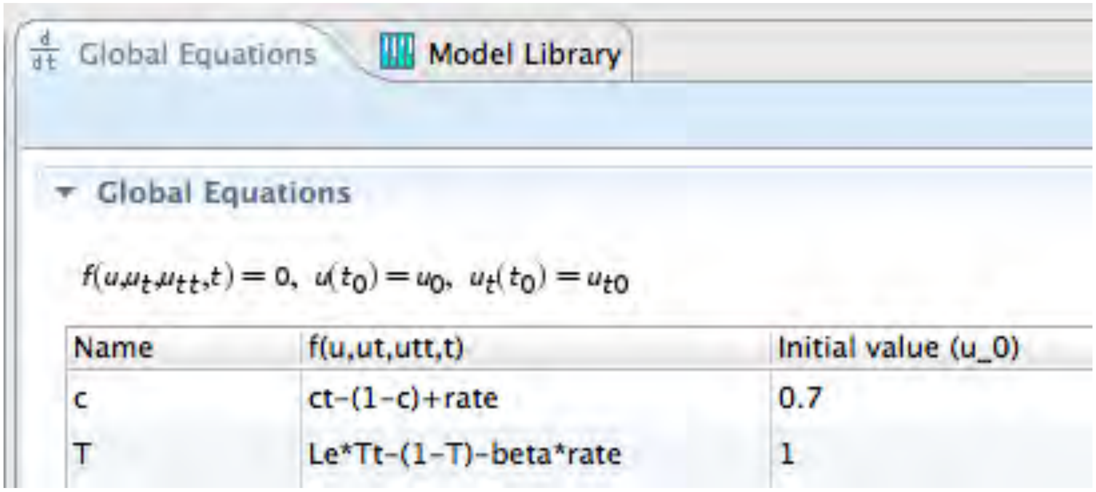
Problem from Eq. (8.58), p. 165

Proceed as before except choose Transient rather than Stationary. This time the variables are:

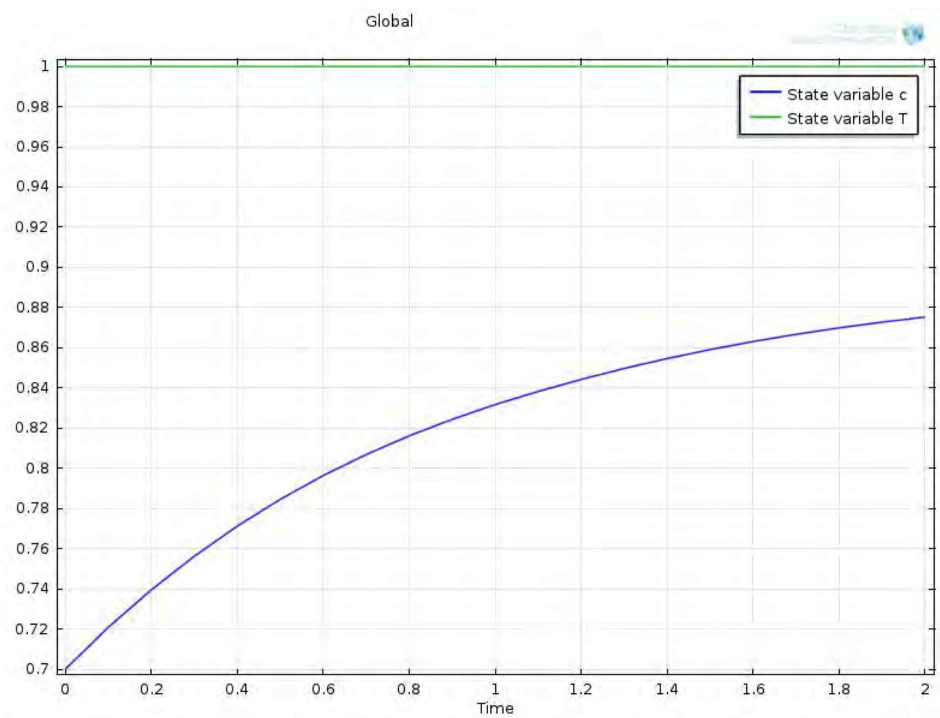


Name	Expression
gamma	30
beta	0.15
Da	0.115
Le	1080
rate	c*Da*exp(gamma*(1-1/T))

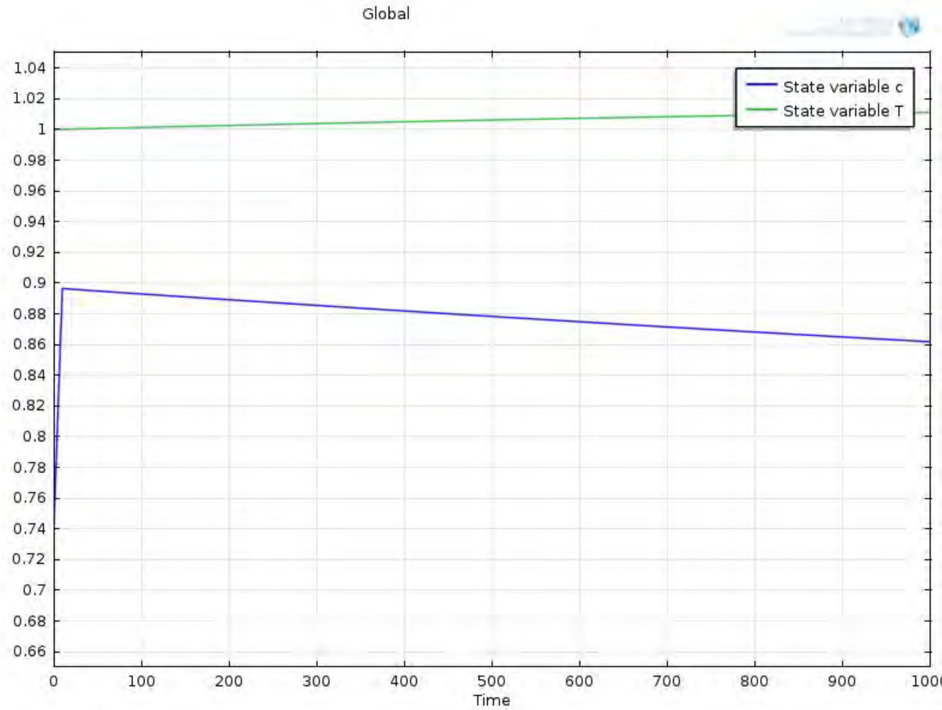
The equations can be written in one panel as follows.



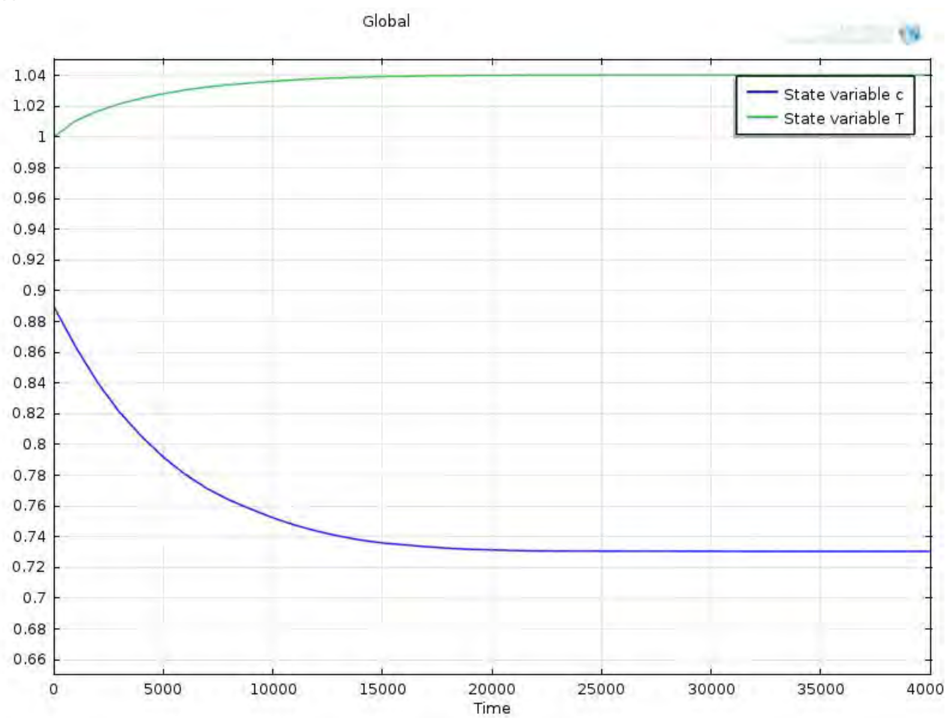
Open Study 1 and set the time range in Step 1: Time Dependent as 0 to 2 with increments of 0.1. Right click Study 1 and choose Compute. The result is shown in the figure below.



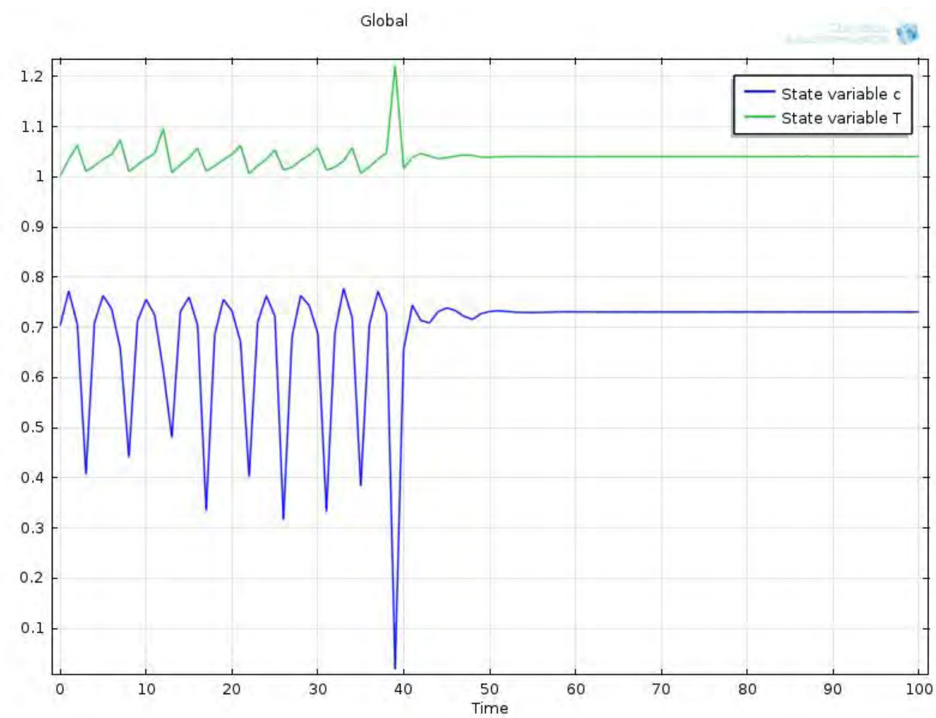
Next solve from 0 to 1000 using steps of 10. The result is shown below.



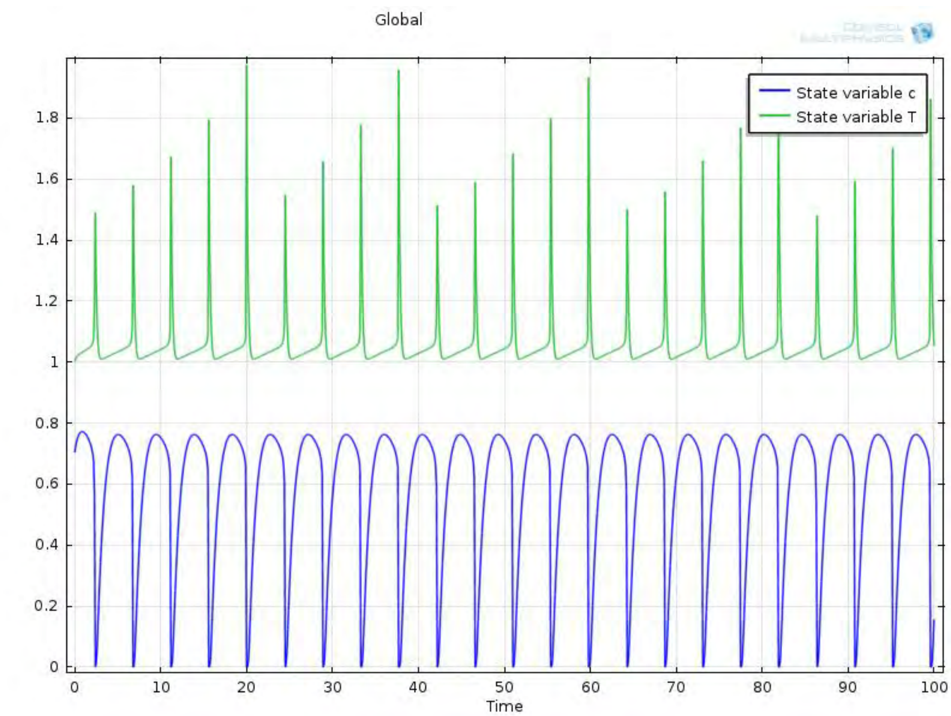
As discussed on page 167, the temperature responds very slowly. Thus, one must solve for a much longer time. Do that for time from 0 to 40,000 with steps of 1000. The result is shown below.



Finally change the Lewis number from 1080 to 0.1 and change the final time to 100, using a step size of 1. The solution is shown in the figure below. It is weird. The problem is that the tolerances are too large and numerical accuracy is a problem.



Thus, change the relative tolerance to 1e-5 (Study 1, Time Dependent, Relative Tolerance) and the absolute tolerance to 1e-5, too (Study 1, Solver Configuration, Solver 1, Time Dependent Solver. The solution still looks ragged, but the raggedness repeats. That is because the time step is too large and the only points plotted are those at which we specified in the steps. So integrate from 0 to 100 with step sizes of 0.1 and a decent figure results below.



Summary: A nonlinear ordinary differential may have solutions which oscillate. If they are very stiff (have widely different time constants) then the tolerance parameters may have to be adjusted to get a good solution.