Solving nonlinear algebraic equations with Comsol Multiphysics

Problem in Eq. (4.15)

Consider the chemical equilibrium problem posed in Eq. (4.15), p. 53.[1] This governs the water-gas shift reaction at equilibrium. The equation that must be solved is

$$f(x) \equiv 148.4 - \frac{x^2}{(1-x)^2} = 0, \text{ find } x$$

While this can easily be solved by taking the square root and solving a linear equation, here we solve it 'as is'; the method is applicable to more complicated problems that don't have an easy solution.

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 'x' for the name and 148.4-(x^2)/(1-x)^2 for the f. Insert 0.5 for the initial value. (The window uses u, but you can think in terms of your variable, *x*.)

Step 3, Solve the Problem: Right click on Study 1 and choose Compute. If you look at the Log, you see that the ErrEst goes from about 1 to 5.8e-5 in 6 iterations. It looks like the problem has been solved.

Step 4, Examine and check the Solution: Open the Results arrow and then open Derived Values. Listed there is State variable x, click that and then in the Global Evaluate window click the = sign or 'Evaluate'. In results a new column is formed labeled as 'State variable x', and the answer is 1.08943. Is that the solution? You can evaluate it and see. If you paste the expression for 'f' into Expression, using mod1.x for the variable x, the answer comes out -0.0133. This is not as accurate as the ErrEst of 5.8e-5. (On a calculator, using x = 1.08943 gave 0.00058.) But, the solution should never be above 1.0, since x represents the number of moles of carbon monoxide reacting and total available is 1.0. So something is wrong. What is wrong is that most nonlinear algebraic equations have more than one solution and the solution you obtain depends upon your initial guess.

Step 5, Change the initial condition are redo: Go back to Global Equations and change the initial guess to 0.9; right click on Study and the problem is solved again. Click on Results/Derived Values/State variable, and click on the = sign. Now the Results Table lists 0.924140. This is the solution found in Excel and MATLAB, although there the solution was more accurate.

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

Problem in Eq. (4.16)

This problem has two equations:

$$10x + 3y^2 = 3$$
$$x^2 - \exp(y) = 2$$

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 'x' for the name and 3-10*x-3*y*y for the function. Insert 1.5 for the initial value. Then in the next line, type in 'y' for the name and 2-x*x+exp(y) for the function. Insert 2.5 for the initial value.

Step 3, Solve the Problem: Right click on Study 1 and choose Compute. You will find that the iterations do not converge. Change the initial guesses to 0,0 and Compute. This time the error gets small (see the Log). Choosing Derived Values/State variable x shows the solution is =–1.44555; Choosing Derived Values/State variable y shows the solution is –2.41216. These are the correct solutions.

Obviously the initial guess of the solution determines whether convergence occurs or not. This is not a problem when solving a problem that is self-contained, but if this problem were in the middle of another problem, it could be a problem: you would have go figure out how to give it an initial guess that would always work.