Solving nonlinear algebraic equations with Comsol Multiphysics

Problem in Eq. (3.9) – Vapor-liquid equilibrium

Consider the vapor-liquid equilibrium problem posed in Eq. (3.9), p. 32.[1] The equation that must be solved is

$$\sum_{i=1}^{4} \frac{(K_i - 1)z_i}{1 + (K_i - 1)v'} = 0$$

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). In Model/Definitions right click and choose variables. Insert the values of K1, K2, K3, and K4, as well as z1, z2, z3, z4. I choose to define var1 as (K1–1)*z1/(1+(K1-1)*v). Then I can copy that for var2 through var4 and change the 1 to 2, etc. Then in Global ODEs/Global Equations, put v as the variable and value as the function.

Step 3, Solve the Problem: Right click on Study 1 and choose Compute. The problem converges and gives the answer (Results/Derived Values, click on State variable v and =) 0.425838. This compares with the Excel solution 0.425837.

It would be nice if variables could be defined as vectors, but that is harder. Of course, it could be done using LiveLink with MATLAB, but if you have MATLAB it is easier just do solve the problem in MATLAB, as shown in Chapter 3. The exercise shown here is just to show you how to solve vapor-liquid equilibrium problems in Comsol Multiphysics.

---

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