

Solving nonlinear algebraic equations with Comsol Multiphysics

Problem Figure 2.1, p. 14

The cubic Redlich-Kwong equation of state is solved as shown in Figure 2.1, p. 14 (using Excel) and p. 17 (using MATLAB)¹. The equation of state is

$$pv^3 - RTv^2 + (a_{RK} - pb_{RK}^2 - RTb_{RK})v - a_{RK}b_{RK} = 0$$

The pressure, p , and temperature, T , are given, and the Redlich-Kwong coefficients depend upon the critical pressure and temperature of the substance, here n-butane. The cubic equation is then solved for the specific volume, v .

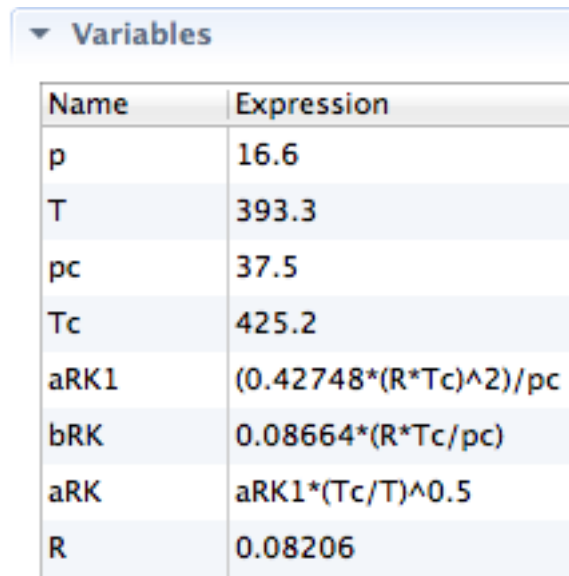
Step 1, Begin: Open Comsol Multiphysics and choose the 0D option, right arrow; then Global ODEs and DAEs (ge) (under Mathematics/ODE and DAE Interfaces); then right arrow and finally Stationary and the Finish flag.

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

$$p*v^3 - R*T*v^2 + (a_{RK} - p*b_{RK}^2 - R*T*b_{RK})*v - a_{RK}*b_{RK}$$

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

Step 3, Insert the Variables and their values:



Name	Expression
p	16.6
T	393.3
pc	37.5
Tc	425.2
aRK1	$(0.42748*(R*Tc)^2)/pc$
bRK	$0.08664*(R*Tc/pc)$
aRK	$aRK1*(Tc/T)^{0.5}$
R	0.08206

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 =.

a. The answer (under Derived Values, v , click the =) is 0.18147. This is not what was obtained in Excel or MATLAB. But, the cubic equation has three unknowns.

b. So, try again but this time use the initial guess of v as $R \cdot T / p$. This time the solution is 1.50648. This differs slightly from the solutions in the book, which are 1.5064.

c. So, change the tolerance. Open Study/Solver Configurations/Solver/Stationary Solver. The relative tolerance is 0.001. Change that to $1e-6$ and resolve. Now the answer is 1.5064, which agrees with the other solutions.

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.