Problems on Mass-Radius relation and Van Der Waals EOS

October 30, 2013

1 The van der Waals equation of state

The van der Waals equation of state is an idealized equation of state that takes into account the finite volume occupied by molecules and the inter-molecular forces.

By scaling the pressure, density and pressure to gas-dependent values p_r, T_r and ρ_r , the equation of state can be written in universal (gas-independent) form:

$$(\tilde{p}+3\tilde{\rho}^2)(\tilde{\rho}^{-1}-\frac{1}{3}) = \frac{8}{3}\tilde{T}$$
 (1)

where $\tilde{p} \equiv p/p_r$ and so forth. Note that at small $\tilde{\rho}$ this reduces to the idealgas equation of state, which makes sence since at low densities molecules are far apart and there is less chance for them to interact. The extra term in the first factor on the left hand side represents the intermolecular forces and the subtraction of $\frac{1}{3}$ in the second factor takes into account the finite volume occupied by the molecules.

The van der Waals equation immediately gives an expression for $\tilde{T}(\tilde{\rho}, \tilde{p})$, and can with a little algebra be solved for $\tilde{p}(\tilde{\rho}, \tilde{T})$. In either case, the formula immediately implies that there is a unique \tilde{T} or $\tilde{\rho}$ corresponding to the other two thermodynamic variables. However to determine $r\tilde{h}o$ in terms of of \tilde{p} and \tilde{T} , one must solve a cubic equation (generally one would do it numerically using Newton's method). The cubic can have more than one real root, and in fact it does for $\tilde{T} < 1$. This can be shown analytically, but you can easily verify the property by plotting $\tilde{p}(\tilde{\rho}, \tilde{T})$ for several different values of \tilde{T} , and looking for which curves are monotonic and which have a maximum (in which case the line of constant $\tilde{\rho}$ intersects the curve in three places). Make it so, and show some graphs illustrating this point. The phase transition in van der Waals is qualitatively like what happens in actual gases, but it fails to obey certain important thermodynamic constraints. Hence, the van der Waals equation of state is most useful away from the phase transition, and in particular for supercritical fluids (which avoid the phase transition).

For many applications, it is sufficient to compute \tilde{p} or \tilde{T} in terms of the other thermodynamic variables, but sometimes it is necessary to compute $\tilde{\rho}$ given \tilde{p} and \tilde{T} . There are two convenient ways to do this numerically. The first is to use Newton's method to solve the cubic for $\tilde{\rho}$. The second method, which is only really workable if your system does not encounter a phase transition, consists of using the explicit $\tilde{p}(\tilde{\rho}, \tilde{T})$ expression to pre-compute a table of $\tilde{\rho}$ and the corresponding \tilde{p} on a suitable list of values of $\tilde{\rho}$ covering your range of interest. For the isothermal case, you'd compute this table for constant \tilde{T} , but for an adiabatic case you'd compute the table assuming \tilde{T} is on the adiabat. Then you can interpolate from the table to get the value of $\tilde{\rho}$ for any given \tilde{p} . This amounts to a digital version of plotting the graph $p(\rho)$ and then rotating it to read off $\rho(p)$.

2 Problems

Problem 2.1 Adiabat for non-ideal EOS

For a non-idea equation of state, it is easiest to compute the adiabat in the form $\rho(T)$ by using the First Law in the form

$$0 = c_v dT + p d\frac{1}{\rho} \tag{2}$$

Then, if you need T(p), you can compute it from the equation of state using these results.

Carry out this calculation using a numerical integration of the First Law, assuming the van der Waals equation of state written in universal form. Assume that c_v is constant. Plot results for $\tilde{T}(\tilde{\rho})$ and $\tilde{T}(\tilde{\rho})$, and discuss the corresponding dimensional values for H₂, N₂ and CO₂.

Problem 2.2 Mass-radius relation for non-ideal EOS

Using the van der Waals equation, compute the mass-radius relation for an isothermal planet made of H₂. For a planet made of CO₂. Do the problem for several different values of the temperature, and discuss how the temperature affects the "puffiness" of the planet. In order to avoid the problem of dealing with the phase transition in the van der Waals equation, you may restrict attention to temperatures such that no phase transition (i.e. multiple solutions for ρ corresponding to a given p) occurs.

Python Tips: If you use Newton's method to get ρ , you can use the class newtSolve in ClimateUtilities to carry out the calculation. Newton's method requires a sufficiently good initial guess at the solution, and when you are carrying out the integration of the hydrostatic relation, you can save the solution from the previous r as the initial guess for the next r. In a case with a phase transition, the solution you get depends on what initial guess you use, but this isn't an issue if you avoid the phase transition. If you use the tabulation and interpolation method, which is only good in a case without a phase transition, then the class interp can be used to create an interpolation function for you.