Example 15.4 Molecules of H_2O in a 100-ml beaker

Assuming α is about 100 at room temperature and $\rho = 1$ g/cm^3, estimate the moles of H_2O monomer in a 100 ml beaker of liquid water.

Solution: Note that the problem statement requests moles of H_2O not $(H_2O)_2$ or $(H_2O)_3$ etc., so we are interested in the true number of H_2O monomer moles. We know $n_0 = 5.556$ from our previous calculation (see “Mass Balances” on page 544), but $n_M = x_M{\cdot}n_T$, so we must convert from our superficial basis. Proceeding, using Eqn. 15.62

$$x_M = [-1 + \sqrt{1 + 4\alpha}\,]/2\alpha = 0.095;\ n_T/n_0 = x_M = 0.095 = n_T/n_0$$

$$\Rightarrow n_M = 0.095{\cdot}(n_T/n_0){\cdot}n_0 = 0.095^2{\cdot}n_0 = 0.05 \text{ moles}$$

Therefore, the true number of moles is 100 times less than the superficial number of moles.

Solving the Equation of State for Density

We can see that Eqn. 15.51 is not truly a cubic in density because x_M depends on density. Also, its functional dependence is nonlinear, which makes implementation more difficult. However, α is a monotonic function of density, and successive substitution of density has been found to quickly yield converged values for density. The algorithm is given in Fig. 15.7.

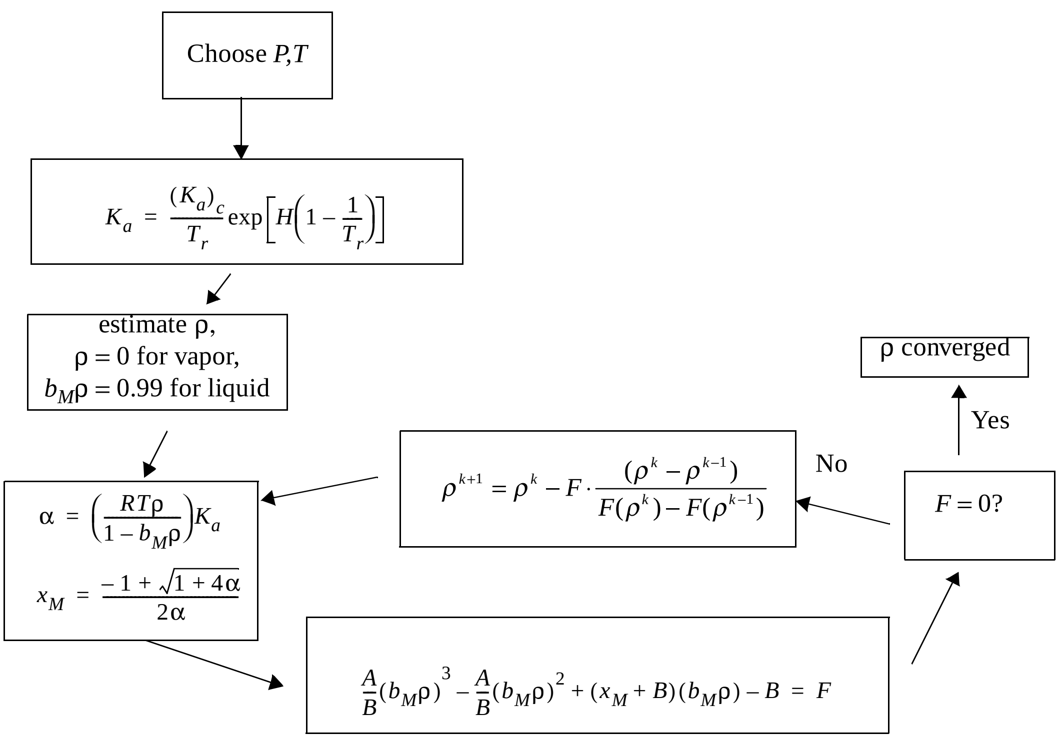

Figure 15.7 *Flowsheet for calculating density by the van der Waals associating fluid model.*