

Example 7.8: Generalized Graphs

Calculate the fugacity of benzene at $T = 64^\circ\text{C}$, $P = 34$ bar using the Lee-Kesler method.

Solution With $T_c = 562.1$ K, $P_c = 48.9$ bar, the given conditions correspond to $T_r = 0.6$, $P_r = 0.7$. From tables E13, E15, we find by interpolation, $\phi^0 = 0.04415$, $\phi^1 = 0.02145$. Notice that these values are printed in italics indicating that the state is liquid. The fugacity coefficient is

$$\phi = (0.04415)(0.02145)^{0.210} = 0.0197$$

and the fugacity is $f = \phi P = (0.0197)(34) = 0.67$ bar.

Fugacity from Cubic Equations of State

Writing the residual Gibbs energy as $G^R = H^R - TS^R$, the fugacity coefficient is expressed as

$$\ln \phi = \frac{H^R}{RT} - \frac{S^R}{R}.$$

Therefore, the calculation of the fugacity coefficient by a cubic equation of state does not require much in terms of additional computations, since the required expressions for the residual enthalpy and entropy have been obtained already. In particular, the result for the Soave-Redlich-Kwong and the Peng-Robinson equation are

- Soave-Redlich-Kwong

$$\ln \phi = Z - 1 - \ln(Z - B') - \frac{A'}{B'} \ln \frac{Z + B'}{Z}. \quad (7.21)$$

- Peng-Robinson

$$\ln \phi = Z - 1 - \ln(Z - B') - \frac{A'}{2\sqrt{2}B'} \ln \frac{Z + (1 + \sqrt{2})B'}{Z + (1 - \sqrt{2})B'}. \quad (7.22)$$

In both cases the dimensionless parameters A' and B' are given by:

$$A' = \frac{aP}{(RT)^2}, \quad B' = \frac{bP}{RT}. \quad [2.36]$$

This calculation requires the compressibility factor at the pressure and temperature of interest. If the polynomial equation for Z has three real roots, the proper root must be selected based on the phase of the system.