ABE 303 Homework Project: FFF: Phases, Fugacity, Fun, and the Peng-Robinson EOS

Using the Peng-Robinson EOS, do the following: (a) Construct a P-V diagram for methane. Use Isotherms in 10 degree increments starting at 75 degrees Kelvin until you are approximately 40 degrees above the critical point.

(b) Calculate the vapor pressure of methane as a function of temperature.

(c) Compare your computed results with the literature and describe the similarities and differences.

(d) On the P-V diagram, use the limits of stability derived in class to construct the metastable regime in your computer code.

(e) Use the requirement that fugacities are equal in the liquid and vapor states to construct the coexistence lines. Compare the envelope of coexistence curves with the result in part (d).

Helpful Hints to find fugacity coefficient for Peng-Robinson EOS

$$\ln \frac{f^V(T,P)}{P} = \frac{1}{RT}\int_{\underline{V}=\infty}^{\underline{V}=Z^V RT/P}\left(\frac{RT}{\underline{V}}-P\right)d\underline{V} - \ln Z^V + \left(Z^V-1\right) \tag{1}$$

$$= \left(Z^V-1\right) - \ln\left(Z^V-B\right) - \frac{A}{2\sqrt{2}B}\ln\left[\frac{Z^V+\left(1+\sqrt{2}\right)B}{Z^V+\left(1-\sqrt{2}\right)B}\right] \tag{2}$$

$$\ln \frac{f^L(T,P)}{P} = \frac{1}{RT}\int_{\underline{V}=\infty}^{\underline{V}=Z^L RT/P}\left(\frac{RT}{\underline{V}}-P\right)d\underline{V} - \ln Z^L + \left(Z^L-1\right) \tag{3}$$

$$= \left(Z^L-1\right) - \ln\left(Z^L-B\right) - \frac{A}{2\sqrt{2}B}\ln\left[\frac{Z^L+\left(1+\sqrt{2}\right)B}{Z^L+\left(1-\sqrt{2}\right)B}\right] \tag{4}$$