ENGG 201 – Real Gas (Single Component) Example

<u>Fall 1993 (Final) (MODIFIED)</u>

A spherical vessel, 7 m in diameter, is used for storing *n*-butane (C_4H_{10}) at 407.2°C and 7.6 MPa. Estimate the molar volume <u>and</u> the mass of *n*-butane in the vessel using the following methods. The critical pressure and temperature of n-butane are 37.5 atm and 425.2 K, and the acentric factor is 0.197.

(a) The ideal gas law.

$$PV_m = RT \qquad V_m = \frac{RT}{P}$$

$$V_m = \frac{RT}{P} = \frac{8.314\frac{kPa.m^3}{kmol.K}680.35K}{7.6x10^3 kPa} = \boxed{0.744\frac{m^3}{kmol}}$$

(b) The generalized compressibility chart method.

$$PV_m = ZRT \qquad V_m = \frac{ZRT}{P} \qquad T_r = \frac{T}{T_c} = \frac{680.35K}{425.2K} = 1.60 \qquad P_r = \frac{P}{P_c} = \frac{7.6MPa}{3.8MPa} = 2.00$$

$$V_m = \frac{ZRT}{P} = \frac{(0.89)8.314\frac{kPa.m^3}{kmol.K}680.35K}{7.6x10^3 kPa} = \boxed{0.662\frac{m^3}{kmol}}$$

(c) The Pitzer-Curl tables

$$PV_m = ZRT \qquad V_m = \frac{ZRT}{P} \qquad T_r = \frac{T}{T_c} = \frac{680.35K}{425.2K} = 1.60 \qquad P_r = \frac{P}{P_c} = \frac{7.6MPa}{3.8MPa} = 2.00$$

$$Z = Z^{(0)} + \omega Z^{(1)} = 0.872 + 0.197(0.17) = 0.905$$

$$V_m = \frac{ZRT}{P} = \frac{(0.905)8.314\frac{kPa.m^3}{kmol.K}680.35K}{7.6x10^3 kPa} = \boxed{0.674\frac{m^3}{kmol}}$$

(d) The van der Waals equation of state.

Use actual T and P in vdW – only use T_c and P_c to calculate a and b.

$$V_m^3 - [b + \frac{RT}{P}]V_m^2 + \frac{a}{P}V_m - \frac{ab}{P} = 0$$

$$a = \frac{27}{64}\frac{R^2T_c^2}{P_c} = \frac{27}{64}\frac{\left(0.08205\frac{atm.m^3}{kmol.K}\right)^2(425.2K)^2}{37.5atm} = 13.69atm\left(\frac{m^3}{kmol}\right)^2$$

$$b = \frac{RT_c}{8P_c} = \frac{\left(0.08205\frac{atm.m^3}{kmol.K}\right)(425.2K)}{(8)(37.5atm)} = 0.1163\frac{m^3}{kmol}$$

$$V_m^3 - [0.1163 + \frac{0.08205 * 680.35}{75atm}]V_m^2 + \frac{13.69}{75}V_m - \frac{13.69 * 0.1163}{75} = 0$$

$$V_m^3 - 0.8606V_m^2 + 0.18253V_m - 0.02123 = 0$$ *Divide by V_m^2*

$$V_m - 0.8606 + \frac{0.18253}{V_m} - \frac{0.02123}{V_m^2} = 0$$

$$V_m = 0.8606 - \frac{0.18253}{V_m} + \frac{0.02123}{V_m^2}$$

Start with Ideal Gas V_m as first guess for Successive Substitution

$$V_{m1} = 0.744\frac{m^3}{kmol} \qquad V_{m2} = 0.8606 - \frac{0.18253}{0.744} + \frac{0.02123}{(0.744)^2} = 0.6536\frac{m^3}{kmol}$$

$$V_{m2} = 0.6536\frac{m^3}{kmol} \qquad V_{m3} = 0.8606 - \frac{0.18253}{0.6536} + \frac{0.02123}{(0.6536)^2} = 0.6310\frac{m^3}{kmol}$$

$$V_{m3} = 0.6310\frac{m^3}{kmol} \qquad V_{m4} = 0.8606 - \frac{0.18253}{0.6310} + \frac{0.02123}{(0.6310)^2} = 0.6246\frac{m^3}{kmol}$$

$$V_{m4} = 0.6246\frac{m^3}{kmol} \qquad V_{m5} = 0.8606 - \frac{0.18253}{0.6246} + \frac{0.02123}{(0.6246)^2} = 0.6228\frac{m^3}{kmol}$$

$$V_{m5} = 0.6228\frac{m^3}{kmol} \qquad V_{m6} = 0.8606 - \frac{0.18253}{0.6228} + \frac{0.02123}{(0.6228)^2} = \boxed{0.6222\frac{m^3}{kmol}}$$