

## SFE Questions/Answers

1. Using the *Peng-Robinson EOS* determine the  $\rho$  of the supercritical CO<sub>2</sub> when  $T = 60^\circ\text{C}$ ,  $P = 90 \text{ bar}$ ,  $R = 8.31451 \times 10^{-2} \text{ L}\cdot\text{bar}/\text{K}\cdot\text{mol}$  and  $\omega = 0.225$ .

$$K_i = 0.37464 + 1.54226(\omega) - 0.26993(\omega^2) = 0.7079838$$

$$T_r = \frac{T}{T_c} = \frac{(60 + 273.15)}{(30.0 + 273.15)} = 1.0959$$

$$b = 0.0778 \left( \frac{R * T_c}{P_c} \right) = 0.0778 \left( \frac{0.0831451 \text{ L} * \frac{\text{bar}}{\text{K}} * \text{mol} * 304 \text{ K}}{73.8 \text{ bar}} \right) = 0.02665047$$

$$a = 0.45724 \frac{(R^2)(T_c^2)}{P_c} [1 + K_i(1 - \sqrt{T_r})]^2 = 3.70178$$

$$B = \frac{b * P}{R * T} = \frac{(0.02665047)(90 \text{ bar})}{(0.0831451)(60 + 273.15)} = 0.086591$$

$$A = \frac{a * P}{R^2 * T^2} = 0.43421$$

$$Z^3 - (1 - B)Z^2 + (1 - 3B^2 - 21B)Z - (AB - B^2 - B^3) = 0$$

$$Z^3 - 0.913409Z^2 - 0.840905Z - .0294514 = 0$$

Using a cubic equation calculator,  $Z=1.49074$

$$\rho = \frac{MP}{ZRT} = \frac{\left(44 \frac{\text{g}}{\text{mol}}\right) (90 \text{ bar})}{1.49074 \left(0.0831451 \frac{\text{L} * \text{bar}}{\text{K} * \text{mol}}\right) (60 + 273.15\text{K})} = 95.947 \text{ g/L} = 96 \text{ g/L}$$

2. When  $P$  is above  $P_c$  and constant. How does increasing  $T$  ( $T$  is already higher than  $T_c$ ) affect density, velocity, solubility, and diffusivity?

*Density is decreased*

*Velocity does increase with increased temperature, but viscosity decreases because it is more dependent on density and density decreases with increased temperatures.*

*Solubility can either increase or decrease depending on what the pressure is. There is an increase in solubility at both low and high pressures (see Supercritical Fluid Extraction (SFE)- An Overview about “cross-over pressure”)*

*Diffusivity increases*

3. Name one aspect about SFE that is BOTH an advantage and disadvantage.

*Several possible. Use of CO<sub>2</sub> as mobile phase (as it is non-polar and needs additives to remove the more polar molecules, but it is non-toxic and cheap), all three parameters can change (gives more flexibility for optimizing results, but also gives too many choices for it at the same time), etc.*

4. Which characteristics of SFE are similar to liquids and which are similar to gases?

*Density and solvent power similar to liquids, viscosity and diffusivity is similar to gases.*