

CH365 Chemical Engineering Thermodynamics

Lesson 29 Residual Properties II

Block 6 Look-Ahead (CDP)

Real Gas Properties

- Residual Properties
- $M = V, U, H, S, \text{ or } G$

$$M^R \equiv M - M^{\text{ig}} \quad (\text{Eq. 6.41})$$

$$M \equiv M^{\text{ig}} + M^R$$

Ideal gas (ig) follows ideal gas law

Real Solution Properties (Liquids)

- Excess Properties
- $M^E = V^E, U^E, H^E, S^E, \text{ or } G^E$

$$M^E \equiv M - M^{\text{id}} \quad (\text{Eq. 6.41})$$

$$M \equiv M^{\text{id}} + M^E$$

$$G^E \equiv G - G^{\text{id}}$$

$$H^E \equiv H - H^{\text{id}}$$

$$S^E \equiv S - S^{\text{id}}$$

Ideal solution (id) follows Raoult's law

GE is related to the activity coefficients

From Gibbs-Duhem:

$$\frac{G^E}{RT} = \sum_i x_i \ln \gamma_i \quad (\text{Eq. 13.10})$$

Margules
(1-constant)

$$\log \gamma_1 = A x_2^2$$

$$\log \gamma_2 = A x_1^2$$

Constants are known from fitting experimental data
("binary interaction parameters" in CHEMCAD and capstone design problem)

Residual Properties from Cubic EOS

Generic cubic equation of state (in Z-Form)

(WPR3)

$$q = q(x) = \frac{\Psi \alpha(x)}{\Omega T_r} \quad (\text{Eq. 3.51})$$

$$\alpha = \alpha(x)$$

(α is found in Table 3.1)

Important: α is written as a function of x where x replaces T_r .

$$\beta = \Omega \frac{P_r}{T_r} \quad (3.50)$$

$$Z = 1 + \beta - q\beta \frac{Z - \beta}{(Z + \epsilon\beta)(Z + \sigma\beta)} \quad (3.48)$$

$$\frac{H^R}{RT} = Z - 1 + T_r \left(\frac{dq}{dT_r} \right) \cdot I$$

(page 497)

$$\frac{S^R}{R} = \ln(Z - \beta) + \left(q + T_r \frac{dq}{dT_r} \right) \cdot I$$

$$I = \frac{1}{\sigma - \epsilon} \ln \left(\frac{Z + \sigma\beta}{Z + \epsilon\beta} \right) \quad \epsilon \neq \sigma$$

$$I = \frac{\beta}{Z} \quad \epsilon = \sigma$$

Homework

Problem 6.141

change: 20 points

Calculate Z , H^R , and S^R by the Redlich-Kwong equation of state for parts (b) through (e).

- (a) Ethylene at 300 K and 35 bar
- (b) Hydrogen sulfide at 400 K and 70 bar
- (c) Nitrogen at 150 K and 50 bar
- (d) n-Octane at 575 K and 15 bar
- (e) Propane at 375 K and 25 bar