CH365 Chemical Engineering Thermodynamics

Lesson 29
Residual Properties II

Agenda
Review
Finish PS10
Start Capstone Calcs.

Block 6 Look-Ahead (CDP)

Real Gas Properties

- Residual Properties
- M = V, U, H, S, or G

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

Ideal gas (ig) follows ideal gas law

Real Solution Properties (Liquids)

- Excess Properties
- M^E = V^E, U^E, H^E, S^E, or G^E

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

$$G^E \equiv G - G^{id} \qquad H^E \equiv H - H^{id} \qquad S^E \equiv S - S^{id}$$

Ideal solution (id) follows Raoult's law

G^E is related to the activity coefficients

From Gibbs-Duhem:

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

Margules (1-constant)

$$\log \gamma_1 = A x_2^2 \qquad \log \gamma_2 = A x_1^2$$

- The constant A is known from fitting experimental data.
- These are the so-called "binary interaction parameters" in CHEMCAD and in the *capstone design problem*.

Residual Properties from Cubic EOS

Generic cubic equation of state (in Z-Form) **(WPR3)**

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

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

(α is found in Table 3.1)

These are the red equations from L28 slide 8 (cleanup).

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

q derivatives must be evaluated before process conditions (T_R, P_r) are entered.

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

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

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

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

$$I = \frac{1}{\sigma - \varepsilon} \ln \left(\frac{Z + \sigma\beta}{Z + \varepsilon\beta} \right) \qquad (13.72)$$

$$\varepsilon \neq \sigma$$

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