CH365 Chemical Engineering Thermodynamics

Lesson 29
Residual Properties II

<u>Agenda</u>
Review
Finish PS10
Start Capstone Calcs.

Block 6 Look-Ahead (CDP)

Real Gas Properties

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

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

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

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

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

Ideal solution (id) follows Raoult's law $\left(y_i P = x_i P_i^{sat}\right)$.

G^E is related to the activity coefficients

From Gibbs-Duhem: $$\frac{G^E}{RT} = \sum_i x_i \ln \gamma_i$$ (Eq. 13.10)

Margules
(1-constant)

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

- 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)**

$$q = q(x) = \frac{\Psi \alpha(x)}{\Omega \cdot x}$$ (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.

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

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

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

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

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

$$\varepsilon \neq \sigma$$

Questions?