CH365 Chemical Engineering Thermodynamics

Lesson 40
Review and Wrap-up

Lesson 40 Agenda

- Online Canvas surveys

- Paper ABET end-of-semester surveys

- TEE exam review

Term-End Exam

Rooms 331, 341

17 December 0730-1100 Wednesday

500 points, 5 problems, 100 points each

- Apply Raoult's Law and Rachford-Rice method to solve VLE with and without activity.

- Calculate T_{pc}, P_{pc}, and ω_{mix} for a mixture and Z, V_R, H_R, and S_R and ϕ from Lee-Kesler tables.

- Calculate properties of ideal gases and ideal gas mixtures ($C_{p,mix}$, V_{ig}, H_{ig}, and S_{ig}).

- Combine residuals and ideal properties to get real properties.

- Calculate residual properties V_R, S_R, and H_R from cubic equations of state from Lee-Kesler tables.

Term-End Exam Review

Calculating Properties

- Pure components – Z, V, H, S, G, and ϕ (or f)

  - Ideal gases $Z = \dfrac{PV}{RT} = 1$ and $\phi = 1$ (ideal gas)

  $$H = H_0^{ig} + R \cdot \int_{T_0}^{T} \left(C_{P_{298}}^{ig} / R \right) dT + H^R$$ (eq 6.50)

  $$S = S_0^{ig} + R \cdot \left(\int_{T_0}^{T} \left(\frac{C_{P_{298}}^{ig} / R}{T} \right) dT - \ln\left(\frac{P}{P_0} \right) \right) + S^R$$ (eq 6.51)

  - Real gas Z, V, and number of phases from cubic EOS

  $$Z = \frac{PV}{RT} \neq 1 \qquad Z = 1 + \beta - q\beta \frac{Z - \beta}{(Z + \varepsilon\beta)(Z + \sigma\beta)}$$ (eq 3.52, real gas)

- Residual properties from EOS or Lee-Kessler

  - Cubic EOS – Lesson 28, 29, Problem 6.141, WPR3

  $$\frac{H^R}{RT} = Z - 1 + T_r \left(\frac{dq}{dT_r} \right) \cdot I \qquad \frac{S^R}{R} = \ln(Z - \beta) + \left(q + T_r \frac{dq}{dT_r} \right) \cdot I \qquad I = \frac{1}{\sigma - \varepsilon} \ln\left(\frac{Z + \sigma\beta}{Z + \varepsilon\beta} \right)$$

  (p. 488) (eq 13.72)

  - Lee-Kessler tables – Lesson 30

- Real - combine ideal and residuals

- Fugacity – Lesson 35, Slides 10-13, computing - slides 12-13

  $$\ln \phi_i = Z_i - 1 - \ln(Z_i - \beta_i) - q_i I_i \qquad \beta_i = \Omega \frac{P_{r_i}}{T_r} \quad \text{(eq 3.50)} \qquad q_i = \frac{\Psi \alpha}{\Omega T_{r_i}} \quad \text{(eq 3.51)}$$

- Mixtures – use average ω, T_C, P_C, C_P

  - Weighted averages with y_i

  (eq 10.26)

  - Ideal gas entropy of mixing

  adds to entropy $R \sum_{i=1}^{3} y_i \ln \frac{1}{y_i}$

Term-End Exam Review

Calculating Properties

- Flash and activity coefficients – modified Raoult's Law

$$y_i P = x_i P_i^{sat}$$

$$K_i = \frac{y_i}{x_i} = \frac{P_i^{sat}}{P}$$

Raoult's Law
K-values
(simple solution,
id vapor phase)

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i P_i^{sat}}{P}$$

Modified Raoult's Law
K-values
(real liquid phase, id
vapor phase)

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i f_i^{sat}}{f}$$

Modified Raoult's Law
K-values with fugacity
(real liquid phase, real
vapor phase)

- Rachford-Rice algorithm – Prob. 13.1

- Fugacity and fugacity coefficients

- Practical applications – CHEMCAD, pipeline diameters – Prob. 6.83

Conceptual Issues

- What does it mean? Be able to define:

  - Simple fluids
  - Acentric factor
  - Enthalpy
  - Entropy
  - Gibbs Energy
  - Partial molar property
  - Chemical potential

  - Pitzer correlation
  - Residual property
  - Excess property
  - Gibbs Energy
  - Partial molar property
  - Chemical potential
  - Pitzer correlation

  - Fugacity
  - Bip
  - Activity coefficient
  - Ideal solution
  - Ideal gas
  - Phase equilibrium
  - Clapeyron's equation

Questions?