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

Room 331

14 December 0730-1100 Thursday

18 December 0730-1100 Monday

500 points, 5 problems, 100 points each

- Calculating properties of mixtures of ideal gases (V_{ig}, S_{ig}, and H_{ig}).
- Properties of mixtures; calculate C_P, T_{pc}, P_{pc}, and ω for a mixture.
- Residual properties V_R, S_R, and H_R. Calculating ϕ and residual properties from the Lee-Kesler tables and cubic equations of state.
- Calculating V and Z from cubic equations of state (Peng-Robinson, SRK, RK, etc.).
- Combining residuals and ideal properties to get real properties.
- Applications of Raoult's Law and Rachford-Rice method to VLE and solutions with and without activity.

Term-End Exam Review

Calculating Properties

- Pure components – Z, V, H, S, G, and ϕ (or f)
  - Ideal gases $Z = \frac{PV}{RT} = 1$ and ϕ=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

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

(p. 488)

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

(eq 13.72)

    - Lee-Kessler tables – Lesson 30
  - Real - combine ideal and residuals
  - Fugacity – Lesson 35, Slides 10-13, computing - slides 12-13

$$\ln \phi_i = Z_i - 1 - \ln(Z_i - \beta_i) - q_i I_i \qquad \beta_i = \Omega \frac{P_{r_i}}{T_r}$$

(eq 3.50)

$$q_i = \frac{\Psi \alpha}{\Omega T_{r_i}}$$

(eq 3.51)

- Mixtures – use average ω, T_C, P_C, C_P
  - Weighted averages with y_i
  - Ideal gas entropy of mixing

(eq 10.26)

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

$y_iP = x_iP_i^{sat}$

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

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