

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

Lesson 40 Agenda

- Online Canvas Surveys

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- ABET end-of-semester surveys

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

Slide 6

Calculating Properties

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

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

$$H = H_0^{\text{ig}} + R \cdot \int_{T_0}^T \left(\frac{C_{P,298}^{\text{ig}}}{R} \right) dT + H^R \quad (eq 6.50)$$

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

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

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

- Residual properties from EOS or Lee-Kessler

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

$$\frac{H^R}{RT} = Z - 1 + T_r \left(\frac{dq}{dT_r} \right) \cdot I \quad \frac{S^R}{R} = \ln(Z - \beta) + \left(q + T_r \frac{dq}{dT_r} \right) \cdot I \quad I = \frac{1}{\sigma - \epsilon} \ln \left(\frac{Z + \sigma\beta}{Z + \epsilon\beta} \right) \quad (p. 488) \quad (eq 13.72)$$

- Lee-Kessler tables – Lesson 30

- Real - combine ideal and residuals

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

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

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

- Weighted averages with y_i

- Ideal gas entropy of mixing

$$\text{adds to entropy} \quad R \sum_{i=1}^3 y_i \ln \frac{1}{y_i} \quad (eq 10.26)$$

Term-End Exam Review

- Flash and activity coefficients – modified Raoult's Law

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

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

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

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

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

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

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

Calculating Properties

- 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?