# 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 $\omega_{mix}$ for a mixture and Z, $V_R$, $H_R$, and $S_R$ and $\phi$ 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 EOS (PR, RK, SRK, vdW).

# Term-End Exam Review



## Calculating Properties

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

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

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

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

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

  - Residual properties from EOS or Lee-Kessler
    - Cubic EOS – Lesson 28, 29, Problem 6.141, WPR3

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

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

    - 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 $\omega$, $T_C$, $P_C$, $C_P$
  - Weighted averages with $y_i$
  - Ideal gas entropy of mixing

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

# Term-End Exam Review

## Calculating Properties

- Flash and activity coefficients – modified Raoult's Law

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

Raoult's Law

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

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?