

## CH365 Chemical Engineering Thermodynamics

### Capstone Design Project – IPR3 Guidance

19 November 2021

#### IPR2 AAR:

- $Z_1$  and  $Z_2$  must be correct. Check your answers with CHEMCAD.

#### IPR3 Guidance – due **Friday 19 November at 1630 hrs.**

- Calculation of  $Z$  using the modified SRK equation in the form of equations 3.48, 3.50, and 3.51, where  $\alpha$  and  $q$  are written as functions of  $x$ , as explained in the IPR2 guidance:

$$Z = 1 + \beta - q \cdot \beta \cdot \frac{Z - \beta}{(Z + \varepsilon \cdot \beta) \cdot (Z + \sigma \cdot \beta)} \quad (\text{eq. 3.48})$$

$$\beta = \Omega \cdot \frac{P_r}{T_r} \quad (\text{eq. 3.50})$$

$$q = \frac{\Psi \cdot \alpha}{\Omega \cdot T_r} \quad (\text{eq. 3.51})$$

- Calculation of  $H^R$  and  $S^R$  using the equations found (un-numbered) on page 488 and highlighted in red font on slide 7 of Lesson 28:

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

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

- Leaning forward (not graded in IPR3 but needed for final submission): Absolute stream enthalpy and entropy are calculated from Equations 6.50 and 6.51:

$$H = H_0^{\text{ig}} + \int_{T_0}^T C_p dT + H^R \quad (\text{eq. 6.50})$$

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

Note that  $H_0^{\text{ig}}$  and  $S_0^{\text{ig}}$  are the standard enthalpy and entropy of formation from CHEMCAD.

- Leaning forward (not graded in IPR3 but needed for final submission): Fugacity coefficients have not been covered in class yet but can be calculated with equation 13.85.
- Leaning forward (not graded in IPR3 but needed for final submission): Begin work on Aspen+.
- Update your summary table and abstract as appropriate.
- MMA and CHEMCAD files must also be in SharePoint.
- Cover sheet and Mathematica combined into single CAC-signed pdf in SharePoint.
- 30 points (25 tech, 5 writing)