Capstone Project - 300 points **Due: Lesson 40**

Objectives: In this project, you will (1) calculate thermodynamic properties (enthalpy, entropy, fugacity coefficient, and compressibility) at two different states, (2) assess your results using Aspen Plus and CHEMCAD, and (3) repeat your calculations for a second molecule.

Go to the "cadet assignments" link on the course web page to find your assigned substances and states (temperatures and pressures), then proceed to the following assignments:

1. 50 points. Use Mathematica and DIPPR Equation 107 to calculate H^{ig} and S^{ig} for your gas-phase substance

   (a) at T_1 and P_1,

   (b) at T_2 and P_2, and

   (c) verify your calculations for 1(a) and 1(b) using Aspen Plus.

2. 75 Points. Use the SRK equation of state to calculate the compressibility (Z), enthalpy departure (H^R), entropy departure (S^R), and fugacity coefficient (ϕ) for your substance

   (a) at T_1 and P_1,

   (b) at T_2 and P_2, and

   (c) verify your calculations for 2(a) and 2(b) using Aspen Plus.

3. 25 Points. Combine your answers from Problems 1 and 2 to obtain overall H and S values for your gas-phase substance

   (a) at T_1 and P_1,

   (b) at T_2 and P_2, and

   (c) verify your calculations for 3(a) and 3(b) using Aspen Plus.

4. 50 Points. Calculate Z, ϕ, H, and S at states 1 and 2 using CHEMCAD.

5. 50 Points. Repeat Problems 1 to 5 for your second molecule.

6. 50 Points. Writing assignment. Design and prepare an appropriately formatted table that summarizes your results. Your table must show calculated properties (H^{ig}, H^R, H, S^{ig}, S^R, S, Z, and ϕ) from Mathematica, Aspen Plus, and CHEMCAD. Your table must be designed to clearly show any differences in the properties.

Suggested IPR due-outs: IPR1 – Problem 1 complete; IPR2 – Z calculation is complete; IPR3 – Problems 1 through 5 complete (except fugacity).

Final Deliverables: (1) Mathematica file containing Problems 1, 2, 3 and 5 for both molecules. (2) Aspen+ files for both molecules, (3) CHEMCAD files for both molecules, (4) Word document containing your table, (5) PDF bundle containing a cover sheet plus deliverables 1 and 4 only, and (6) results input into master excel table on course website.