Homework Set 6

Due: Thursday, October 13 (sections 001, 003, and 004)/Friday, October 14 (section 002)

This assignment is to be completed individually. The number in parentheses next to each problem shows how many points the problem is worth in the overall assignment. Please show all work and use correct significant figures to receive full credit. Be sure to follow the problem formatting instructions to avoid unnecessary deductions. If you use an equation-solving tool (calculator, APEx, Solver, MATLAB), write out the equation(s) and note the tool that you used; otherwise, show all hand calculations used to solve any equations.

1. (10 pts) Using the SRK equation of state (or any other cubic equation of state) to determine a specific volume from a specified temperature and pressure requires a trial-and-error calculation or the use of root-finding software (like Solver or APEx). The goal of this problem is to use Excel's GoalSeek to determine (L/mol) for CO_2 at the following conditions: (i) 200K and 6.8 atm; (ii) 250K and 12.3 atm; (iii) 300K and 6.8 atm; (iv) 300K and 21.5 atm; and (v) 300K and 50.0 atm.
   (a) Starting with Equation 5.3-8, derive the following equivalent expression for the SRK equation of state: $f(\hat{V}) = P\hat{V}^3 - RT\hat{V}^2 + (a\alpha - b^2P - bRT)\hat{V} - a\alpha b = 0$
   (b) Prepare a spreadsheet with inputs to include: a species identifier (such as CO_2), the critical temperature, critical pressure, Pitzer acentric factor, and the temperatures and pressures for which is to be calculated, and to calculate using Equations 5.3-8 to 5.3-13 for each of the specified conditions.

   The spreadsheet should have the following structure:

Species	CO2				
Tc(K)	304.2				
Pc(atm)	72.9				
w	0.225				
a	*.****				
b	*.****				
m	*.****				
T(K)	P(atm)	alpha	V(ideal)	V(SRK)	f(V)
200	6.8	1.3370	2.4135	2.1125	*.**E-**
250	12.3	*.****	*.****	*.****	*.**E-**
300	6.8	*.****	*.****	*.****	*.**E-**
300	21.5	*.****	*.****	*.****	*.**E-**
300	50.0	*.****	*.****	*.****	*.**E-**

   Single digits should appear in place of each asterisk shown on the table. Formulas should be entered into the row for 200K and 6.8 atm and copied into the next four rows. The Goal Seek tool should be used to determine each $\hat{V}$ (SRK), starting with the ideal-gas value as an initial guess and varying the cell value to make f($\hat{V}$) as close as possible to zero.

Please print and submit the Excel spreadsheet for part (b) of this problem with the homework set. You will also need to submit the Excel file via Moodle. Please name your file LastName_Section_HW 6.xlsx (e.g. Bullard_002_HW6.xlsx). *Review the syllabus instructions about academic integrity related to spreadsheets.*

2. (10 pts) The oxidation of nitric oxide

$$NO + 1/2\,O_2 \rightleftharpoons NO_2$$

takes place in an isothermal batch reactor at constant volume. The reactor is charged with a mixture containing 20.0 volume percent NO and the balance air at an initial pressure of 380 kPa (absolute).
(a) Assuming ideal gas behavior, determine the composition of the mixture (component mole fractions) and the final pressure (kPa) if the conversion of NO is 90%.
(b) Suppose the pressure in the reactor eventually equilibrates at 360 kPa. What is the equilibrium percent conversion of NO? Calculate the reaction equilibrium constant at the prevailing temperature, K_p ($atm^{-0.5}$), defined as

$$K_p = \frac{\left(p_{NO_2}\right)}{\left(p_{NO}\right)\left(p_{O_2}\right)^{0.5}}$$

where p_i (atm) is the partial pressure of species i (NO_2, NO, O_2) at equilibrium.

3. (10 pts) Dry ice (solid CO_2) has been used as a mine explosive in the following manner. A hole is drilled into the mine wall, filled with dry ice plus a small charge of gunpowder, and then plugged. The gunpowder is lit with a fuse, vaporizing the CO_2 and building an explosively high pressure within the hole. Use each of the following correlations to estimate the pressure in kPa that will develop if 5.00 g of dry ice is placed in a 50.0 mL hole and heated to 1000 K: (a) the ideal gas equation of state, (b) the compressibility-factor equation of state, and (c) the SRK equation of state.

4. (10 pts) The product gas from a coal gasification plant consists of 60.0 mole % CO and the balance H_2; it leaves the plant at 150°C and 2000 psia. The gas expands through a turbine, and the outlet gas from the turbine is fed to a boiler furnace at 100°C and 1 atm at a rate of 15,000 ft^3/min. Estimate the inlet flow rate to the turbine in ft^3/min using Kay's rule. What percentage error would result from the use of the ideal gas equation of state at the turbine inlet?

5. (8 pts) Ethyl alcohol has a vapor pressure of 20.0 mm Hg at 8.0°C and a normal boiling point of 78.4°C. Estimate the vapor pressure at 45°C using (a) the Antoine equation; (b) the Clausius–Clapeyron equation and the two given data points; and (c) linear interpolation between the two given points. Taking the first estimate to be correct, calculate the percentage error associated with the second and third estimates. **Work this one in problem session – cover linear interpolation.**

6. (52 pts) The remainder of the assignment (8 problems) will be completed online using WileyPLUS. *You do not have to turn in any paperwork with this portion of the assignment.* Use the link for your class on the Moodle site, and then you can access the Assignment within WileyPLUS. The due date for the WileyPLUS completion is the same as for the homework assignment – the beginning of your class period. Note that the WileyPLUS assignment cannot be submitted late.

Challenge Problem: FR&B 5.31