CH2010: Chemical Engineering Thermodynamics

Assignement I

(Dated: September 20, 2020)

In order to ensure that each of you can work out the problem in an independent fashion, variables in each problem are either random or related to your roll number. Therefore we expect no two students will have the same numbers while working out the solutions.

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1. The following second virial coefficients have been reported for a mixture of n-butane (1) and carbon dioxide (2) at 313.2 K

$$B_{11} = -625 cm^3/mol$$
$$B_{22} = -110 cm^3/mol$$
$$B_{12} = -153 cm^3/mol$$

   From these data, do the following:

   - Predict the molar volume of a mixture of x% butane in carbon dioxide at 313.2 K and 10 bar. You can take x to be the following: If CHmnBpqr is your roll number, take $x = (mn + pqr)/150$.
   - Estimate the value of the binary interaction parameter, k_{12}, at 313.2 K.

2. Calculate the volume occupied by m kg of an alkane, C_lH_{2l+2} at P bar and T°C, using the following:

   - the ideal gas model
   - The Redlich–Kwong equation of state
   - The Peng–Robinson equation of state
   - The compressibility charts

   Use the following numerical values for variables. If CHmnBpqr is your roll number, take the alkane to be made up of $l = r$ if $r \geq 2$, else l to be a number of your choice. Take the numerical values of other variables as $m = pqr$, $P = 10 + (pqr/mn)$ and $T = 273.15 + (2 \times pqr)$.

3. Consider the Berthelot equation of state given below.

$$P = \frac{RT}{v - b} - \frac{a}{Tv^2} \tag{1}$$

   (a) Show how to calculate the constants a and b using only critical point data.

   (b) Find the reduced form of the Berthelot equation of state

   (c) Repeat the calculation in problem 2 using Berthelot equation of state.

4. Calculate the van der Waals parameters from critical point data for the three gases of your choice. Explain the relative magnitudes of a and b from a physical basis.

   To make sure that you are selecting different combinations, let us ensure that (i) molecular weight of one of the gases be close to your roll number (ii) the first alphabet of the name of one of the gases be a neighbouring alphabet of your name (first, middle or last).

5. Consider a mixture of two gases (say, species a and b) from problem 4. Write down expressions for the attractive interactions Γ_{aa}, Γ_{bb} and Γ_{ab} as a function of distance between the molecules, r. Sketch (qualitatively) this potential as a function of r.

[End]
