CHEG 231 Chemical Engineering Thermodynamics I
Semester Project
Due Friday, December 6, 2019, 11:55 p.m.

Content, Thermodynamic Data and Charts

Prepare the following information for your compound and include these in your report. Parts of this were previously assigned as components of your homework, so these can be adapted for the corresponding components in your report.

1. For your project compound, answer the following questions: Who produces it? How is it produced? What commercial significance of your compound?
2. For your compound, find:
    a. The constants $\boldsymbol{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$ for the Antoine equation (and the form of the equation for which they apply) or a similar model correlation. Include also the range of temperatures for which this equation is valid.
    b. The sublimation, vaporization, and fusion enthalpies ($\Delta\underline{\boldsymbol{H}}^{sub}$, $\Delta\underline{\boldsymbol{H}}^{vap}$, and $\Delta\underline{\boldsymbol{H}}^{fus}$), together with the temperatures and pressures at which they are measured or calculated.
    c. The temperature, pressure, and molar volume(s) corresponding to the triple point, critical point, and normal melting point.
3. Find the acentric factor, $\boldsymbol{\omega}$, and the critical compressibility, $\boldsymbol{Z_c}$, for your project compound using your vapor pressure correlation(s) and compare with any literature reports you can find in which $\boldsymbol{\omega}$ is provided. Also, obtain $\boldsymbol{a(T)}$ and $\boldsymbol{b}$ for the Peng-Robinson equation of state (P-R EOS) for your compound. In your report, be sure to discuss whether the P-R EOS truly is suitable for predicting the behavior of your compound. (In some cases, it may not be! To maintain similarity in the computational efforts required of the project, you will still use it regardless of how applicable it truly is.)
4. Using the P-R EOS , plot $\boldsymbol{C_P - C_V}$ as a function of $\boldsymbol{T}$ for reduced temperatures in the range $\boldsymbol{T_{r,tp} \le T_r \le 2.5}$ with $\boldsymbol{P_r = 1.00}$.
5. Using the P-R EOS, plot $\boldsymbol{C_P(T, P)}$ versus T for temperatures ranging from the triple point to $\boldsymbol{T_r = 2.5}$ with three isobars at $\boldsymbol{P_r = 0.00, 0.50}$ **and** $\boldsymbol{1.00}$. Comment on the trend in deviation of your compound from ideal gas behavior. Include a simulation of the gas phase heat capacity ($P \rightarrow 0$ limit) for your compound using the Joback Group Contribution Method as discussed in class. Comment on how this compares with any real data and available model correlations based on real data for your compound.
6. Using the P-R EOS, Plot $\boldsymbol{Z = P\underline{V}/RT}$ as a function of the reduced pressure, P_r, in the range $\boldsymbol{0 \le P_r \le 8}$ and for each of the following reduced isotherms: $\boldsymbol{T_r = 1.00, 1.10, 1.25, 1.50, 1.75,}$ ***and*** $\boldsymbol{2.00}$ (see for example Figure 6.6-3 in the textbook to compare with the Corresponding States compressibility factor behavior). On a separate graph, plot $Z = P\underline{V}/RT$ as a function of the reduced pressure, $\boldsymbol{P_r}$, for $\boldsymbol{0 \le P_r \le 8}$ and for the reduced isotherm $\boldsymbol{T_r = 1.00}$, ***using P-R EOS, vdW EOS, and values obtained from*** **Figure 6.6-3**. Which EOS provides predictions that are closest to the CS values?
7. Using the P-R EOS, plot the coefficient of thermal expansion, $\boldsymbol{\alpha}$, and the Joule-Thomson coefficient, $\boldsymbol{\mu_{JT}}$, versus reduced temperature in the range $\boldsymbol{T_{r,tp} \le T_r \le 2.5}$ for three isobars at $\boldsymbol{P_r = 0.00, 0.50,}$ **and** $\boldsymbol{1.00}$.
8. Plot $\boldsymbol{P - \underline{V}}$ phase diagram using the P-R EOS at $\boldsymbol{T_r = 0.70, 0.80, 0.90, 1.00, 1.25,}$ ***and*** $\boldsymbol{1.5}$ showing equilibrium (binodal) limits and stability (spinodal) limits for the liquid-vapor

envelopes (see for example Figure 7.3-4 in the textbook). Make sure your $\boldsymbol{P}$ and $\underline{\boldsymbol{V}}$ ranges clearly display the co-existence envelope (*i.e.* – not too small and not too large).

9. Plot $\boldsymbol{P-T}$ phase diagram using P-R EOS and quantitative $\boldsymbol{P^{vap}(T)}$ and $\boldsymbol{P^{sub}(T)}$ curves, with comparisons to Clausius-Clapeyron and Antoine curves for $\boldsymbol{P^{vap}(T)}$. If you have other vapor or sublimation correlations, you may find it useful to include them as well. (Note: Plot $\boldsymbol{P}$ versus $\boldsymbol{T}$ once in Cartesian coordinates and once on a semi-log plot, logarithmic in $\boldsymbol{P}$), to have a better view of the solid-vapor, solid-liquid, and liquid-vapor equilibrium lines. See Figure 7.3-6 in the textbook for a not-to-scale example.) The fusion curve may be difficult to describe with more than a straight line. At the least, you should be able to use the triple point and normal melting point to determine a line for this. Check to see if there are multiple solid phases known for your compound and include representations of these in your phase diagram. Make sure your $\boldsymbol{P}$ and $\boldsymbol{T}$ ranges clearly display the main features found on a $\boldsymbol{P-T}$ phase diagram (*i.e.* – not too small and not too large).

Report Outline

You need to prepare a report (single spacing, one line between paragraphs, Times New Roman, font size 11) following the outline below. The length suggestions are only for general guidance and may vary somewhat from person to person.

1. Cover page
It must include the course information (and section number), project title, your name, your project compound name, and date.

2. Abstract (on its own page, 250 words)

3. Introduction (no more than 500 words)
- **(a)** Basic chemistry
- **(b)** Compound uses
- **(c)** Safety issues
- **(d)** Environmental issues
- **(e)** Manufacturing processes

4. Methods (no more than 500 words)
- **(a)** Peng-Robinson EOS description
- **(b)** Critical properties
- **(c)** Outline of numerical procedures used to generate the thermodynamic charts

5. Results (no more than 500 words)
- **(a)** Thermodynamic charts with brief descriptions
- **(b)** Tables of values (process conditions, etc.) used in the charts

6. Discussion (no more than 500 words)
- **(a)** Discuss your diagrams in detail and compare them to experimental data if available.
- **(b)** Discuss the industrial or environmental significance of your compound and how that relates to its thermodynamic behavior.

7. Conclusion (no more than 250 words)

8. References
Please use ACS reference style. Details can be found at http://pubs.acs.org/paragonplus/submission/jacsat/jacsat_authguide.pdf.

9. Appendix (length will vary with computer code)
Any supporting information, the procedure of calculations, a copy of your MATLAB code, etc.

Report Submission

You must submit your project report electronically by 11:55 p.m. on December 7, 2018. **Both .doc(x) AND .pdf files are required for the electronic submission.** Name your files using this convention: [your compound name]_[your last name].doc(x)/.pdf (for example, Aniline_Enszer.docx). Late reports will earn partial credit, and no credit will be earned for reports submitted more than three days past the deadline. Technical difficulties are not an acceptable excuse for missing the deadline; be sure your file is not too large and not corrupted before submitting it. <u>**You are encouraged to submit your project WELL BEFORE the deadline.**</u>

<u>**Academic Honesty**</u>

The Delaware Code of Conduct states:

Plagiarism is the inclusion of someone else's words, ideas, images, or data as one's own. When a student submits academic work that includes another's words, ideas, images, or data, whether published or unpublished, the source of that information must be acknowledged with complete and accurate references and, if verbatim statements are included, with quotation marks as well. By submitting work as his or her own, a student certifies the originality of all material not otherwise acknowledged. Plagiarism includes, but is not limited to:

i. The quotation or other use of another person's words, ideas, opinions, thoughts, or theories (even if paraphrased into one's own words) without acknowledgment of the source; or
ii. The quotation or other use of facts, statistics, or other data or materials (including images) that are not clearly common knowledge without acknowledgment of the source.

In the context of this project, you are expected to hand in 100% original work. All text, code, plots, and calculations must be your own. References must be cited.