ChE 63b Chemical Engineering Thermodynamics

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Texts:

Engineering and Chemical Thermodynamics, Milo D. Koretsky, Wiley, 2004.

Statistical Mechanics: A Concise Introduction for Chemists, B. Widom, Cambridge, 2002.

Grading Scheme:

Homework (approx. 1 per week)	30%
Mid-term exam	30%
Final exam	40%

Collaboration Policy:

For problem sets, you may consult any texts that you wish, but you may not look at problem set solutions or exams from previous years. You are encouraged to discuss problem sets together, and with the TA, but the work that you turn in should reflect your own understanding of the material. While you may use software such as Mathematica, Maple, Matlab, etc. on the homework, you should be aware that you will not be allowed to use such programs on the exams.

Course Outline:

1. Review (1)
   Work, heat and energy;
   First law for closed systems; enthalpy; heat capacity; open systems;
   Second law; definition of entropy; mathematical statement of second law; microscopic interpretation of entropy; maximum and minimum work; heat engine and Carnot cycle;
   Helmholtz and Gibbs free energies; chemical potential; fundamental equations; Maxwell relations.

2. Review (2)
   Equilibrium condition; stability criteria;
   Ideal gas; corrections for non-ideality;
   PVT behavior of single component fluids: EOS; V-L equilibrium; melting; Clapeyron equation.

3. Mixtures
   Ideal gas mixtures; entropy of mixing; partial molar properties; fugacity and excess functions; reversible work of mixing and separation.

4. Solutions
   Ideal and/or dilute solutions; Raoul's law and Henry's law; colligative properties of dilute solutions; osmotic pressure; vapor-liquid equilibria in solutions; phase diagrams.

5. Models for solutions
   Regular solution model; Margule's model; Flory-Huggins theory for polymer solutions and blends.

6. Chemical equilibria
   Standard Gibbs free energy change and the equilibrium constant; effects of temperature and pressure on chemical equilibrium; aggregation (micellization) as a chemical reaction.

7. Introductory statistical thermodynamics
   Boltzmann entropy formula; Boltzmann distribution law; partition functions; connection to thermodynamics; 2-state and lattice models; Maxwell-Boltzmann velocity distribution; partition function for monatomic and diatomic gases; 2nd virial coefficient.