MSE 3000: CHEMICAL THERMODYNAMICS OF MATERIALS
Prof. R. F. Speyer

COURSE OUTLINE

1. EMPIRICAL PROPERTIES OF GASES

   Ideal gases. Molecular view of pressure. Dalton's law of partial pressures. Gas energy, average velocity, and velocity distribution. Real gases.

2. THE FIRST LAW OF THERMODYNAMICS

   Temperature. Work. Path dependence/independence. Maximum and minimum work. Heat and the First Law. Special conditions: constant volume, constant temperature, constant pressure, adiabatic. Relation between C_p and C_V.

3. THE SECOND LAW OF THERMODYNAMICS

   Carnot engine and the Clausius inequality. Two types of entropy. Statistical thermodynamics. Configurational entropy: diffusion and polymer conformations. Carnot cycle revisited.

4. AUXILIARY FUNCTIONS

   Combined 1st and 2nd laws. Maxwell relations and applications: Debye heat capacity and achieving cryogenic temperatures. Use of the Helmholtz energy in predicting equilibrium. The competing terms for the Gibbs energy: thermodynamics of vacancy formation in solids.

5. CHEMICAL THERMODYNAMICS

   The reversibility of phase transformations. Chemical potential and unary phase equilibria. Osmotic pressure. The conditions of equilibrium. The Clapeyron equation and unary phase equilibria. LeChatelier's principle.

6. TEMPERATURE DEPENDENCE OF THERMODYNAMIC FUNCTIONS

   Sensible and latent heats. Temperature dependence of entropy and the third law. Formation reactions. Useful approximations. Calorimetry.

7. GASEOUS REACTION EQUILIBRIA

   Combustion. Adiabatic flame temperature. Standard Gibbs energy of reaction and the equilibrium constant. Equilibria between pure condensed phases and a gas. Reduction of metals. Extractive metallurgy. The Gibbs-Helmholtz relation. Two methods of obtaining thermodynamic data.

8. SOLUTIONS

   Raoult's and Henry's laws. Measurement of vapor pressure. Gibbs energy of mixing. The Gibbs-Duhem equation. Graphical determination of the partial molar Gibbs energy of mixing.

9. BINARY PHASE EQUILIBRIA

   Fully miscible solid and liquid solutions. Refining of fully miscible binary systems: fractional crystallization, zone melting, liquid-vapor systems. Limited miscibility: regular solutions. Intermediate compounds. Experimental methods for phase equilibria.

10. THE PHASE RULE

    Foundations. Applications: unary equilibria, reaction equilibria among gases and pure condensed phases, reaction equilibria among gases and condensed solutions, binary phase equilibria.

11. TERNARY PHASE EQUILIBRIA

    Ternary equilibria with pure solids. The CaO-Al_2O_3-SiO_2 system. Ternary equilibria with solid solutions.

REFERENCES

1. D. R. Gaskell, *Introduction to the Thermodynamics of Materials*, 3rd Ed., Taylor and Francis, Washington, DC, 1995.
2. G. W. Castellan, *Physical Chemistry*, 3rd Ed., Addison-Wesley, Reading, MA, 1983.
3. K. Denbigh, *The Principles of Chemical Equilibrium* 4th Ed., Cambridge University Press, Cambridge, UK.
4. C. G. Bergeron and S. H. Risbud, *Introduction to Phase Equilibria in Ceramics*, American Ceramic Soc., Westerville, OH, 1984.
5. F. N. Rhines, *Phase Diagrams in Metallurgy, Their Development and Application*, McGraw-Hill, New York, 1956.
6. H. B. Callen, *Thermodynamics and an Introduction to Thermostatics*, 2nd Ed., John Wiley and Sons, New York, 1985.
7. O. Kubaschewski, C. B. Alcock, and P. J. Spencer, *Materials Thermochemistry*, 6th Ed., Pergamon Press, New York, 1993.

EXAMS

There will be 7 exams during the semester, all equally weighted. The seventh exam will be given during the final exam period. Exam dates: August 30, September 15, October 1, October 15, November 3, November 17, December 6 (final exam period). The exams will ask for derivations from the lecture and lecture handouts, written explanations of concepts presented in lecture and lecture handouts, and problem solving very closely related to example problems (and solutions) handed out in lecture.