CH272: APPLIED PHASE AND CHEMICAL EQUILIBRIA
Spring 2008

Catalog Data: CH272 Applied Phase and Chemical Equilibria
Fugacities, activities, thermodynamics of solutions, phase equilibria, reaction equilibria, and flash calculations. Engineering applications, safety and design considerations.
Pre-requisites: CH271
Course Type: Required
Textbook: Engineering and Chemical Thermodynamics
M. Koretsky, Wiley, NY, 2004
Instructor: Ross Taylor (CAMP 222, 268-6652, taylor@clarkson.edu)
Office hours: Open door policy or by appointment

Learning Objectives:

1. To introduce a bewildering array of thermodynamic properties some of which have names like *Gibbs excess energy*, Helmholtz energy, *activity*, fugacity, and *K-constants* (even though they're not - constant that is).
2. To study law (the laws of Raoult, Henry, and Ideal Gas will do for a start).
3. To understand how to calculate activity coefficients, fugacity coefficients and other strange quantities that help when those laws fail (which is most of the time).
4. To know what the acronyms NRTL, UNIQUAC, UNIFAC, ASOG, SRK, and PR stand for, what to calculate with them, when to use them, and - more importantly - when *not* to use them.
5. To carry out phase equilibrium calculations for multiphase systems (e.g. vapor-liquid, liquid-liquid).
6. To understand chemical reaction equilibria.
7. To understand and *create* phase diagrams for multiphase systems.
8. To understand and create residue curve and distillation boundary maps.
9. To model single equilibrium stage operations (e.g. flash).

Learning Outcomes[1]:

1. Students will become familiar with fugacity coefficients, activity coefficients, K-values, and other thermodynamic properties of mixtures [1-8] (1)
2. Students will know how to choose from a menu of models for calculating these properties [7,8] (1)
3. Students will be able to recognize different kinds of vapor-liquid and liquid-liquid phase diagrams [1-8] (1)
4. Students will be able to sketch distillation boundary maps and residue curve maps and understand the significance of these diagrams [5,7,8] (1)
5. Students will be able to perform flash calculations. (1)

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1 Numbers in [] refer to evaluation methods used to assess student performance
Numbers in () refer to the program outcomes

Evaluation:

Grades will be based on your performance on a number of assignments, some of which will be done by yourself and others in small groups. Major assignments (not in chronological order) are shown below. Some of these will require writing a formal report.

1. Presentation on either someone of importance in the history of thermodynamics, or on some aspect of thermodynamics – 10%
2. Activity coefficients – 15%
3. Bubble and dew points, phase diagrams – 15%
4. High pressure VLE – 15%
5. Liquid-liquid equilibria – 10%
6. Equilibrium topic to be determined – 10%
7. A small number of surprise quizzes – 10%
8. Final exam (multiple choice, past exams will be made available) – 15%

Course Topics:

1. Equilibrium in one-component systems
2. Equilibrium in multicomponent systems
3. K-values and relative volatility
4. Equilibrium data
5. Ideal behavior
6. Nonideal behavior
7. Activity coefficient models
8. Parameter fitting
9. Fugacity coefficients for mixtures from equations of state
10. K-value models
11. Bubble and dew point calculations
12. Computer creation of phase diagrams
13. Phase diagrams for vapor-liquid systems
14. Phase diagrams for liquid-liquid systems
15. High-pressure phase behavior - retrograde behavior
16. Flash calculations
17. Azeotropes
18. Three-phase behavior
19. Complex mixtures – crude oil
20. Electrolytes
21. Solid-liquid systems
22. Gas-liquid systems
23. Reaction equilibrium
24. Residue curves and distillation boundaries

Class Time: MWF 9:00 AM, SC162
Prepared by: Ross Taylor, January 8, 2008