**CHEN 3370 - PHASE AND REACTION EQUILIBRIA (3)
Required Core Course**

**2015-2016 Catalog Data Lec (3).** Molecular thermodynamics of phase and chemical reaction equilibria including non-ideal thermodynamics and multicomponent applications.

**Prerequisites** Pr: MATH 2630 or MATH 2637, Completion of CHEN 2100 and ENGR 2010 with grades of C or better, P/C CHEN 3600

**Schedule** Three one-hour class sessions per week.

**Course Objectives** This course teaches chemical engineering students applications of thermodynamics principles to gas and liquid mixtures, non-ideal solutions, phase equilibria, and chemically reacting systems.

**Textbooks** *(Instructor’s choice)*

Elliott, Introductory Chemical Engineering Thermodynamics, 2e, 2011, 0136068545, Prentice-Hall

Smith, Introduction to Chemical Engineering Thermodynamics, 7e, 2004, 9780073104454, McGraw-Hill

**Topics Covered {outcome numbers}**

1. Selection and use of equations of state (1.67 weeks) {1,2}
2. Thermodynamic property relations (2.00 weeks) {3-6}
3. Phase equilibrium single component systems (1.67 weeks) {7-11}
4. Phase equilibrium multicomponent systems (3.33 weeks) {12-20}
5. Use of Gamma-Phi formulation of VLE to solve phase equilibrium problems based on reasonable assumptions (1.67 weeks) {21-22}
6. Introduction to the molecular basis of thermodynamic parameters and extension to other types of phase equilibria (0.67 week) {23-24}
7. Chemical reaction equilibria (2.00 weeks) {25-27}
8. Exams (1.00 weeks)

**Course Outcomes:** Upon successful completion of this course, students should be able to:

1. Predict the P-V-T properties of gases and liquids using equations of state including the ideal gas law, van der Waals equation, virial equation, generalized cubic equations of state, the Rackett equation and generalized compressibility factor charts.
2. Demonstrate the ability to select an appropriate equation of state or generalized correlation or chart based on the temperature, pressure, chemical composition and required level of precision in the answer.
3. Explain the concepts and definitions of enthalpy (H), entropy (S), Helmholtz energy (A), Gibbs free energy (G), heat capacity at constant pressure (Cp) and volume (Cv), volume expansivity, and isothermal compressibility.
4. Use multivariate calculus (partial and total derivatives) to develop general fundamental property (Gibbs) relations for differential changes in fundamental thermodynamic properties (U, H, A, G) in a simple closed system.
5. Apply multivariable calculus to derive the Maxwell relations and then develop the “Fundamental Property Equations” to relate easily measured experimental properties (P,V, T) to thermodynamic quantities (dU, dA, dH, dG).
6. Demonstrate the ability to use Fundamental Property Equations, Maxwell relations, and Equations of State in conjunction with one another to solve problems involving process changes starting from either P-V-T data or thermodynamic property data.
7. Explain the concepts of departure functions, residual and excess properties and evaluate these functions for practical engineering applications using equations of state or generalized correlations.
8. Explain the concepts underlying phase equilibria for a pure gas, liquid or solid.
9. Explain the concepts of fugacity and fugacity coefficient.
10. Calculate the fugacity coefficient using the equations of state and generalized correlations.
11. Identify and explain the Clapeyron equation, Clausius-Clapeyron equation, shortcut vapor pressure equation, Poynting correction, and Rackett equation.
12. Explain the concepts of chemical potential, partial molar properties, partial molar excess properties, component fugacity, component fugacity coefficient, activity, activity coefficient, standard state fugacity, ideal solution, thermodynamic properties of mixing, and Lewis-Randall rule.
13. Explain the concepts underlying phase equilibria for multicomponent systems.
14. Evaluate component fugacity coefficients as a function of composition for ideal gas mixtures, ideal solutions and real gas mixtures. Explain the concept of mixing rules.
15. Read accurately and extract thermodynamic vapor liquid equilibrium (VLE) data from phase diagrams.
16. Construct P-x-y and T-x-y diagrams from experimental VLE data and various VLE models.
17. Explain the concepts of activity coefficient as a correction factor for non-ideal solution behavior and the thermodynamic relationship between activity coefficient and the partial molar excess Gibbs energy. Explain what is meant by an activity (or activity coefficient) model.
18. Calculate activity coefficients from experimental VLE data at a limited number of compositions, develop (or fit) a model for the composition dependence of excess Gibbs energy and, after differentiating, obtain a mathematical expression for predicting activity coefficients across the composition range for use in engineering VLE problems including the construction of phase diagrams.
19. Demonstrate the ability to use graphical techniques and the Gibbs-Duhem equation to test for thermodynamic consistency between experimental and predicted data.
20. Explain the advantages and limitations of empirical activity models (Margules equations and van Laar equation), regular solution models (Scatchard-Hildebrand) and local composition models (Wilson, UNIQUAC, and UNIFAC).
21. Write the mathematical expression for the General VLE Equation (Gamma-Phi formulation) including liquid and vapor nonideality and the Poynting correction and explain and discuss the significance of each symbol in the equation.
22. Demonstrate the ability to simplify the General VLE Equation (non-ideal liquid, non-ideal gas) based on the problem statement and solve equilibrium, bubble point, dew point, and flash problems.
23. Demonstrate awareness of the molecular basis for thermodynamics by explaining the basic concepts of intermolecular potentials, the origin of the second virial coefficient and the sign of excess properties.
24. Demonstrate an awareness that the basic principles for solving VLE problems apply to other types of equilibrium such as VLLE, LLE, and SLE.
25. Explain the concepts underlying chemical reaction equilibrium, minimization of Gibbs energy, reaction coordinate, standard state Gibbs energy of reaction, equilibrium constant, equilibrium conversion and yield.
26. Explain the effects of concentration, temperature, pressure and the addition of an inert component on equilibrium conversion in gas phase reactions.
27. Calculate the equilibrium conversion and composition at a given temperature and pressure for gas phase reactions using ideal gas mixture, ideal solution and real gas mixture models.

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| **Contribution of Course to Meeting ABET Criteria 5 (Curriculum)** |
| **Math and Basic Sciences** | **Engineering Topics** | **General Education** |
| 0 Credits | 3 Credits | 0 Credits |

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| **Relationship of Course to Student Outcomes (PO’s)** |
| **Student Outcome** | **A** | **B** | **C** | **D** | **E** | **F** | **G1** | **G2** | **H** | **I** | **J** | **K** |
| **Level of Coverage** | **S** | **S** |  |  | **R** | **I** |  |  |  |  |  | **I** |

 **Date of Preparation and Person(s) Preparing This Description:**

June 11, 2016. Virginia A. Davis, Ronald Neumann, and Allan David.