## Readings

Chapter readings in the table are from the course text, Tester, J. W., and Michael, Modell. *Thermodynamics and Its Applications*. Upper Saddle River, NJ: Prentice Hall PTR, 1997.

| SES # | TOPICS | READINGS |
|---|---|---|
| *Part I - Fundamental Principles* | | |
| 1 | Course Outline, Motivation to Connect Classical Concepts and Laws to Physical Properties from Macroscopic to Molecular, Definitions, Nomenclature, Exams+Homework Policy, Approach to Solving Problems, Constitutive Property Models and the Ideal Gas State, Postulatory Approach, 1st Law Concepts | Handouts |
| 2 | Postulatory Approach<br>1st Law Concepts (Work, Heat, and Energy), Closed and Open System Treatments, including PE+KE Effects, Tank Blowdown [Demonstration - CO2 Fire Extinguisher] | Ch 1-2 (all sections), 3.1-3.8 |
| 3 | 1st Law Open | 3.7-3.9 |

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| | Systems, Tank Blowdown and Filling - Class Examples, Problem 3.9 | |
| 4 | 2nd Law Concepts, Reversible Heat Engines, Carnot Efficiency, Entropy, Clausius Theorem, Reversibility[Demo-drinking Bird] | 4.1-4.5 |
| 5 | Entropy Balance, 1st and 2nd Laws Combined [Demo - Hilsch Vortex Tube] | 4.6-4.7 |
| 6 | 2nd Law Concepts and Applications, Steady State and Transient Flow Work | 4.8-4.9 |
| 7 | Availability and Exergy Concepts, Heat Integration and Pinch Analysis, Power Cycle Analysis [Demo - Stirling Engine] | 14.1-14.3, 14.5-14.6 |
| 8 | Calculus of Thermodynamics, Gibbs Fundamental Equation, Graphical Interpretation of Fundamental Surface | 5.1-5.4<br><br>Thermodynamic Properties of Pure Materials (PDF) |
| 9 | Derivative Transformation and Manipulation, Maxwell Relations, | 5.1-5.4 |

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| | Jacobian Transformations | |
| 10 | Legendre Transformations, Equivalent Forms of the Fundamental Equation, Examples | 5.5-5.7 |
| 11 | Legendre Transforms Continued, Connections to the Gibbs Surface and Other Derived Properties | 5.5-5.7 |
| 12 | Equilibrium Criteria Concepts and Applications---Phase, Chemical, and Membrane, Phase Rule, Examples of Simple Phase Diagrams | 6.1-6.7 |
| 13 | Stability Criteria, Concepts and Applications, Critical States | 7.1-7.2 |
| 14 | Pure Component Properties, Fund. Eq., Theorem of Corresponding States, Constitutive Property Models - Stress Connections to Molecular Level Interactions and Effects | 8.1-8.2 |
| 15 | Real Fluid Properties, *PVTN* Equations of State, | 8.3-8.4 |

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| | Ideal Gas Heat Capacity Cp* | |
| 16 | Departure Functions, Concepts and Applications, Standard ΔG° and ΔH° of Formation | 8.5, 8.7-8.9 |
| 17 | Mixtures, *PVTN EOSs* , Partial Molar Properties, Gibbs-Duhem Relation, Mixing Functions, Discuss Problem 9.2, Ideal Gas Mixtures and Ideal Solutions, Fugacity and Fugacity Coefficients, Standard States | 9.1-9.7 |
| 18 | Ideal Solution Conditions, Excess Properties, Activity and Activity Coefficients, ΔGEX- γi Models (See Table 11.1), Standard States, Thermodynamic Consistency using the Gibbs-Duhem Relation | 9.8, 11.2, 11.4, 11.7, 11.9 |
| 19 | Mixture Equations of State, Continued and Needs | 11.7, 11.9 |
| 20 | *Review for Exam 1* | |
| | *Exam I: 2 hours* | |
| *Part II - Introduction to Statistical Mechanics for* | | |

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| *the Interpretation of Thermodynamic Functions and the Computation of Thermodynamic Properties* | | |
| 21 | Fundamental Principles of Quantum and Classical Statistical Mechanics - N-body Problem, Phase Space, Statistics and Distribution Functions and Averaging Methods, Boltzmann Distribution | 10.1, handouts<br><br>Fundamental Principles of Quantum and Classical Statistical Mechanics (PDF) |
| 22 | Postulates of Statistical Mechanics, Gibbs ensembles - Micro-canonical and Canonical; States of System, Probabilities | 10.1, handouts<br><br>Postulates of Statistical Mechanics, Gibbs Ensembles (PDF) |
| 23 | Computation of Ideal Gas Properties from Intramolecular Effects - Translation, Rotation, Vibration using Statistical Mechanics I | 10.1, handouts<br><br>Computation of the Properties of Ideal Gases (PDF) |
| 24 | Computation of Ideal Gas Properties from Intramolecular Effects - Translation, Rotation, Vibration using Statistical Mechanics II | 10.1, handouts<br><br>Computation of the Properties of Ideal Gases (PDF)<br><br>Appendix to Session 21-24 Statistical |

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| | | Mechanics Readings: Connection to Thermodynamics and Derivation of Boltzmann Distribution (PDF) |
| 25 | Classical Statistical Mechanics; Hamiltonian and Ideal Gases, Factoring the Partition Function with the Semi-classical Approximation, *PVTN* Properties via Configuration Integral from Intermolecular Effects, Grand Canonical Ensemble I | 10.1, handouts |
| 26 | Semi-classical Approximation, *PVTN* Properties via Configuration Integral from Intermolecular Effects, Grand Canonical Ensemble II -- Examples | 10.1, handouts |
| 27 | Gibbs Ensembles Continued: Micro-canonical Ensemble Revisited, Grand Canonical, NPT, etc., Including Equivalence of Ensembles; Time Averaging and | 10.1, handouts |

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| | Ergodicity, and Fluctuations; Macroscopic Connection | |
| 28 | Intermolecular Forces and Potentials, Role of Quantum Mechanics, Commonly used Potential Functions, Pairwise Additivity | 10.2-10.3 |
| 29 | Virial Equation of State and Molecular Corresponding States from Statistical Mechanics; Connection of *PVTN* Equations of State to Statistical Mechanics and Molecular Simulations | 10.4-10.6 |
| 30 | Mean Field Theory, Connecting the van der Waals EOS Model to Statistical Mechanics, Hard Sphere Fluids, Perturbed Hard Sphere Fluids, Lattice Models | 10.6, 10.8 |
| 31 | Statistical Mechanical Models of Fluids I - Expanding the Virial EOS to Mixtures, Radial Distribution Functions, Structure | 10.7 |

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| | of Fluid and Solid Phases, Critical Phenomena (Fluctuations, Critical Opalescence) | |
| 32 | Statistical Mechanical Models of Fluids II - Biological Materials and Protein Applications | 10.7 |
| 33 | Foundations of Molecular Simulations - Monte Carlo and Molecular Dynamics | 10.9 |
| 34 | Application of Molecular Simulations to Estimating Pure Component and Mixture Properties | 10.9 |
| *Part III - Multi-scale Thermodynamics of Pure Fluids and Mixtures - Physical Properties and Phase and Chemical Equilibria* | | |
| 35 | Calculation of Pure Component Properties (Vapor Pressure, Δ *Hvap*, … etc.) Using Equation of State and Other Models--Departure Functions | 8.5, 8.7, 8.9 |
| 36 | Review of Mixture Thermodynamics, Fugacity, Fugacity Coefficient, | 9.1-9.8 |

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| | Activity, Activity Coefficient, Standard States and Constitutive Models for Capturing Non-Ideal Effects | |
| 37 | Phase Equilibrium and Stability - Gibbs Phase Rule, Phase Diagrams, Using Constitutive Property Models for Capturing Non-Ideal Effects | 15.1-15.2, 15.8 |
| 38 | Applications of Mixture Thermodynamics to VLE Phase Equilibria, Minimum Work of Separation, etc. | 9.7-9.9, 11.4, 11.7, 11.9 |
| 39-40 | *Review for Exam II* -- Review of Statistical Mechanics Principles and Applications, and Pure Fluid and Mixture Properties | |
| | *Exam II: 2 hours* | |
| 41 | Phase Equilibria, Differential Approach, Constitutive Property Models Continued, *P-T* Relationships | 15.3-15.4, 11.1-11.7 |
| 42 | Phase Equilibria, Integral Approach, | 15.5 |

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| | Applications, Solubility - Gas - Liquid, Liquid - Liquid, and Solid - Liquid Systems | |
| 43 | Phase Equilibria Applications - Examples Colligative Properties, Ternary Diagrams, S-L-V Three Phase Monovariant Binary Equilibria, Biological Examples | |
| 44 | Phase Stability Applications, Spinodal Decomposition, Critical Points, Uses of Equations of State and Gibbs Free Energy Models, Polymer and Materials Examples, Pictures of Crystalization | 7.1-7.2, 15.6-15.7 |
| 45 | Chemical Equilibrium - General Approach, Nonstoichiometric and Stoichiometric Formulation, Statistical Mechanical Approach | 16.1-16.4, 16.9 |
| 46 | Equilibrium Constants and Standard States, Gibbs Phase Rule | 16.5-16.6 |

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| | Applications | |
| 47 | Chemical Equilibria Applications and Example Problems, Combined Phase and Chemical Equilbria | 17.1-17.3 |
| 48 | *Review Session* | |
| | *Final Exam: 3 hours* | |

**Supplementary References***

**CLASSICAL THERMODYNAMICS**


Bejan. *Advanced Engineering Thermodynamics.* Wiley, New York: 1988. [Graduate Level, mechanical engineering emphasis, generalized exergy/availability analysis].*

Bett, Rowlinson, and Saville. *Thermodynamics for Chemical Engineers.* MIT Press, 1975. [General text from a Chemical Engineering perspective].

Callen. *Thermodynamics and an Introduction to Thermostatistics.* Wiley, 1985. [Physics approach, recommended section on Legendre transformations].*

Denbigh. *Principles of Chemical Equilibrium.* 4th ed. London: Cambridge University Press, 1981. [Well-written, alternative intermediate text from a Chemistry perspective].*

Gibbs. *Collected Works I: Thermodynamics.* Yale University Press, 1963. [Historical reference].*

Gyftopoulos, and Beretta. *Thermodynamics: Foundations and Applications.* Macmillan, 1991. [Comprehensive mechanical engineering approach, power cycles, availability/exergy analysis].

Hatsopoulous, and Keenan. *Principles of General Thermodynamics.* Wiley, 1964. [Detailed theoretical, postulatory approach].

Hougen, and Watson. *Chemical Process Principles I: Thermodynamics.* 2nd ed. Wiley, 1959. [Corresponding-states principle, a classic Chemical Engineering Thermodynamics text].

Keenan, et al. *Steam Tables: Thermodynamic Properties of Water Including Vapor, Liquid, and Solid Phases,* International System of Units. Wiley, 1978. [Good reference].

Pitzer. *Thermodynamics.* 3rd ed. McGraw-Hill, 1995. [Well-written, revision of classic 1923 text by G.N. Lewis and M. Randall, treats electrolytes].

Milora, and Tester. *Geothermal Energy as a Source of Electric Power.* MIT Press, 1976. [Thermodynamic treatment of low-temperature power cycles].

Prausnitz, Lichtenthaler, and Azevedo. *Molecular Thermodynamics of Fluid Phase Equilibria.* 3rd ed. Prentice-Hall, 1999. [Intermolecular forces, bridges the gap between Classical and Statistical Thermodynamics, presents many practical models for non-ideal behavior].

Prigogine, and Defay. *Chemical Thermodynamics.* London: Longmans, 1954. [Detailed, theoretical, good on mixtures and phase equilibria].

Reid, Prausnitz, and Poling. *The Properties of Gases and Liquids.* 4th ed. McGraw-Hill, 1987. [Essential for estimating thermodynamic properties].

Sandler. *Chemical and Engineering Thermodynamics.* Wiley, 1999. [Introductory, well-organized].

Smith, van Ness, and Abbott. *Introduction to Chemical Engineering Thermodynamics.* 5th ed. McGraw-Hill, 1996. [Introductory, classic chemical engineering undergrad text, well-organized].

Tisza. *Generalized Thermodynamics.* MIT Press, 1966. [Theoretical, detailed discussion of Legendre transformations].

Walas. *Phase Equilibria in Chemical Engineering.* Buttersworth, 1985. [Excellent, practical treatment of VLE and LLE].

Weber, and Meissner. *Thermodynamics for Chemical Engineers.* 2nd ed. Wiley, 1957. [Well-written, introductory text].

**STATISTICAL MECHANICS**

Chandler. *Introduction to Modern Statistical Mechanics.* Oxford, New York, 1982. [Concepts and modern theory, particularly helpful for phase transitions.]

Callen. *Thermodynamics and an Introduction to Thermostatistics.* 2nd ed. Wiley, 1985. [Critical-point scaling theories.]

Debenedetti. *Metastable Liquids.* Princeton University Press, 1996. [Modern treatment of experimental data and theories regarding stability and criticality.]

Hill. *Statistical Mechanics - Principles and Selected Applications.* Dover, 1987. [Advanced text covering basic aspects of liquid state theory.]

Hirshfelder, Curtiss, and Bird. *Molecular Theory of Gases and Liquids.* Wiley, 1954. [Excellent comprehensive treatment of theory and early work.]

Huang. *Statistical Mechanics.* Wiley, 1987. [Advanced text with extensive discussion of Ising models.]

McQuarrie. *Statistical Mechanics.* Harper Row, 1976. [Good detailed treatment of classical statistical mechanics.]*

Pathria. *Statistical Mechanics.* 2nd ed. Butterworth-Heinemann, 1996. [Intermediate text, with a thorough coverage of phase transitions and condensed matter theory.]

Reed, and Gubbins. *Applied Statistical Mechanics.* Butterworth-Heinemann, 1973. [Intermediate level text with a solid treatment of intermolecular potentials and some liquid state theory.]

Reif. *Fundamentals of Statistical and Thermal Physics.* McGraw-Hill, 1965. [Introductory text with clear explanations of basic concepts of statistical mechanics, motivated from probability theory.]

Rowley. *Statistical Mechanics for Thermophysical Property Calculations.* Upper Saddle River, NJ: Prentice-Hall, 1994. [Clear basic treatment, including simulation methods, written by a Chemical Engineer.]

Stanley. *Introduction to Phase Transitions and Critical Phenomena.* Clarendon Press-Oxford, 1971. [A classic text in its field, with clear discussions of scaling relations and critical exponents.]

Yeomans. *Statistical Mechanics of Phase Transitions.* Clarendon Press-Oxford, 1992. [An introductory text, simpler than Stanley, with discussions of a number of techniques commonly used in studying the behavior of many-body systems.]

**MOLECULAR SIMULATIONS**

Allen, and Tildesley. *Computer Simulation of Liquids.* Oxford, 1987. [Classic treatment.]

Frenkel, and Smit. *Understanding Molecular Simulation.* Academic Press, 1996. [Good overview with more recent advances than Allen and Tildesley.]

*Starred references are of particular value in supplementing text readings.