Calendar

SES #	TOPICS	KEY DATES
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	
2	Postulatory Approach 1st Law Concepts (Work, Heat, and Energy), Closed and Open System Treatments, including PE+KE Effects, Tank Blowdown [Demonstration - CO2 Fire Extinguisher]	
3	1st Law Open Systems, Tank Blowdown and Filling - Class Examples, Problem	Assignment 1 due

	3.9	
4	2nd Law Concepts, Reversible Heat Engines, Carnot Efficiency, Entropy, Clausius Theorem, Reversibility[Demo-drinking Bird]	
5	Entropy Balance, 1st and 2nd Laws Combined [Demo - Hilsch Vortex Tube]	
6	2nd Law Concepts and Applications, Steady State and Transient Flow Work	
7	Availability and Exergy Concepts, Heat Integration and Pinch Analysis, Power Cycle Analysis [Demo - Stirling Engine]	Assignment 2 due
8	Calculus of Thermodynamics, Gibbs Fundamental Equation, Graphical Interpretation of Fundamental Surface	
9	Derivative Transformation and Manipulation, Maxwell Relations, Jacobian Transformations	
10	Legendre	

	Transformations, Equivalent Forms of the Fundamental Equation, Examples	
11	Legendre Transforms Continued, Connections to the Gibbs Surface and Other Derived Properties	Assignment 3 due
12	Equilibrium Criteria Concepts and Applications---Phase, Chemical, and Membrane, Phase Rule, Examples of Simple Phase Diagrams	
13	Stability Criteria, Concepts and Applications, Critical States	
14	Pure Component Properties, Fund. Eq., Theorem of Corresponding States, Constitutive Property Models - Stress Connections to Molecular Level Interactions and Effects	
15	Real Fluid Properties, *PVTN* Equations of State, Ideal Gas Heat Capacity Cp*	
16	Departure	

	Functions, Concepts and Applications, Standard ΔG° and ΔH° of Formation	
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	Assignment 4 due
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	
19	Mixture Equations of State, Continued and Needs	Assignment 5 due
20	*Review for Exam 1*	
	Exam I: 2 hours	
Part II - Introduction to Statistical Mechanics for 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	
22	Postulates of Statistical Mechanics, Gibbs ensembles - Micro-canonical and Canonical; States of System, Probabilities	
23	Computation of Ideal Gas Properties from Intramolecular Effects - Translation, Rotation, Vibration using Statistical Mechanics I	
24	Computation of Ideal Gas Properties from Intramolecular Effects - Translation, Rotation, Vibration using Statistical Mechanics II	
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	
26	Semi-classical Approximation, *PVTN* Properties via Configuration Integral from Intermolecular Effects, Grand Canonical Ensemble II -- Examples	
27	Gibbs Ensembles Continued: Micro-canonical Ensemble Revisited, Grand Canonical, NPT, etc., Including Equivalence of Ensembles; Time Averaging and Ergodicity, and Fluctuations; Macroscopic Connection	Assignment 6 due
28	Intermolecular Forces and Potentials, Role of Quantum Mechanics, Commonly used Potential Functions, Pairwise Additivity	

29	Virial Equation of State and Molecular Corresponding States from Statistical Mechanics; Connection of *PVTN* Equations of State to Statistical Mechanics and Molecular Simulations	
30	Mean Field Theory, Connecting the van der Waals EOS Model to Statistical Mechanics, Hard Sphere Fluids, Perturbed Hard Sphere Fluids, Lattice Models	
31	Statistical Mechanical Models of Fluids I - Expanding the Virial EOS to Mixtures, Radial Distribution Functions, Structure of Fluid and Solid Phases, Critical Phenomena (Fluctuations, Critical Opalescence)	Assignment 7 due
32	Statistical Mechanical Models of Fluids II - Biological Materials and Protein Applications	

33	Foundations of Molecular Simulations - Monte Carlo and Molecular Dynamics	
34	Application of Molecular Simulations to Estimating Pure Component and Mixture Properties	
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	Assignment 8 due
36	Review of Mixture Thermodynamics, Fugacity, Fugacity Coefficient, 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-	Assignment 9 due

	Ideal Effects	
38	Applications of Mixture Thermodynamics to VLE Phase Equilibria, Minimum Work of Separation, etc.	
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	
42	Phase Equilibria, Integral Approach, 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	
45	Chemical Equilibrium - General Approach, Nonstoichiometric and Stoichiometric Formulation, Statistical Mechanical Approach	Assignment 10 due
46	Equilibrium Constants and Standard States, Gibbs Phase Rule Applications	
47	Chemical Equilibria Applications and Example Problems, Combined Phase and Chemical Equilbria	Assignment 11 due
48	*Review Session*	
	Final Exam: 3 hours	