
Course Outline and Outcomes

Thermodynamic Properties

- Define and articulate some of the critical language and concepts of Thermodynamics
 - Distinguish between the universe, system, surroundings, and boundary [Ch 1.1-1.2]
 - Define open system, closed system, and isolated system [Ch 1.1-1.2]
 - Define adiabatic, isothermal, isobaric, and isochoric processes [Ch 1.1-1.2]
 - Distinguish between extensive and intensive thermodynamic properties [Ch 1.3]
 - Explain the difference between state and path variables [Ch 1.5]
 - Distinguish between equilibrium and steady state [Ch 1.4]
 - Define the term phase and explain what it means for phases to be in equilibrium [Ch 1.4]
- Relate properties to phase behavior [Ch 1.6-1.8]
 - Relate the measured thermodynamic properties of temperature and pressure to molecular behavior
 - Describe phase and chemical reaction equilibrium in terms of dynamic molecular processes
 - Apply the state postulate and the Gibbs phase rule to determine the number of required independent properties needed to constrain the state of a system (pure species)
 - Identify the phases present on a PT and/or Pv diagram as well as the critical point and triple point
 - Describe the difference between the saturation and vapor pressures
- Determine thermodynamic properties using both calculations and tabulated data [Ch 1.6-1.7]
 - Read desired thermodynamic properties from steam tables
 - Using linear, sometimes double, interpolation to calculate property values from sparse tabular data
 - Use equations of state to calculate unknown properties from measured properties

The First Law of Thermodynamics

- Explain and manipulate the first law [Ch 2.4]
 - Write the integral and differential forms of the first law
 - Describe the physical meaning of each of the terms within both the integral and differential form of the first law
 - Identify when the open and closed forms of the first law are applicable
 - Determine when each term in the first law is zero or negligible
- Establish whether the ideal gas law is appropriate or if more advanced approaches are necessary (including tabulated data) [Ch 1.8]
- Identify, formulate, and solve simple engineering problems (such as expansion/compression in piston-cylinder systems and power cycles) [Ch 2.7-2.9]
- Describe the molecular basis for internal energy, heat transfer, work, and heat capacity [Ch 2.1-2.2]
- Explain the difference between a reversible and irreversible process [Ch 2.3]
- Distinguish between reversible and irreversible processes [Ch 2.3]
- Explain the utility of enthalpy, flow work, and shaft work [Ch 2.5]

- Calculate enthalpy changes associated with sensible heat, latent heat, and chemical reaction [Ch 2.6]

Entropy and The Second Law of Thermodynamics

- Explain and manipulate the second law [Ch 3.3-3.6]
 - State and illustrate by example the second law of thermodynamics
 - Write both the integral and differential forms of the second law
 - Identify when the open and closed forms of the second law are applicable
 - Determine when each term in the second law is zero or negligible
- Identify, formulate, and solve simple engineering problems (such as expansion/compression and power cycles) [Ch 3.5-3.9]
- Derive and use the mechanical energy balance equation to solve engineering problems [Ch 3.8]
- Devise and use strategies for entropy change calculations
 - Develop hypothetical reversible paths between two states in order to calculate entropy changes [Ch 3.1-3.2]
 - Use the heat capacity to calculate entropy changes
 - Use tables to calculate entropy changes
 - Calculate entropy changes for materials undergoing phase changes and/or reaction
- Perform power cycle problems [Ch 3.9]
 - Solve for the net power obtained and efficiency of reversible power cycles
 - Calculate the coefficient of performance of a reversible refrigeration cycle
 - Correct reversible calculations for real systems using isentropic efficiencies

Equations of State

- From molecular considerations, identify which intermolecular interactions are significant (including estimating relative strengths of dipole moments, polarizability, etc.)
- Apply simple rules for calculating P, v, or T
 - Calculate P, v, or T from non-ideal equations of state (cubic equations, the virial equation, compressibility charts, and ThermoSolver)
 - Apply the Rackett equation, the thermal expansion coefficient, and the isothermal compressibility to find v for liquids and solids
- State the molecular components that contribute to internal energy
- Relate macroscopic thermodynamic properties/behaviors with their molecular origins, including point charges, dipoles, induced dipoles, dispersion interactions, repulsive forces, and chemical effects
- Define van der Waals forces and relate it to the dipole moment and polarizability of a molecule
- Define a potential function
- Write equations for ideal gas, hard sphere, Sutherland, and Lennard-Jones potentials and relate them to intermolecular interactions
- Explain the origin of an use "complex" equations of state
 - State the molecular assumptions of the ideal gas law
 - Explain how the terms in the van der Waals equation relax these assumptions
 - Describe how cubic equations of state account for attractive and repulsive interactions

- State and use the principle of corresponding states to develop expressions for the critical property data of a species
- Describe the purpose of the acentric factor and its role in the construction of compressibility charts
- Adapt our approach to mixtures [Ch 4.5]
- Write the van der Waals mixing rules and explain their functionality in terms of molecular interactions
- Write the mixing rules for the virial coefficients and for pseudo-critical properties using Kay's rule
- Using mixing rules to solve for P , v , and T of mixtures
- Write the exact differential of one property in terms of two other properties [Ch 5.1, 5.2]
- Use departure functions to calculate property data for real fluids (and use them to solve engineering problems) [Ch 5.4]
- Calculate departure functions from Lee-Kesler charts
- Use equations of state to calculate departure functions

Phase Equilibrium: Conditions for Equilibrium

- Write down the conditions for equilibrium for: a pure single phase system, a pure multi-phase system, and a multi-phase mixture [Ch 6.1, 6.2]
- Explain how energetic and entropic effects balance at equilibrium [Ch 6.2]
- Use the Clapeyron equation and/or the Clausius-Clapeyron equation to relate T and P for pure species phase equilibrium [Ch 6.2]
- Use the Antoine equation to relate T and P for pure species phase equilibrium [Ch 6.2]
- Explain the relationship between the Clausius-Clapeyron equation and the Antoine equation [Ch 6.2]
- Write exact differentials for extensive properties in terms of $m+2$ independent variables for mixtures of m species [Ch 6.3]
- Define and explain the difference between the terms: pure species property, total solution property, and partial molar property [Ch 6.3]
- Calculate total solution properties from partial molar properties [Ch 6.3]
- Calculate partial molar properties [Ch 6.3]
 - using graphical methods
 - using equations of state
 - using the Gibbs-Duhem equation
- Explain the origin of enthalpy, entropy, and volume changes due to mixing [Ch 6.3]
- Calculate the enthalpy of solution from the enthalpy of mixing and vice versa [Ch 6.3]
- Explain why the chemical potential is the relevant property for determining solution equilibrium [Ch 6.4]

Phase Equilibrium: Fugacity and Equilibrium Calculations

- Relate the fugacity and the chemical potential (or the partial molar Gibbs free energy) [Ch 7.1, 7.2]
- Use the fugacity coefficient to calculate the vapor phase fugacity [Ch 7.3]
- Use the activity coefficient to calculate the liquid (or solid) phase fugacity [Ch 7.4]
- Identify conditions when a liquid or solid mixture would form an ideal solution [Ch 7.4]

- Explain when Lewis-Randall versus Henry ideal solution reference states are appropriate [Ch 7.4]
- Use the Gibbs-Duhem equation to relate activity coefficients in a mixture [Ch 7.4]
- Perform bubble-point and dew point calculations [Ch 8.1]
 - using Raoult's Law
 - using complete fugacity relations (assuming known fugacity coefficients and activity coefficients)
- Draw and read Txy and Pxy diagrams for VLE [Ch 8.1]
- Use Henry's Law to calculate VLE for gases dissolved in liquids [Ch 8.1]

Chemical Reaction Equilibrium

- Explain the relationship between energy and entropy in reacting systems (i.e., show why the Gibbs Free Energy is still the proper state function for equilibrium) [Ch 9.2]
 - Write balance chemical reaction expressions with associate reaction stoichiometry [Ch 9.3]
 - Relate extent of reaction expressions to the equilibrium constant(s) [Ch 9.3]
 - Use thermochemical data to calculate the equilibrium constant and its dependence on temperature [Ch 9.4]
 - Determine the equilibrium composition for a single-phase, single-reaction system (i.e., calculate the extent of reaction) [Ch 9.5]
 - in vapor phase reactions
 - in liquid phase reactions
 - Determine the equilibrium composition for a multiphase, single-reaction system [Ch 9.5]
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