AE/ME 6765 Kinetics and Thermodynamics of Gases

Catalog Description: AE/ME 6765: Kinetics and Thermodynamics of Gases. 4-0-4
Thermodynamics of nonreacting and reacting gas mixtures. Introductory quantum theory, statistical thermodynamics and gas kinetic theory.

Text: At the level of

The Principles of Chemical Equilibrium, 4th edition, Kenneth Denbigh, Cambridge, 1981
Introduction to Physical Gas Dynamics, Walter Vincenti and Charles Kruger, Jr., Krieger, 1965.

Coordinator: Dr. Jerry M. Seitzman, Assistant Professor

Learning Objectives:

1. Thermodynamics of nonreacting and reacting gas mixtures.
2. Equilibrium properties of gas mixtures.
3. Quantum states and energy levels of molecules.
4. Equilibrium population distribution of molecular energy levels.
5. Equilibrium kinetic theory of gases.
6. Transport properties of gases.

Prerequisites:

Exposure to thermodynamics, e.g., thermodynamics properties, and First and Second Law of Thermodynamics.

Lecture Topics:

Classical Thermodynamics (18 Lectures)
- Overview and Thermodynamic Definitions
- The State Postulate and Reversible Work Modes
- Zeroth, First, and Second Laws of Thermodynamics
- Gibbs Equation and Entropy Transfer
- Entropy Analysis for a Control Mass, and Availability Analysis for a Control Volume
- Properties of the Enthalpy
- Useful Work for Flowing and Reacting Systems (Control Volume Analysis)
- General Conditions for Chemical Equilibrium of a Mixture; Chemical Potential and Chemical/Phase Equilibrium
- Maxwell's Relations and Other Mathematical Relationships
- Measurable Quantities in Thermodynamics (Specific Heats, Compressibility Coefficients, Heats of Reaction and
  Phase Change)
- Calculation of Changes in Thermodynamic Properties
- Molar and Partial Molar Quantities
- State Equations for a Single Perfect Gas, a Perfect Gas Mixtures, and Imperfect Gases
- Equilibria of Reactions Involving Gases, Equilibrium Constant Kp and Law of Mass Action
- Standard Reference States: Gibbs Free Energies and Enthalpies of Formation
- Mixed Phase Equilibria
- Stoichiometric Reactions, Independent Reactions, and a General Method for Solving Equilibrium Composition
  (Major-Minor Species Model)

Quantum Theory and Wave Mechanics (5 lectures)
- Molecular Models
- Origin of Quantum Theory of Matter - Bohr Model of Atom
- Quantum Mechanics/Wave Theory (Schrodinger Equation)
- Free Particle, Particle in a Box, Harmonic Oscillator, Rigid Rotor
- H atom (Electronic Energy)

Statistical Mechanics (5 lectures)

- Enumeration of Microstates
- Most Probable Macrostate
- Distribution over Energy States
- Statistical Thermodynamics and Thermodynamic Properties (7 lectures)
- Thermodynamic Relations
- Independent Energy Modes
- Translational Properties; Monatomic Gas with Electronic Excitation
- Diatomic Gas and Boltzmann Fractions
- Improved Models/Corrections
- Polyatomic Molecules

Chemically Reacting Gas Mixtures (3 lectures)

- Equilibrium Constant: Statistical Mechanics Approach
- Equilibrium Constant: Combined Thermo./Stat. Mech. Approach
- Specific Heats of Reacting Mixtures

Gas Radiation and Optical/Laser Diagnostics (3 lectures)

- Aborption/Emission Lines and Einstein Coefficients
- Scattering and Overview of Optical Diagnostic Methods

Introductory Gas Kinetic Theory (6 lectures)

- Models of Molecular Potentials
- Pressure, Temperature and Internal Energy from Collisions
- Mean Free Path
- Transport Phenomena
- Molecular Magnitudes

Equilibrium Gas Kinetic Theory (9 lectures)

- Velocity Distribution Function
- Equation of State for a Perfect Gas
- Equilibrium and Maxwellian Distribution
- Collision Rate and Mean Free Path
- Energy Involved in Collisions
- Inelastic Collision Rates
- Transport Properties