ME 501 Combustion Fundamentals
Tuesday, Thursday 1-2:50 260 MEB
Text: *Combustion* 4th Edition. By Glassman and Yetter. Academic Press.
Instructor: Nick Glumac (MEL 2111 x4-8333 glumac@illinois.edu)
Office Hours: TBA

Course Outline

Part I: Fundamentals

1) Thermodynamics - Chapter 1[2 weeks]
General review. 1st and 2nd Laws. Gibbs free energy. Chemical equilibrium. van't Hoff relation. Entropy of formation. Adiabatic flame temperature. Results from statistical mechanics. Vapor pressure and the Clausius-Clapyron equation. Energy content of fuels and oxidizers. Thermodynamic references, databases. Modern computational tools for equilibrium calculations.

2) Chemical Kinetics - Chapter 2 and Chapter 3 [2]
The structure of a gas. Maxwell distribution. Collision theory. Arrhenius and transition state rate expressions. Unimolecular reactions. Organic chemistry terminology. Atomic and molecular structure. Types of reaction. Steady-state approximation. Partial equilibrium. Reaction chains and mechanisms. Modern computational tools for chemical kinetics calculations. CHEMKIN, Cantera.

3) Transport [1]
Kinetic theory of transport. Collision integrals. Maxwellian molecules approximation. Diffusion; Fick's law, multi-component diffusion, barodiffusion and thermal diffusion. Thermal conductivity and the heat equation. Viscosity. References, equations, and tables for obtaining transport coefficients.

4) The Fundamental Equations of Combustion [1]
Continuity, momentum, and energy equations for a laminar, gaseous, multi-component,reacting system. Common approximations and their ranges of validity. Extensions to multi-phasic and turbulent systems.

Part II: Classical Applications

5) The Hydrogen/Oxygen System [1]
Full reaction mechanisms. Schematic overview. Solving the full equations computationally. Detailed analysis of a low pressure stoichiometric flame: flame structure, key reactions, validity of common assumptions. Experimental verification of results.

6) Laminar Flames - Chapter 4 [1]
Important dimensionless parameters (Lewis, Peclet, Schmidt, Prantl, and Damkohler numbers). Thermal theory of flames. Classical (i.e. Zeldovich) approaches. Flame speed. Flame temperature calculations. Quenching distance. Flammability. Stabilization. System design using basic flame parameters.

7) Non-premixed and Multi-phasic Flames - Chapter 6 [2]
Burke-Schuman solution. Actual structure of a laminar 'diffusion' flame. Modern computational solution of an axisymmetric laminar non-premixed flame. Counterflow non-premixed flames. Droplet evaporation and burning. Introduction to combustion of solids (e.g. coal and metals).

8) Detonation - Chapter 5 [1]
Gas dynamic 1-D thermodynamics of detonations/deflagrations. Hugoniot curve. Calculation of detonation velocity. Chapman-Jouguet diagram. ZND structure of detonation waves. Computational tools for CJ velocity calculation.

Part III: Modern Applications

9) Environmental Combustion Considerations - Chapter 8 [1]
Common pollutants and sources. Photochemical smog. Low and high temperature mechanisms for NO_x formation. SO_x formation. Ozone production. Stratospheric ozone depletion. Soot formation. CO_2 production in combustion systems. Sequestration of CO_2. Modern strategies for minimizing emissions. GRI mechanism. Hydrogen combustion opportunities and challenges.

10) Combustion Measurements [1]
Spectroscopic fundamentals. Flame spectra. Intrusive and non-intrusive flame probes: gas chromatograpy, mass spectrometry, emission and absorption spectroscopy, laser induced fluorescence, Raman and Rayleigh scattering.

11) Catalytic combustion [1]
Catalysis. Classical and emerging catalytic materials. Automotive catalytic converters. Heterogeneous reaction mechanism. Role of support materials. Temperature dependence and emissions characteristics of catalytic combustion. Design of a catalytic combustor. CHEMKIN SPIN code.

12) Heterogenous combustion Chapter 9 [1]
Mechanism of coal combustion. Combustion of solid propellants. Transport and kinetic limitations. Metal combustion and energetics.

13) Energetic materials [1]
Common explosives, propellants, and pyrotechnics. Detonation in solids. Applications and design criteria for explosives. Emerging explosives systems (nanometals, nanothermites, high nitrogen materials).

Homework

Homework will be issued each week and be due the following week. Homework is an important part of the course, and is worth 30% of the grade. I encourage students to work together and to consult each other on the problems. However, each student must write out the problems separately and complete the programming and electronic assignments individually. If you have any questions regarding this policy, please ask me.

Exams

There will be a 2 hour mid-term exam covering the first half of the course, and a 1 hour final exam covering the final half of the course.

Project - Short paper

In the second half of the course, homework will consist of shorter assignments, and students are expected to use the rest of the time to work on a short paper. The paper will consist of a review of three journal articles on a specific topic in combustion. The length of the paper should be between four and six single spaced, 12 pt font pages with 1" margins. The three references should be attached, and the student can refer to the figures in these papers, rather than replicate them in the text. The following are the relevant due dates for the paper:

- April 8: Topic chosen
- April 22: Three papers chosen
- May 6 (last day of class): Complete paper due

Grading

Grades will be based on homework (30%), mid-term (30%), short paper (20%), and the final (20%).