

**Spring 2002**

**ME 536: Chemically Reacting Flows**

Instructor: Professor S.K. Aggarwal  
Room 2059 ERF, Phone: 996-2235, email: ska@uic.edu

Textbook: No specific textbooks will be extensively used. I recommend that you buy the book, "Combustion Theory" by F. A. Williams. Most of the material will be from the following sources, especially the first three reference books. Additional material will be taken from combustion journals.

Reference: Stephen R. Turns, **An Introduction to Combustion, 2nd Edition**

- F.A. Williams, "Combustion Theory"
- I. Glassman, "Combustion"
- K. K. Kuo, "Principle of Combustion"
- D.B. Spalding, "Some Fundamentals of Combustion"
- R.A. Strehlow, "Combustion Fundamentals"

Journals: Combustion and Flame (1956-present)  
Combustion Science and Technology (1969-present)  
N'th Symposium (International) on Combustion, 29th in 2002.

**MAJOR TOPICS**

**1. Governing Equations for Chemically Reacting Flows**

**Source: Turns' Book and additional material covered in class**

- Mass Conservation Equation
- Species Conservation Equation
  - Reaction rate terms
  - Multicomponent diffusion
  - Fickian diffusion
- Momentum Conservation Equation
- Energy Conservation Equation
  - Shvab Zeldovich variables
- Conserved scalars
- Various conserved scalars
- Mixture fraction
- Conservation equation for mixture fraction
- Conserved scalar energy equation

**2. Chemical Kinetics**

**Source: S. Turns, I. Glassman**

**William C. Gardiner: Combustion Chemistry, See chapter by Warnatz**

**B. Lewis & G. Van Elbe: Combustion Flames & Explosion of Gases**

## **Additional material covered in class, and project**

- Elementary Reaction Rates
  - Reaction rate constant, Preexponential factor, activation energy
  - Equilibrium constant
- Bimolecular reactions and collision theory
- Reaction rate for multistep reactions
- Elementary reactions
- Radicals and chain reactions
- Molecularity and reaction order
  
- **Some Important Chemical Mechanisms**
  - H<sub>2</sub>-O<sub>2</sub> System
  - CO oxidation
  - Oxidation of Higher Paraffins
  - Methane oxidation
  - Propane oxidation
  - n-Heptane Oxidation
  - NO<sub>x</sub> mechanisms

### **3. Laminar Nonpremixed (Diffusion) Flames**

**Source: Turns' Book and additional material covered in class**

- Introduction
- Nonreacting Laminar Jet
- Laminar Jet Flame
- Flame Lengths for Circular (Axisymmetric) and Slot burners
- Counterflow flames
- Partially Premixed Flames

### **4. Turbulent Combustion**

**Source: Turns' Book (Chapters 11-13), additional material covered in class, journal papers**

#### **4.1 Introduction to Turbulence**

- General characteristics of turbulent flows
- Turbulent scales
- Reynolds decomposition
- Closure problem in analyzing turbulent flows
- Turbulent Models
- Nonreacting, Constant-Density Jet-Similarity solution

#### **4.2 Turbulent Nonpremixed Flames**

- Extension of constant-density jet solution to turbulent jet flame
- Scale analysis to estimate flame height for laminar and turbulent jet flames
- Conventional-averaged and Favre-averaged governing equations for turbulent reacting flows
- Turbulence models
- k-e turbulence model for variable density flows
- Conserved Scalar or Laminar Flamelet Approach
- Probability density function of mixture fraction
- Governing equations for Favre-averaged mixture fraction and its variance
- Solution for turbulent nonpremixed flames using assumed PDF function
- Global properties of turbulent nonpremixed flames
- Flame liftoff and blowout characteristics

## **5. Premixed Flames**

### **Introduction, general concepts**

#### **5.1 Laminar Premixed Flames**

- Flame speed
- Qualitative features of laminar premixed flames
- Scale analysis for laminar flame speed and thickness
- Discussion of one-dimensional premixed flames

#### **5.1 Turbulent Premixed Flames**

- Basic concepts
- General methodology for solving turbulent premixed flames
- Turbulent flame speed
- Relevant scales for turbulent nonreacting and reacting flows
- Turbulent flame regimes-Borghi's Diagram
- Empirical equations for turbulent flame speed