Preliminary Syllabus August 2008

ME 599-001: Energy Processes for Novel Fuels

COURSE TITLE: ME599-01: Energy Processes for Novel Fuels

TERMS OFFERED: Fall, 2008

PREREQUISITES: Thermodynamics I. It is recommended to check with the instructor at the beginning of the semester.

INSTRUCTOR: Angela Violi - *Department of Mechanical Engineering, Chemical Engineering and Biomedical Engineering*

CATALOG DESCRIPTION: This class deals with the energy processes for the production of fuels. After an overview of the broader aspects of energy use from viewpoints of sustainability, resource availability, environmental effects and economics, a review of the fundamentals for the combustion chemistry of novel fuels will be presented. The material covered in this class is intended to provide the students with the tools and understanding to handle basic problems involving chemical systems and rates of simple chemical reactions.
This course deals with the theoretical aspects of chemical reaction kinetics, including transition-state theories, estimation of rate constants, modeling complex reacting mixtures, and uncertainty/sensitivity analyses. Reactions in the gas phase are discussed with examples drawn from combustion chemistry. The students will be introduced to the CHEMKIN software and if time allows, to the Gaussian package to compute the energetics of reactions.
Various fuels will be considered, including oxygenated. Kinetic mechanisms for fossil fuels and biodiesels will be studied. This course will also examine state of the art technologies aiming at cost effective biomass conversion along with economics, environmental impact, and policy issues.
Guest lectures are brought in to cover environmental and societal issues.
Grading will be largely based on a term-long project, proposed by the students themselves.

Technical Requirements:
CHEMKIN® software and Gaussian software.

AUDIENCE: Graduate students. The class is also open to senior undergraduate students – please check with the instructor.

COURSE TOPICS:

1. Sustainable Energy

Introduction to Sustainable Energy: Definition of Sustainable Energy; Technical Performance; Thermodynamics; Allowability, Second Law, Importance of Rate Processes

2. Fossil Fuels and Combustion Modeling

Fossil Fuel – Type of fuels – Sustainability – Harvesting Energy and Energy Products from fossil fuels; Fuel Combustion – General Structure of a Theoretical Model – Governing Equations for Combustion Modeling

3. Chemical Thermodynamics

The first Law of Thermodynamics; The second Law of Thermodynamics Enthalpies of Formation; Thermochemical Laws; Bond Energies and Heats of Formation; heats of Reaction; Equilibrium Constants; Chemical Equilibrium Calculations

4.Chemical Kinetics and Reaction Mechanisms

Rates of Reaction and their functional dependence; One-step chemical reactions of various orders; Consecutive reactions; Competitive reactions; Chain reactions; Chain branching explosions

5. Chemkin analysis and code application for gas-phase kinetics

The Chemkin code; Procedure and application of sensitivity analysis; Reaction flow analysis
Reaction mechanisms of H2/O2 systems; Gas-phase reaction mechanisms of aliphatic hydrocarbon and oxygen systems; Formation mechanisms of nitrogen oxides; Formation and control of CO and particulates; Reaction Mechanisms for Biofuels