Department of Chemistry
Franklin College of Arts and Sciences

School of Environmental, Civil, Agricultural, and Mechanical Engineering
College of Engineering

CHEM 8970 | MCHE 8970 Combustion Science
Fall 2022

Instructor: Professor Brandon Rotavera, Ph.D.
College of Engineering | Department of Chemistry
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Topical Outline:
Molecular structure of hydrocarbons and biofuels;
Mathematical formulation of fundamental combustion equations;
Chemical thermodynamics and thermochemistry;
Collision theory;
Classification of chemical reactions;
Chemical kinetics;
Potential energy surfaces;
Transition state theory;
Chemical kinetics mechanisms, rate rules, and group additivity theory;
Rate coefficient codes (Master Equation solvers, MESS, MESMER, etc.);
Oxidation mechanisms of hydrogen and of functionalized organic molecules;
Pollutant formation mechanisms;
Atmospheric implications from combustion-generated pollutants;

Description: Fundamental concepts related to the use of combustion as a source of transportation energy and advanced combustion technologies are covered from the perspective of physical chemistry and thermodynamics. Topics include mathematics of combustion, chemical thermodynamics/thermochemistry, chemical kinetics, potential energy surfaces, collision theory, and molecular structure of hydrocarbons and biofuels. Rate theory codes are used to predict and analyze the kinetics and dynamics of gas-phase chemical reactions.

Credit Hours: 3 (lecture)

Prerequisites:
CHEM 3212 – Modern Physical Chemistry II (or equivalent)
MCHE 3150 – Engineering Thermodynamics II (or equivalent)

Lecture Times: Tuesday/Thursday 2:20 P – 3:35 P

Lecture Location: STEM-I (Room 1023)

Website: eLC

Required Text: *Combustion* (5th Edition)
Authors: Irvin Glassman, Richard A. Yetter, and Nick G. Glumac
ISBN: 978-0-12-407913-7

Supplemental Text: Physical Chemistry textbook

Grading:

Problem Sets (5)	70%
Oral Problem Solution	30%

Oral Problem Solution: Two important components to graduate school coursework are a deepening of fundamental science principles and the development of technical communication skills. To connect both, the *oral problem solution* part of the grading involves preparing lecture notes built around the solution of a problem that will be assigned in advance. Tutorials that are no longer than 30 min. in length will then be delivered to the class on the whiteboard (i.e. no PowerPoint slides). The notes are to include (i) conceptual elements explaining the fundamentals of the problem, (ii) derivation and/or explanation of underlying equations from first principles, (iii) a step-by-step solution of the assigned problem, and (iv) a brief summary.

Departmental Grading Policy Regarding Communication Skills: 30% of the grade on all written assignments (e.g. reports, projects, and papers) and oral presentations will be based on quality of communication. Spelling, grammar, punctuation, and clarity of writing are evidence of written communication quality. Enunciation, voice projection, clarity and logical order of the presentation and effective use of visual aids are evidence of oral communication quality.

Problem Sets: Working homework problems is a necessity for practicing and learning the material, and is a tool that leads to a deeper understanding beyond the lecture content. Homework will be assigned on an approximately bi-weekly basis, approximately 10 – 12 problems. Diligently working through the assignments and detailing the results in an organized, professional format is strongly encouraged. Points of emphasis on the assignments include detailing each step of the methodology applied (i.e. application of assumptions, equations), reaching the correct solution, analysis and interpretation of the result(s), and organizational merits. An important component of the solution is writing comments on the context/meaning of the result.

Academic Honesty: Ethical behavior and academic honesty are expected and required of students and even more so of engineers and scientists. Evidence of cheating during an exam or other assignment for credit may result in failure of the entire course for the student(s) in question. The University of Georgia requires academic honesty and personal integrity among students and other members of the University Community. A policy on academic honesty has been developed to serve these goals. All members of the academic community are responsible for knowing the policy and procedures on academic honesty. The document for academic honesty may be found at the website for The University of Georgia Office of Senior Vice President for Academic Affairs and Provost. All academic work must meet the standards contained in "A Culture of Honesty". Students are responsible for informing themselves about the standards before performing any academic work.

Americans with Disabilities Act (ADA) Policy Statement:
The Americans with Disabilities Act (ADA) is a federal anti-discrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you believe you have a disability requiring an accommodation, please contact Disability Resource Center, in Clark Howell Hall, call 706-542-8719, or email at dsinfo@uga.edu. For additional information visit https://drc.uga.edu/.

Course Objectives and Expected Learning Outcomes: By the end of the course, students will have (at a minimum) developed the ability to (a) identify types of chemical reactions involved in combustion reactions, (b) formulate basic reaction mechanisms, (b) understand and apply advanced-level thermodynamics analysis of reacting flows, (c) learned interdisciplinary concepts and problem solving skills in chemistry and engineering that are relevant to combustion science, (d) understand the role of combustion in transitioning to lower carbon-intensive transportation energy and the relevant short-term scientific problems that require attention, and (e) gained the ability to analyze reacting systems and assess the utility of next-generation biofuels in current and future combustion technologies.