University Of California, Berkeley
Department of Mechanical Engineering

ME 154 – Thermophysics for Applications (3 units)

Undergraduate Elective

Syllabus

CATALOG DESCRIPTION

Development of classical thermodynamics from statistical treatment of microscale molecular behavior; Boltzmann distribution; partition functions; statistical-mechanical evaluation of thermodynamic properties; equilibrium; chemical equilibrium; phase transitions; molecular collisions; Maxwell-Boltzmann distribution; collision theory; elementary kinetic theory; molecular dynamics simulation of molecular collisions; kinetic Monte Carlo simulations of gas-phase and gas-surface reactions. Implications are explored for a variety of applications, which may include advanced combustion systems, renewable power systems, microscale transport in high heat flux electronics cooling, aerospace thermal management, and advanced materials processing.

COURSE PREREQUISITES

ME40

TEXTBOOK(S) AND/OR OTHER REQUIRED MATERIAL

Statistical Thermodynamics and Microscale Thermophysics, by V.P. Carey, Cambridge University Press, New York, 1999.

or

Statistical Thermodynamics: Fundamental and Applications, N. Laurendeau, Cambridge University, 2005.

COURSE OBJECTIVES

To introduce students to the statistical foundation of thermodynamics and provide skills to perform advanced calculations for analysis of advanced energy conversion processes and devices.

DESIRED COURSE OUTCOMES

Students ability to calculate partition functions, perform equilibrium calculations, and undertake molecular-dynamics and Monte-Carlo simulations of non-equilibrium systems. This course will provide a foundation for design analysis of energy conversion systems and transport phenomena encountered in a variety of applications.

TOPICS COVERED

Statistical ensembles, Boltzmann distribution; partition functions; statistical-mechanical evaluation of thermodynamic properties; equilibrium; chemical equilibrium; phase transitions; molecular collisions; Maxwell-Boltzmann distribution; collision theory; elementary kinetic theory; molecular dynamics simulation of molecular collisions; kinetic Monte Carlo simulations of gas-phase and gas-surface reactions; applications. Coverage of these fundamental topics will emphasize connections to modern applications such as advanced combustion systems for power and propulsion, renewable power systems, microscale transport in high heat flux electronics cooling, aerospace thermal management, and advanced materials processing.

CLASS/LABORATORY SCHEDULE

Three hours of lecture per week.

CONTRIBUTION OF THE COURSE TO MEETING THE PROFESSIONAL COMPONENT

This course is an elective course in the Mechanical Engineering undergraduate Program. It has a primarily engineering science focus, providing undergraduates with and advanced foundation for energy technology development. Project assignments in the class prepare students for advanced project development work in energy-related applications.

RELATIONSHIP OF THE COURSE TO ABET PROGRAM OUTCOMES

The following list the outcomes that will apply to this course:

(a) an ability to apply knowledge of mathematics, science, and engineering

(c) an ability to design a system, component, or process to meet desired needs within realistic constraints such as economic, environmental, social, political, ethical, health and safety, manufacturability, and sustainability

(d) an ability to function on multi-disciplinary teams

(e) an ability to identify, formulate, and solve engineering problems

(g) an ability to communicate effectively

(j) a knowledge of contemporary issues

(k) an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.

ASSESSMENT OF STUDENT PROGRESS TOWARD COURSE OBJECTIVES

30% Homeworks
30% Midterms or Projects
40% Final Exam or Final Project

SAMPLE OF WEEKLY AGENDA

Week 1-2	Introduction, Review of classical thermodynamics, Basic classical and quantum mechanics
Week 3	Statistical ensembles, Boltzmann's distribution, Partition functions
Week 4	Evaluation of translational partition function, Particle distinguishability
Week 5-6	Evaluation of rotational, vibrational, and electronic partition functions
Week 7-8	Application of partition functions, Chemical equilibrium
Week 9	Condenses phases: Crystals and liquids
Week 10	Maxwell-Boltzmann distribution
Week 11	Potentials and forces (Mie, Lennard-Jones, Morse, Tersoff, …)
Week 12	Kinetic theory of gases and molecular collisions, Transport properties

Week 13	Simple collision and transition-state theories of reaction rates
Week 14	Master equations of energy transfer
Week 15	RRR
Week 16	Final Week

ADDITIONAL COMMENTS/CONCERNS

Room-Share with ME 254

This is a room-share course that will be taught concurrently with ME254. ME154 and ME254 will share a common lecture, but project assignments for graduate students in ME254 will be different than those for undergraduate students in ME154. Compared to the projects assigned to undergraduates, graduate students taking ME254 will be given project assignments that require modeling of more physically complex systems, and use of more sophisticated computational tools. Final exam questions or final projects for graduate students in ME254 will be different than those for undergraduate students in ME154.

PERSON(S) WHO PREPARED THIS DESCRIPTION

Prof. Michael Frenklach, September 20, 2018
Prof. Van P. Carey, September 20, 2018

ABBREVIATED TRANSCRIPT TITLE (19 SPACES MAXIMUM): ADV THERMODYNMCS
TIE CODE: LECT
GRADING: Letter
SEMESTER OFFERED: Fall and Spring
COURSES THAT WILL RESTRICT CREDIT: ME 254
INSTRUCTORS: M. Frenklach and V. P. Carey
DURATION OF COURSE: 15 Weeks
EST. TOTAL NUMBER OF REQUIRED HRS OF STUDENT WORK PER WEEK: 9
IS COURSE REPEATABLE FOR CREDIT? No
CROSSLIST: None