TO: The Engineering Faculty

FROM: The Faculty of the School of Mechanical Engineering

RE: New Course – ME 61700 Applied Thermal Physics and Molecular Spectroscopy

The Faculty of the School of Mechanical Engineering has approved the following new course. This action is now submitted to the Engineering Faculty with a recommendation for approval.

ME 61700 Applied Thermal Physics and Molecular Spectroscopy, 3 credits
Prerequisites: Thermodynamics I, Heat Transfer I, Chemistry I.
Attributes: Graduate Students and Upper Level Undergrads

Course Description: The fundamentals of statistical mechanics, kinetic theory, and molecular spectroscopy will be taught in order to predict and characterize the behavior of non-equilibrium gases using optical and laser diagnostics. This material will be taught within the context of applications involving combustion, plasmas, propulsion, energetic materials, shock waves and laser radiation.

History: This course has previously been offered two times since 2018 as a ME 597 course titled "Applied Thermal Physics and Infrared Spectroscopy." The student enrollment in the course and student evaluations were as follows:

- Fall 2018: 23 students
  - Response rate: 15/23, course rating: 4.7/5, instructor rating: 4.9/5
- Fall 2020: 10 students
  - Response rate: 8/10, course rating: 5/5, instructor rating: 5/5

Details of this course are outlined in the appended material below.

Eckhard A. Groll

Eckhard Groll, Head
William E. and Florence E. Perry Head of Mechanical Engineering,
and Reilly Professor of Mechanical Engineering

ME 61700
Applied Thermal Physics and Molecular Spectroscopy

Course Outcomes

Students will learn the concepts below in order to understand how to *model and experimentally characterize* the dynamic behavior of non-equilibrium gases as they transition from one equilibrium state to another (e.g., due to chemical ignition, shock heating/compression, and laser radiation).

1. *Statistical Mechanics:* to understand how energy is distributed (i.e., partitioned) on the molecular level
2. *Kinetic Theory:* to understand how energy is transferred and transformed on the molecular level and how quickly
3. *Spectroscopy and Laser Diagnostics:* to understand radiative-energy transfer and how these processes are exploited by optical sensors to rapidly and non-invasively monitor thermodynamic conditions (e.g., temperature, pressure, and chemical composition).

This material will be covered in the context of real-world applications, with an emphasis on: combustion, plasmas, propulsion, shock-wave physics, energetic materials, and optical diagnostics.

1. Basic Quantum Mechanics (1 week)

1. Wave-particle duality of matter and light
2. Heisenberg Uncertainty Principle
3. Schrodinger's Equation

Application: particles in a box

2. Quantization of Energy Levels (1 week)

1. Electronic energy and the H-atom
2. Translational energy
3. Rotational energy, rigid rotors, ro-vibrational coupling
4. Vibrational energy, harmonic oscillators, and anharmonicity

Application: absorbance spectrum of O_2

3. Statistical Mechanics (1 week)

1. Partition Function
2. Boltzmann Distribution
3. Boltzmann temperatures: translational, rotational, vibrational, and electronic

Application: "temperature" in a plasma

4. Kinetic Theory of Gases (3 weeks)

1. Molecular energy and speeds
2. Maxwell-Boltzmann Velocity Distribution Function
3. Collision theory
4. Unimolecular and bimolecular reactions and Arrhenius kinetics

Application: kinetic models for combustion

5. Rovibrational Energy Transfer (3 weeks)

1. Rotational-energy transfer
2. Vibrational-energy transfer via vibration-translation and vibration-vibration collisions
3. Vibrational relaxation and dissociation

Application: modeling vibrational relaxation in shock-heated air

6. Absorption and Emission Spectroscopy (3 weeks)

1. Absorption spectroscopy of gases
   - Line/band position, strength, shape, and Beer's Law
2. Emission spectroscopy of gases, liquids, and solids

Application: laser-absorption diagnostics for propulsion and IR imaging

7. Laser-Induced Fluorescence and Photochemical Kinetics (3 weeks)

1. Laser-induced fluorescence basics
2. Kinetics of collisional quenching and radiative-excitation and -decay
3. Multi-level models for predicting LIF signals

Application: Planar-LIF diagnostics for imaging *T*, *P*, *X*, and *V* in reacting flows

COURSE NUMBER: ME 61700

COURSE TITLE: Applied Thermal Physics and Molecular Spectroscopy (3 credits)

SHORT TITLE (max 30 char): Apl Therm Physics & Mol Spect

REQUIRED COURSE OR ELECTIVE COURSE: Elective

PROPOSED EFFECTIVE TERM: Spring 2022
TERMS OFFERED: Every other Spring Semester (once in two years)

JUSTIFICATION FOR THE COURSE: This course is highly relevant to the PhD research of approximately 75-100 graduate students conducting their MS and PhD research in laser spectroscopy, combustion, plasma, and propulsion science within the Schools of ME and AAE alone. The course has previously been offered two times (to 33 students) as an ME 597 course, and has received instructor and course ratings between 4.7 and 5.0 out of 5.0, thereby demonstrating this.

JUSTIFICATION OF THE NEED FOR THE COURSE:

This is the only class at Purdue University which focuses on the intersection of absorption and emission spectroscopy diagnostics for molecular species, and their applicability to combustion, plasma, and propulsion science. The need for this course is also justified by the number of students who have taken this course to date, and the extremely positive feedback they have provided.

JUSTIFICATION THAT THE COURSE WILL BE TAUGHT AT GRADUATE LEVEL: None of the course material is taught to undergraduate ME or AAE students. Further, this class has already been successfully taught at the graduate level twice.

JUSTIFICATION FOR ONLINE/DISTANCE DELIVERY: N/A

TEXTBOOK/REQUIRED MATERIAL:

- *Molecular Physical Chemistry for Engineers*, J. Yates Jr. and J.K. Johnson
- *Spectroscopy and Optical Diagnostics for Gases,* R.K. Hanson, R.M. Spearrin, and C.S. Goldenstein
- Lecture notes provided by instructor

PRE-REQUISITIES:

- Thermodynamics I
- Heat Transfer I
- Chemistry I

ATTRIBUTES: Graduate Level & Upper Undergraduate Students
RESTRICTIONS: Upper Level
COURSE REPEATABLE? Yes

COORDINATING FACULTY: Christopher S. Goldenstein

COURSE DESCRIPTION: The fundamentals of statistical mechanics, kinetic theory, and molecular spectroscopy will be taught in order to predict and characterize the behavior of non-equilibrium gases using optical and laser diagnostics. This material will be taught within the context of applications involving combustion, propulsion, energetic materials, shock waves and laser radiation.

COURSE OUTCOMES:

Students will learn the concepts below in order to understand how to *model and experimentally characterize* the dynamic behavior of non-equilibrium gases as they transition from one equilibrium state to another (e.g., due to chemical ignition, shock heating/compression, and laser radiation).

1. *Statistical Mechanics:* to understand how energy is distributed (i.e., partitioned) on the molecular level

ASSESSMENTS TOOLS:

1. Weekly homework (typically 3-4 exam style problems) for students to learn and apply concepts taught in lecture on statistical mechanics, kinetic theory, spectroscopy and laser diagnostics.
2. One lab report and group presentation completed by analyzing experimental data acquired in a laser-absorption-spectroscopy experiment in order to demonstrate their ability to apply theoretical concepts on laser spectroscopy to real world experimental data.
3. One mid-term examination to test students' understanding of concepts taught in first half of class (statistical mechanics, kinetic theory). The exam will consist of HW style problems.
4. One project report (< 10 pages) describing a student-defined (and instructor approved) research project involving modeling the chemical kinetics governing a practical application (e.g., combustion of methane).
5. A final examination to test students' understanding of concepts taught in last half of class (spectroscopy and laser diagnostics). The exam will consist of HW style problems.

PROVIDE ADDT'L INFO ABOUT THE ASSESSMENT METHOD(s) THAT ADDRESS THE LEARNING OUTCOMES LISTED ABOVE (few sentences describing assignment, prj, etc and how they address learning objectives):
See above.

NATURE OF DESIGN CONTENT: N/A

PROFESSIONAL COMPONENT:
1. Engineering Topics: Engineering Science – 3 credits (100%)

COMPUTER USAGE: MATLAB or Python

COURSE STRUCTURE/SCHEDULE:

Lecture - 2 days per week at 75 minutes per lecture, 16 weeks

2. *Kinetic Theory:* to understand how energy is transferred and transformed on the molecular level and how quickly
3. *Spectroscopy and Laser Diagnostics:* to understand radiative-energy transfer and how these processes are exploited by optical sensors to rapidly and non-invasively monitor thermodynamic conditions (e.g., temperature, pressure, and chemical composition).

This material will be covered in the context of real-world applications, with an emphasis on: combustion, plasmas, propulsion, shock-wave physics, energetic materials, and optical diagnostics.

RELATED ME PROGRAM OUTCOMES:
N/A

GRADE MODE (Regular; Pass/No Pass; Audit; Satisfactory/Unsatisfactory: Regular	**FINAL GRADING CRITERIA (%):** **Exams & Quizzes: 60%** **Papers & Projects: 10%** **Homework: 15%** **Laboratory Exercises: 15%** **Class Preparation: %** **Other:**
LIBRARY RESOURCES (describe any library resources that are currently available or the resources needed to support this proposed course. If none needed, explain how the students will complete their research for the course): **The students may need to access archival journal publications within journals that Purdue University subscribes to (e.g., Applied Optics, Journal of Quantitative Spectroscopy and Radiative Transfer, Combustion and Flame).**	**ADDITIONAL FEES:** No **EXPLANATION OF COURSE FEES (Coop, Lab, Rate Request): N/A**
ADDITIONAL COURSE INFORMATION: None	
PREPARED BY: Christopher S. Goldenstein	**REVISION DATE:** 06-08-21