Engineering Tripos Part IIB, 4A9 Molecular Thermodynamics, 2020-21

Module leader

Dr A J White [1]

Lecturers

Dr A J White and Dr A M Boies

Timing and Structure

Michaelmas term. 14 lectures + 2 examples classes. Assessment: 100% exam.

Content

This module provides an introduction to the relationship between the microscopic and macroscopic descriptions of thermodynamics and fluid mechanics. The module is equally divided between the two main microscopic approaches, kinetic theory and statistical mechanics, each of which has its place for solving different types of problem. If you have ever wondered about the interpretation of viscosity and thermal conductivity at a molecular level; why the Lewis number is taken as unity for combustion calculations; how to estimate the rate of a gaseous chemical reaction; why the speed of sound in a gas isn't faster (or slower); what are the interpretations of heat, work and entropy at a molecular level; how you can estimate the specific heat of a gas just by counting, how the conservation equations of fluid flow can be derived from microscopic considerations; what the Boltzmann distribution is and why it is so important; why the no-slip boundary condition is such a good approximation for continuum flow; when the Navier-Stokes equations lose their validity; how gases behave under highly rarefied conditions; how to set about calculating the surface temperature of the space shuttle during re-entry; and many other allied phenomena; then you should find many things to interest you in this module.

The main objective is to obtain a good physical understanding of the relationship between the microscopic and macroscopic viewpoints of thermodynamics and fluid mechanics. At first exposure, this can be a profound experience as it gradually emerges that the macroscopic thermo-fluid-dynamic behaviour of gases can be explained, almost in its entirety, by the results of collisions between molecules. On completion of the module students will have a good appreciation of the microscopic basis of a wide range of macroscopic phenomena.

Kinetic theory and statistical mechanics are complementary theories which are used to give quantitative estimates of macroscopic phenomena, often by using quite simple mathematics. Students will be equipped with the tools to estimate, from microscopic data, many macroscopic thermodynamic properties which would otherwise need to be obtained experimentally. They will also be in a position to construct their own simple molecular models to provide working solutions to specific problems where no data exists. To this end, the lectures will stress the importance of physical understanding backed up by simple mathematical modelling.

More accurate and advanced calculations require a more formalised and complex mathematical approach. Examples occur in rarefied gas dynamics where the fluid cannot be treated as a continuum and the Navier-Stokes equations no longer apply, and in statistical mechanical calculations where inter-molecular forces dominate. Although the lectures will not address such topics in detail, a further objective is to put the student in a position where he or she is ready to assimilate the more advanced literature in both kinetic theory and statistical mechanics.

GAS KINETIC THEORY Dr A J White (7 lectures + 1 examples class)

- Elementary kinetic theory
  Intermolecular forces and molecular models, Density, Pressure, Internal energy, Kinetic and thermodynamic

temperature, Specific heat capacity, Molecular degrees of freedom, Equipartition of energy, Rôle of intermolecular forces, Imperfect gases.

- Transport properties and chemical equilibrium
  Collision rates, Mean free path, Viscosity, Thermal conductivity, Prandtl number, Mixtures of different gases, Diffusion, Schmidt and Lewis numbers, Chemical equilibrium, Law of mass action.

- Molecular velocity distributions
  Velocity distribution functions, Effect of collisions, Maxwell-Boltzmann distribution, Statistical averages, Nonequilibrium velocity distributions, Boltzmann's equation, Relaxation time to equilibrium.

- Molecular gas dynamics
  Derivation of mass, momentum and energy conservation equations from kinetic theory, Isentropic flow, Navier-Stokes equations, Rarefied gases, Knudsen number, Boundary slip, Collisionless flow and heat transfer.

STATISTICAL MECHANICS Dr A M Boies (7 lectures + 1 examples class)

- Introduction to Statistical Mechanics
  Motivation, microstates, statistical analogues of entropy, the Boltzmann relation, probability examples and averaging procedures.

- The Partition Functions
  Microcanonical, canonical and grand canonical ensembles, the system partition function and its relation to thermodynamic properties, the single-particle partition function.

- Quantum Mechanics and Energy States
  Key results from quantum mechanics, the de Broglie wavelength, the Schrodinger equation and its solution for a particle in a box, density of energy states and energy levels, degeneracy.

- The Ideal Gas Model
  The statistical basis of the ideal gas, the high temperature limit and the Boltzmann distribution, the Sackur-Tetrode equation, temperature-dependence of specific heats (vibrational, rotational and electronic excitation energy modes), the equipartation of energy.

- Relationship to Thermodynamics and Probability
  Statistical interpretation of heat and work transfers and the First Law. Thermodynamic probability and property fluctuations.

- Other Statistical Models
  Other counting methods, the Einstein crystal and the rubber band model.

Booklists

Please refer to the Booklist for Part IIB Courses for references to this module, this can be found on the associated Moodle course.

Examination Guidelines

Please refer to Form & conduct of the examinations [2].

UK-SPEC

This syllabus contributes to the following areas of the UK-SPEC [3] standard:

Toggle display of UK-SPEC areas.

GT1

Develop transferable skills that will be of value in a wide range of situations. These are exemplified by the Qualifications and Curriculum Authority Higher Level Key Skills and include problem solving, communication, and working with others, as well as the effective use of general IT facilities and information retrieval skills. They also include planning self-learning and improving performance, as the foundation for lifelong learning/CPD.

IA1

Apply appropriate quantitative science and engineering tools to the analysis of problems.

IA2

Demonstrate creative and innovative ability in the synthesis of solutions and in formulating designs.

KU1

Demonstrate knowledge and understanding of essential facts, concepts, theories and principles of their engineering discipline, and its underpinning science and mathematics.

KU2

Have an appreciation of the wider multidisciplinary engineering context and its underlying principles.

E1

Ability to use fundamental knowledge to investigate new and emerging technologies.

E3

Ability to apply mathematical and computer based models for solving problems in engineering, and the ability to assess the limitations of particular cases.

US1

A comprehensive understanding of the scientific principles of own specialisation and related disciplines.

US2

A comprehensive knowledge and understanding of mathematical and computer models relevant to the engineering discipline, and an appreciation of their limitations.

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