COURSE CONTENT

MOLECULAR GAS DYNAMICS								
VIII Semester: AE								
Course Code	**Category**	**Hours / Week**			**Credits**	**Maximum Marks**		
AAED61	**Elective**	**L**	**T**	**P**	**C**	**CIA**	**SEE**	**Total**
		3	0	-	3	40	60	100
Contact Classes: 48	**Tutorial Classes: Nil**	**Practical Classes: Nil**			**Total Classes: 48**			
Prerequisite: Thermodynamics, Gas Dynamics								

I. COURSE OVERVIEW:

The course is about microscopic approach to understanding the behavior of a gas which states that all substances are composed of a large number of very small particles (molecules or atoms). The observable properties of gas are the consequence of the actions of the molecules making up the gas. We will cover gas dynamic phenomena that require the molecular description such as the structure of shock wave, high-altitude aerodynamics and expansions into vacuum, velocity slip and aerodynamic forces in nano/Microsystems.

II.COURSES OBJECTIVES:

The students will try to learn:

I. The basic gas properties such as temperature, pressure, flow velocity, gas stresses and fluxes from the molecular velocity distribution function.
II. The gas flow regimes (continuum, slip, transitional, free molecular) and applicable governing equations.
III. The equilibrium fluxes to solve basic free-molecular flow problems.
IV. To setup and conduct direct simulation Monte Carlo modeling for rarefied flow problems.

III.COURSE OUTCOMES:

After successful completion of the course, students should be able to:

CO1 Understand the real gas properties in their macroscopic form for their mathematical modelling.
CO2 Make use of statistical mechanics to describe the behavior of gases at the molecular level.
CO3 Apply the kinetic theory of gases for deriving macroscopic gas laws
CO4 Calculate transport properties of gases, including viscosity, thermal conductivity, and diffusion, based on molecular principles.
CO5 Utilize molecular gas dynamics concepts for modelling the behavior of gases in high-altitude flight.
CO6 Make use of direct simulation Monte Carlo approach for solving Boltzmann Equation

IV.SYLLABUS:

MODULE–I: GAS PROPERTIES (10)

Introduction, perfect and real gases, intermolecular forces, gas internal energy, distribution of the molecules on the available energy states, the internal energy of polyatomic molecules, the specific heats and their ratio, the molecular velocity distribution. averaged values, the mean free path and, the transport coefficients, classical dynamics of binary collisions, the collision integrals, effusive sources, different regimes of a gas in thermal equilibrium, on the possibility of a macroscopic description of, the gas behavior, gas in equilibrium, gas in non-equilibrium.

MODULE–II: MOLECULAR MODEL & COLLISIONS (10)

Need for a molecular description of fluid flow, continuum breakdown, concepts of equilibrium, degree of non-equilibrium, Molecular model, elastic collisions, concept of collision cross-section, collision frequency, mean free path, collision rate constant, hard sphere model, variable hard sphere model, inelastic collisions.

MODULE–III: BASIC KINETIC THEORY (10)

Introduction, Molecular Model, Pressure, Temperature, and Internal Energy, Mean Free Path, Transport Phenomena, Molecular Magnitudes, Velocity Distribution Function, Equation of State for a Perfect Gas

Maxwellian Distribution-Condition for Equilibrium, Maxwellian Distribution-Final Results, Collision Rate and Mean Free Path, Chemical Equilibrium and the Law of Mass Action.

MODULE–IV: NONEQUILIBRIUM KINETIC THEORY (09)

Introduction, the conservation equations of gas dynamics, the Boltzmann equation, equilibrium and entropy, the equations of equilibrium flow, moments of the Boltzmann equation, dynamics of a binary collision, the evaluation of collision cross-sections, the evaluation of collision integrals, gas mixtures.

MODULE–V: BOLTZMANN EQUATION (09)

Solution of the Boltzmann Equation: Introduction to particle-based approach, Direct Simulation Monte Carlo (DSMC) method, how it works, different processes modelled, gas-surface interactions, calculation of macroscopic properties, scope/mandates of the method, example problems.

V.TEXTBOOKS:

1. G.A. Bird, “Molecular Gas Dynamics and the Direct Simulation of Gas Flows”. Oxford Science, 1994.
2. Y. Sone, “Molecular Gas Dynamics: Theory, Techniques and Applications”. Birkhauser, 2006.

VI.REFERENCE BOOKS:

1. W. G. Vincenti and C. H. Kruger, “Introduction to Physical Gas Dynamics”, R. Krieger Publishing Company (1982).

VII. ELECTRONICS RESOURCES:

1. http://www.efunda.com/smhome/sm.cfm
2. https://www.iitk.ac.in/cce/courses/2019/molecular-gas-dynamics/

VIII.MATERIALSONLINE:

1. Course template
2. Tutorial question bank
3. Tech talk topics
4. Open end experiments
5. Definitions and terminology
6. Assignments
7. Model question paper – I
8. Model question paper - II

9. Lecture notes
10. E-learning readiness videos (ELRV)
11. Power point presentation