TEE-906 Advanced Combustion Kinetics

Course Objectives

1. The objectives of “Advanced Combustion Kinetics” course are:
   a. To develop fundamental understanding of chemical kinetics relevant for thermal engineering applications
   b. To develop in-depth understanding of transition state theory and Lindemann theory
   c. To identify advantages and limitations of various experimental techniques used in chemical kinetics

Course Contents

2. Contents with suggested contact hours

No.	Topics	Contact Hours
a.	**Introduction to Chemical Kinetics** • Reaction Orders • Molecularity • Determination of reaction orders and rate coefficients • A comparison of the techniques • Dependence on temperature • Thermodynamics and its relationship to kinetics • Parallel and consecutive reactions	6
b.	**Experimental Techniques** • Classical Techniques • Discharge flow • Detection technique for discharge flow apparatus • Liquid and stopped-flow systems • Flash photolysis	6

	• Detection technique for flash photolysis experiments • Shock tubes • Relative rate determinations • Relaxation techniques • Temperature control and measurement	
c.	**Bimolecular Reactions** • Collision theory • Transition state theory (TST) • Thermodynamic formulation of TST • Experimental evidence for transition state theory • Applications of transition state theory	6
d.	**Reaction Dynamics** • Collision of real molecules • Experimental reaction dynamics • Reaction dynamics and potential energy surfaces • Calculation of kinetic properties from potential energy surfaces • Variational transition state theory	6
e.	**Unimolecular and Associated Reactions** • Lindemann Theory • Comparison of experimental data with Lindemann theory • Contribution of the rate of reaction • Hinshelwood-RRK Modifications • High pressure limit • Low pressure rate coefficient • Strong collision assumptions	9

	• Vibrational energy redistribution • Associated reactions • Physical basis for association reactions	
f.	**Explosions and Branched Chain Reactions** • Thermal explosion • Branched chain reactions • Hydrocarbon oxidation	6
g.	**Negative Feedback and Oscillatory Behavior** • Oscillatory behavior in well stirred reactor • Cool flames • Belousov-Zhabotinskill reaction • Representation of oscillatory behavior	6
		45

Outcomes

3. By the end of this course students will be able to:
   a. Recall the basic concepts of chemical kinetics
   b. Have in depth understanding of biomecular reactions, unimolecular and association reactions
   c. Distinguish between numerous experimental techniques used in chemical kinetics
   d. List the advantages and limitations of numerous laser diagnostic techniques
   e. Propose experimental setup to perform combustion kinetics measurements
   f. Details of lab work, workshops practice (if applicable).

4. **Recommended Reading (including Textbooks and Reference books).**

	Title	Author(s)	Remarks
a.	Reaction Kinetics	Pilling and Seakins	Text Book
b.	Chemical kinetics and dynamics	Steinfeld, Francisco and Hase	Reference Book