**Subject Code: 01CH0602**
**Subject Name: Chemical Reaction Engineering-1**
**B.Tech. Year – III (Semester – VI)**

**Objective:** This subject introduces concepts of reaction rate, derivation of rate expressions from reaction mechanism, ideal reactor types, integral method of analysis, differential method of analysis, principles of chemical reactor analysis and design.

**Credits Earned:** 4 Credits

**Course Outcomes:** After completion of this course, student will be able to:

1. To build basic knowledge and Understanding of classification of reactions.
2. Understand kinetics of competing reactions and their influence on product yield and selectivity.
3. Understand fundamentals of kinetics including definitions of rate and forms of rate expressions and relationships between moles, concentration, extent of reaction and conversion.
4. Derive batch, CSTR, and PFR performance equations from general material balance.

**Pre-requisite of course:** Basic knowledge of material and energy balances in chemical engineering applications, laws of thermodynamics.

**Teaching and Examination Scheme**

| Teaching Scheme (Hours) | | | Credits | Theory Marks | | | Tutorial/ Practical Marks | | Total Marks |
|---|---|---|---|---|---|---|---|---|---|
| Theory | Tutorial | Practical | | ESE (E) | CSE | Internal (I) | Viva (V) | Term work (TW) | |
| 3 | 0 | 2 | 4 | 50 | 20 | 30 | 25 | 25 | 150 |

**Theory Contents:**

| Unit | Topics | Contact Hours |
|---|---|---|
| 1 | **Introduction to Reaction Engineering**<br>Classification of reactions, definitions of reactions rate, variables affecting reaction rate. | 4 |
| 2 | **Kinetics of homogenous reactions**<br>Simple reactor types, the rate equation, concentration dependent term of rate equation. Molecularity and order of reaction. Rate constant k, representation of an elementary and nonelementary reaction. Kinetic models for nonelementary reactions. Testing kinetic models. Temperature dependant term of rate equations | 6 |

| | | |
|---|---|---|
| | from Arrhenius theory and comparison with collision and transition state theory. Activation energy and temperature dependency. | |
| 3 | **Interpretation of Batch reactor data**<br>Constant volume batch reactor, analysis of total pressure data, Integral and differential methods of analysis of data for constant volume and variable volume cases. | 6 |
| 4 | **Introduction to reactor design & Ideal reactors for single reaction**<br>Mass and energy balances around a volume element. Ideal batch reactor, steady-state mixed flow reactor, steady-state plug-flow reactor, holding and space time for flow reactors. | 6 |
| 5 | **Design of reactor for single reactions**<br>Size comparison of single reactors, multiple reactor systems, recycle reactor and autocatalytic reactions. | 4 |
| 6 | **Design for multiple reactions**<br>Introduction to multiple reactions, qualitative and quantitative treatment of product distribution and of reactor size, the selectivity. Irreversible first order reactions in series. Quantitative treatment, for plug flow or batch reactor and mixed flow reactor, their performance characteristics. | 6 |
| 7 | **Temperature and pressure effects**<br>Single Reactions: Calculations of heats of reaction and equilibrium constants from thermodynamics, equilibrium conversion, general graphical design procedure. Optimum temperature progression, Energy balances equations in adiabatic and non-adiabatic case. | 6 |
| | **Total Hours** | 36 |

**References:**

1. Octave Levenspiel, Chemical Reaction Engineering, 3rd Edition, Wiley-India Pvt. Ltd.
2. H. Scott Fogler, Elements of Chemical Reaction Engineering, 4th Edition, Prentice Hall of India Pvt. Ltd.
3. J.M. Smith, Chemical Engineering Kinetics, 2nd edition, McGraw-Hill.
4. L. D. Schmidt, the Engineering of Chemical Reactions, Oxford Press.

**Suggested Theory distribution:**

The suggested theory distribution as per Bloom’s taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

| Distribution of Theory for course delivery and evaluation | | | | | |
|---|---|---|---|---|---|
| Remember | Understand | Apply | Analyse | Evaluate | Create |
| 10% | 20% | 25% | 25% | 10% | 10% |

**List of Experiments:**

1. To determine the activation energy of the reaction between sodium thio-sulphate and HCl using Arrhenius Equation.
2. To determine order of reaction for the reaction between sodium thio-sulphate and HCl.
3. To determine the kinetics of the reaction between ethyl acetate and sodium hydroxide at room temperature by the integral method of analysis.
4. To measure the kinetics of a reaction between ethyl acetate and sodium hydroxide under condition of excess ethyl acetate at room temperature.
5. To determine the activation energy and frequency factor for reaction between ethyl acetate and sodium hydroxide at room temperature & at different temperature.
6. To determine the kinetics of the reaction between ethyl acetate and sodium hydroxide at room temperature by the differential method of analysis.
7. To determine the kinetics of the reaction between n- butyl acetate and sodium hydroxide at room temperature by the integral method of analysis.
8. To determine the kinetics of the reaction between n- butyl acetate and sodium hydroxide at room temperature by the differential method of analysis.

**Instructional Method:**

a. The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.

b. The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.

c. Practical examination will be conducted at the end of semester for evaluation of performance of students in laboratory.

d. Students will use supplementary resources such as online videos, NPTEL videos, e-courses, Virtual Laboratory

**Online Web Resources**:

1. http://nptel.ac.in
2. https://ocw.mit.edu

**Design Based Problems (DP)/ Open Ended project (OEP):**

In the beginning of the session, subject faculty will allot an OEP / DP to the students. Students will be free to choose a topic of their choice which will be relevant to the syllabus and they will either prepare a working model/ report / presentation / poster on their topic.