

CHEMICAL REACTION KINETICS**Course Code : 314309**

Programme Name/s : Chemical Engineering
Programme Code : CH
Semester : Fourth
Course Title : CHEMICAL REACTION KINETICS
Course Code : 314309

I. RATIONALE

Chemical reaction kinetics is an engineering activity concerned with the exploitation of chemical reactions on a commercial scale. This course seeks to familiarize the students with concepts of rate of reaction, rate expression derivation from reaction mechanism by integral method, differential method, and half-life method of analysis. Its goal is the successful design and operation of chemical reactors. Knowledge of the course helps in selecting the optimum reactor design for any process by considering the reaction's kinetics, heat and mass transfer effects, and the economics of the process.

II. INDUSTRY / EMPLOYER EXPECTED OUTCOME

Operate various chemical reactors to produce products of desired quality with minimum cost.

III. COURSE LEVEL LEARNING OUTCOMES (COS)

Students will be able to achieve & demonstrate the following COs on completion of course based learning

- CO1 - Perform kinetics of different chemical reactions.
- CO2 - Use appropriate catalyst for enhancing rate of reaction.
- CO3 - Identify the order of reactions based on interpretation of batch reactor data.
- CO4 - Calculate the size of reactor by using the knowledge of design reactor equations.
- CO5 - Identify suitable reactor for best conversion of reactants.

IV. TEACHING-LEARNING & ASSESSMENT SCHEME

Course Code	Course Title	Abbr	Course Category/s	Learning Scheme					Credits	Paper Duration	Assessment Scheme										Total Marks
				Actual Contact Hrs./Week			SLH	NLH			Theory			Based on LL & TL		Based on SL					
				CL	TL	LL					FA-TH	SA-TH	Total		FA-PR	SA-PR	SLA				
													Max	Min			Max	Min	Max	Min	
314309	CHEMICAL REACTION KINETICS	CRK	DSC	4	-	4	-	8	4	03	30	70	100	40	25	10	25@	10	-	-	150

Total IKS Hrs for Sem. : 0 Hrs

Abbreviations: CL- ClassRoom Learning , TL- Tutorial Learning, LL-Laboratory Learning, SLH-Self Learning Hours, NLH-Notional Learning Hours, FA - Formative Assessment, SA -Summative assessment, IKS - Indian Knowledge System, SLA - Self Learning Assessment

Legends: @ Internal Assessment, # External Assessment, *# On Line Examination , @\$ Internal Online Examination

Note :

1. FA-TH represents average of two class tests of 30 marks each conducted during the semester.
2. If candidate is not securing minimum passing marks in FA-PR of any course then the candidate shall be declared as "Detained" in that semester.
3. If candidate is not securing minimum passing marks in SLA of any course then the candidate shall be declared as fail and will have to repeat and resubmit SLA work.
4. Notional Learning hours for the semester are (CL+LL+TL+SL)hrs.* 15 Weeks
5. 1 credit is equivalent to 30 Notional hrs.
6. * Self learning hours shall not be reflected in the Time Table.
7. * Self learning includes micro project / assignment / other activities.

V. THEORY LEARNING OUTCOMES AND ALIGNED COURSE CONTENT

Sr.No	Theory Learning Outcomes (TLO's) aligned to CO's.	Learning content mapped with Theory Learning Outcomes (TLO's) and CO's.	Suggested Learning Pedagogies.
1	<p>TLO 1.1 State the parameters affecting the rate of reaction</p> <p>TLO 1.2 Classify different types of reactions with examples.</p> <p>TLO 1.3 Define reaction rate and rate constant with units.</p> <p>TLO 1.4 Describe Kinetics of non-elementary reaction.</p> <p>TLO 1.5 Calculate the frequency factor and activation energy for the given using given data analytically and graphically.</p> <p>TLO 1.6 Compare the temperature dependency of rate constant in terms of Arrhenius law, transition state theory and collision theory.</p>	<p>Unit - I Kinetics of Homogeneous Reactions</p> <p>1.1 Concept of chemical kinetics, parameters affecting the rate of reaction.</p> <p>1.2 Types of Reaction (Definition and examples): a. Homogenous and Heterogeneous reactions b. Catalytic non catalytic reactions c. Molecularity of reaction d. Exothermic and endothermic reactions e. Order of reaction f. Reversible and irreversible reactions g. Elementary and non-elementary reaction. h. Chain and non-chain reaction.</p> <p>1.3 Reaction rate, rate equation, rate constant, units of rate constant, concentration dependent term of rate equation.</p> <p>1.4 Kinetics of non-elementary reactions (homogeneous reaction)</p> <p>1.5 Activation energy and its significance and numericals.</p> <p>1.6 Derive temperature dependency of rate constant from: a. Arrhenius law b. Transition state theory c. Collision Theory d. Compare Arrhenius, Transition state theory and Collision Theory (Numericals)</p>	<p>Lecture Using Chalk-Board Presentations Video Demonstrations</p>

Sr.No	Theory Learning Outcomes (TLO's) aligned to CO's.	Learning content mapped with Theory Learning Outcomes (TLO's) and CO's.	Suggested Learning Pedagogies.
2	<p>TLO 2.1 State the characteristics of catalytic reaction.</p> <p>TLO 2.2 Define homogeneous and heterogeneous with example.</p> <p>TLO 2.3 Describe the specified properties of catalyst.</p> <p>TLO 2.4 Describe various methods of catalyst preparation.</p> <p>TLO 2.5 Explain the mechanism of solid gas phase catalytic reactions.</p> <p>TLO 2.6 Describe catalyst poisoning.</p> <p>TLO 2.7 Explain catalyst regeneration.</p>	<p>Unit - II Catalysis</p> <p>2.1 Definition of catalysis, characteristics of catalytic reaction</p> <p>2.2 Classification of catalytic reaction: homogeneous and heterogeneous</p> <p>2.3 Properties of catalyst: Activity, specificity, porous and crystalline structure, kindling point</p> <p>2.4 Methods of catalyst preparation: Precipitation, Gel formation, Simple mixing of components, Impregnation.</p> <p>2.5 Mechanism of solid gas phase catalytic reactions</p> <p>2.6 Concept of catalyst deactivation, Concept of Promoters, Inhibitors and Accelerators, Catalyst Poisoning: Deposited poison, chemisorbed poison, selectivity poison, diffusion poison, stability poison.</p> <p>2.7 Catalyst regeneration</p>	<p>Lecture Using Chalk-Board Presentations Video Demonstrations</p>
3	<p>TLO 3.1 Define constant and variable volume batch reactor</p> <p>TLO 3.2 Compare concentration and conversion term for constant volume system.</p> <p>TLO 3.3 : State the different methods to analyse the rate data for various order of reactions by integral method at constant volume batch reactor.</p> <p>TLO 3.4 Derive the integrated rate equations for different order of reactions by integral method at constant volume reactor system.</p> <p>TLO 3.5 Derive the integrated rate equation for first order, second order and zero order reaction in variable volume system by integral method.</p>	<p>Unit - III Interpretation of Batch Reactor Data</p> <p>3.1 Concept of constant volume batch reactor and variable volume batch reactor</p> <p>3.2 Constant Volume Batch Reactor: Relation between concentration and conversion for constant volume system</p> <p>3.3 Methods of analysis of kinetic data/rate data: Integral method, differential method, half-life method, Ostwald isolation method and initial rate method</p> <p>3.4 General procedure for integral method for analysis of kinetic data for constant volume reactor a. Integrated rate expression for Irreversible unimolecular type first order reactions and its characteristics b. Integrated rate expression for irreversible bimolecular type second order reactions ($2A \rightarrow \text{Product}$ and $A+B \rightarrow \text{Product}$) and its characteristics c. Integrated rate expression for zero order reaction and its characteristics d. Integrated rate expression for nth order reaction (Numericals)</p> <p>3.5 Variable Volume Batch Reactor to Analyse the Kinetic Data/Rate Data: a. Concept of ϵ_A b. Integrated rate expression for irreversible unimolecular type first order reaction c. Integrated rate expression for irreversible bimolecular type second order reactions ($2A \rightarrow \text{Product}$) d. Integrated rate expression for zero order reaction (Numericals)</p>	<p>Lecture Using Chalk-Board Presentations Video Demonstrations</p>

Sr.No	Theory Learning Outcomes (TLO's) aligned to CO's.	Learning content mapped with Theory Learning Outcomes (TLO's) and CO's.	Suggested Learning Pedagogies.
4	<p>TLO 4.1 Classify the different reactors with their applications.</p> <p>TLO 4.2 Derive design equation for ideal batch reactor for constant and variable volume system.</p> <p>TLO 4.3 State space time, space velocity and holding time.</p> <p>TLO 4.4 Derive design equation for continuous stirrer tank reactor for constant and variable volume system.</p> <p>TLO 4.5 Derive design equation for tubular flow reactor for constant and variable volume system.</p>	<p>Unit - IV Reactor Design</p> <p>4.1 Classification of Reactors (diagram, brief description and applications): Batch, semi-batch, continuous stirred tank reactor, tubular/plug flow, fixed bed and fluidised bed reactor</p> <p>4.2 Performance/design equation for ideal batch reactor for constant and variable volume system with their graphical representation. (Numericals)</p> <p>4.3 Concept of space time, space velocity, holding time for flow reactors. (Numericals)</p> <p>4.4 Performance/design equation for steady state continuous stirrer tank reactor (CSTR) for constant and variable volume system with their graphical representation. (Numericals)</p> <p>4.5 Performance/design equation for steady state Plug flow reactor (PFR) for Constant and variable volume system with their graphical representation. (numericals)</p>	<p>Lecture Using Chalk-Board Presentations Video Demonstrations</p>
5	<p>TLO 5.1 Compare CSTR and PFR according to the given parameters.</p> <p>TLO 5.2 Determine the optimized arrangement for CSTR and PFR in terms of conversion.</p>	<p>Unit - V Size Comparison of Plug Flow Reactor (PFR) and Continuous stirrer tank reactor (CSTR)</p> <p>5.1 Size comparison of single reactor: CSTR and PFR</p> <p>5.2 Multiple Reactor System: a. CSTR in series (equal size) b. Judgement of the best system for given conversion in PFR and CSTR connected in series c. CSTR connected in parallel d. PFR connected in series or in parallel e. PFR connected in series parallel combination. (Numericals)</p>	<p>Lecture Using Chalk-Board Presentations Video Demonstrations</p>

VI. LABORATORY LEARNING OUTCOME AND ALIGNED PRACTICAL / TUTORIAL EXPERIENCES.

Practical / Tutorial / Laboratory Learning Outcome (LLO)	Sr No	Laboratory Experiment / Practical Titles / Tutorial Titles	Number of hrs.	Relevant COs
<p>LLO 1.1 Prepare 0.1 N solution of NaOH and ethyl acetate</p> <p>LLO 1.2 Determine the effect of temperature on the activation energy</p> <p>LLO 1.3 Plot of $\ln k$ vs $1/T$ give a straight line with slope equal to E/R</p>	1	<p>* Determination of activation energy of saponification of ethyl acetate and sodium hydroxide at various temperatures.</p>	4	CO1
<p>LLO 2.1 Prepare 0.1 N solution of NaOH and methyl acetate</p> <p>LLO 2.2 Determine the effect of temperature on the activation energy</p> <p>LLO 2.3 Plot of $\ln k$ vs $1/T$ give a straight line with slope equal to E/R</p>	2	<p>*Determination of the activation energy of the reaction by hydrolysis of methyl acetate at various temperatures.</p>	4	CO1

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Practical / Tutorial / Laboratory Learning Outcome (LLO)	Sr No	Laboratory Experiment / Practical Titles / Tutorial Titles	Number of hrs.	Relevant COs
LLO 3.1 Titrate against 0.1 N NaOH solution using phenolphthalein indicator LLO 3.2 Calculate conversion of methyl acetate at any time LLO 3.3 Determine the concentration of methyl acetate at any time	3	*Determination of Arrhenius rate constants for acidic hydrolysis of methyl acetate at various temperatures.	4	CO1
LLO 4.1 Titrate against 0.1 N NaOH solution using phenolphthalein indicator LLO 4.2 Calculate conversion of ethyl acetate at any time LLO 4.3 Determine the concentration of ethyl acetate at any time	4	*Determination of Arrhenius rate constant for acidic hydrolysis of ethyl acetate at various temperatures.	4	CO1
LLO 5.1 Standardised NaOH and HCl solution with oxalic acid solution LLO 5.2 Titrate against HCl solution using phenolphthalein indicator LLO 5.3 Calculate concentration of ethyl acetate	5	*Determination of the rate constant for the saponification reaction of ethyl acetate and sodium hydroxide.	4	CO1
LLO 6.1 Measure the weight of the catalyst using weighing balance. LLO 6.2 Measure the change in volume of water after putting catalyst in water. LLO 6.3 Measure the density of water LLO 6.4 Filter the catalyst using filter paper	6	Determination of the void volume of a catalyst particle.	4	CO2
LLO 7.1 Measure the weight of the catalyst using weighing balance. LLO 7.2 Measure the change in volume of water after putting catalyst in water. LLO 7.3 Measure the density of water LLO 7.4 Filter the catalyst using filter paper.	7	*Determination of the solid density of a catalyst particle.	4	CO2

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Practical / Tutorial / Laboratory Learning Outcome (LLO)	Sr No	Laboratory Experiment / Practical Titles / Tutorial Titles	Number of hrs.	Relevant COs
LLO 8.1 Measure the weight of the catalyst using weighing balance. LLO 8.2 Measure the change in volume of water after putting catalyst in water. LLO 8.3 Measure the density of water LLO 8.4 Filter the catalyst using filter paper.	8	Determination of the porosity of a catalyst particle.	4	CO2
LLO 9.1 Prepare 0.1 N sodium hydroxide and ethyl acetate solution LLO 9.2 Titrate against HCl solution using phenolphthalein indicator LLO 9.3 Calculate normality of sodium hydroxide and hydrochloric acid LLO 9.4 Determine concentration of ethyl acetate	9	*Determination of order of reaction for saponification of ethyl-acetate with sodium hydroxide.	4	CO3
LLO 10.1 Prepare 0.1 N sodium hydroxide and methyl acetate solution LLO 10.2 Titrate against HCl solution using phenolphthalein indicator LLO 10.3 Calculate strength of sodium hydroxide and hydrochloric acid LLO 10.4 Determine concentration of methyl acetate	10	Determination of the order of reaction for acidic hydrolysis of methyl acetate.	4	CO3
LLO 11.1 Prepare 0.1 N sodium hydroxide, hydrochloric acid and ethyl acetate solution LLO 11.2 Titrate against 0.1 N NaOH using phenolphthalein indicator LLO 11.3 Calculate the concentration of ethyl acetate	11	*Determination of the kinetics of the reaction between ethyl acetate and sodium hydroxide in an isothermal batch reactor.	4	CO4
LLO 12.1 Prepare 0.1 N sodium hydroxide, hydrochloric acid and ethyl acetate solution LLO 12.2 Titrate against 0.1 N NaOH using phenolphthalein indicator LLO 12.3 Calculate the concentration of ethyl acetate	12	Determination of the kinetics of saponification of ethyl acetate and sodium hydroxide in a Plug Flow Reactor.	4	CO4

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Practical / Tutorial / Laboratory Learning Outcome (LLO)	Sr No	Laboratory Experiment / Practical Titles / Tutorial Titles	Number of hrs.	Relevant COs
LLO 13.1 Prepare 0.1 N sodium hydroxide, hydrochloric acid and ethyl acetate solution LLO 13.2 Titrate against 0.1 N NaOH using phenolphthalein indicator LLO 13.3 Calculate the concentration of ethyl acetate	13	Determination of the kinetics of saponification of ethyl acetate and sodium hydroxide in a continuous stirrer tank reactor.	4	CO4
LLO 14.1 Prepare 0.1 N sodium hydroxide, hydrochloric acid and ethyl acetate solution LLO 14.2 Determine rate constant by plotting the graph between time and concentration.	14	Determination of rate constant by the half-life period of the saponification reaction between ethyl acetate and sodium hydroxide in an isothermal batch reactor.	4	CO4
LLO 15.1 Prepare 1N potassium Hydroxide solution LLO 15.2 Two layers are separated by decantation method.	15	*Determination of kinetics of Bio-diesel synthesis from vegetable oils by Transesterification	4	CO4
LLO 16.1 Prepare 0.02 N sodium hydroxide, 0.05 N hydrochloric acid and ethyl acetate solution LLO 16.2 Calculate the concentration of ethyl acetate and sodium hydroxide	16	*The performance of three equal volumes of CSTR's in series for the saponification of ethyl acetate and sodium hydroxide reactions.	4	CO5

Note : Out of above suggestive LLOs -

- '*' Marked Practicals (LLOs) Are mandatory.
- Minimum 80% of above list of lab experiment are to be performed.
- Judicial mix of LLOs are to be performed to achieve desired outcomes.

VII. SUGGESTED MICRO PROJECT / ASSIGNMENT/ ACTIVITIES FOR SPECIFIC LEARNING / SKILLS DEVELOPMENT (SELF LEARNING)

NA

- NA

Note :

- Above is just a suggestive list of microprojects and assignments; faculty must prepare their own bank of microprojects, assignments, and activities in a similar way.
- The faculty must allocate judicious mix of tasks, considering the weaknesses and / strengths of the student in acquiring the desired skills.
- If a microproject is assigned, it is expected to be completed as a group activity.
- SLA marks shall be awarded as per the continuous assessment record.
- For courses with no SLA component the list of suggestive microprojects / assignments/ activities are optional, faculty may encourage students to perform these tasks for enhanced learning experiences.
- If the course does not have associated SLA component, above suggestive listings is applicable to Tutorials and maybe considered for FA-PR evaluations.

VIII. LABORATORY EQUIPMENT / INSTRUMENTS / TOOLS / SOFTWARE REQUIRED

Sr.No	Equipment Name with Broad Specifications	Relevant LLO Number
1	<p>ISOTHERMAL BATCH REACTOR To determine the kinetic parameters affecting progress of a Chemicals reaction. Power 500 Watt (w), Voltage 240 Volt (v), Materials S S Metal Reactor of Capacity Min. 2 Ltrs fitted with Stirrer having Impeller and shaft coupled with DC Motor. Double walled Water Bath, insulated and fitted with agitator having Impeller and shaft coupled with DC Motor with the help of bearings. Heater whose temperature controlled by PID Controller, 0-199.9° C. Reactor, water bath, Impeller and shaft should be made of stainless steel .RPM of the stirrer should be displayed with the help of RPM sensor .Operating/instruction manual and sample calculations with Photographs, line diagram, detailed design and drawing of the impeller, must be provided with equipment. Equipments has to be demonstrated at college site, results should be repeatable within ± 5 to 10 % of the sample calculations provided.</p>	1,2,3,4,5,9,10,11,14,15
2	<p>ISOTHERMAL PLUG FLOW REACTOR (PFR) To determine the Reaction Rate Constant and effect of temperature on saponification reaction in Isothermal Plug Flow Reactor. Helical Coiled Tube Type Reactor of min Volume 0.5Ltrs. Double walled Water Bath, insulated with Ceramic Wool and reactor fitted with stirrer having Impeller and shaft coupled with motor and Heater whose temperature controlled by PID Controller, 0-199.9° C. Feed Circulation by pump and flow measurement device. Reactor, water bath, Impeller, shaft and feed tanks should be made of stainless steel Temperature measurement done by Temperature Sensors of RTD PT-100 type with Digital Temperature Indicator (0-199.9 °C). Operating/instruction manual consisting of experimental procedure, block diagram etc. and sample calculations should to be provided along with equipment. Equipments has to be demonstrated at college site, results should be repeatable within ± 5 to 10% of the sample calculations provided.</p>	12

Sr.No	Equipment Name with Broad Specifications	Relevant LLO Number
3	<p>ISOTHERMAL CONTINUOUS STIRRED TANK REACTOR To determine the Reaction Rate Constant and effect of temperature on Saponification Reaction in Isothermal CSTR. Reactor of min capacity 2 Ltrs fitted with agitation system and shaft coupled with Motor and min. four Baffles. Double walled Water Bath, insulated with Ceramic Wool should be fitted with Agitator having min 4 square bladed Impeller and shaft coupled with motor and Heater whose temperature controlled by PID Controller, 0-199.9° C. Feed Circulation done by compressed air from Feed Tanks, 1.2 mm thick, capacity 20 liters each, made of stainless steel and Flow Measurement by Rotameter. Reactor, water bath, baffles, Impeller, shaft and feed tanks should be made of stainless steel and Piping of Stainless Steel and PU pipe. Bourdon type pressure gauge of 0-2 Kg/cm² and Pressure Regulator of 0-2 Kg/cm² should be provided. Temperature measurement done by Temperature Sensors of RTD PT-100 type with Digital Temperature Indicator (0-199.9 °C). Electricity Supply: Single Phase, 220 V AC, 50 Hz, 5-15 Amp combined socket with earth connection. Floor Drain. Laboratory Glassware and Chemicals required for analysis as per the system adopted.</p>	13,16

IX. SUGGESTED WEIGHTAGE TO LEARNING EFFORTS & ASSESSMENT PURPOSE (Specification Table)

Sr.No	Unit	Unit Title	Aligned COs	Learning Hours	R-Level	U-Level	A-Level	Total Marks
1	I	Kinetics of Homogeneous Reactions	CO1	10	4	4	2	10
2	II	Catalysis	CO2	6	4	2	2	8
3	III	Interpretation of Batch Reactor Data	CO3	18	4	8	8	20
4	IV	Reactor Design	CO4	16	2	8	8	18
5	V	Size Comparison of Plug Flow Reactor (PFR) and Continuous stirrer tank reactor (CSTR)	CO5	10	2	4	8	14
Grand Total				60	16	26	28	70

X. ASSESSMENT METHODOLOGIES/TOOLS

Formative assessment (Assessment for Learning)

- Two Class Test of 30 Marks Each, Term Work Assessment of 25 Marks

Summative Assessment (Assessment of Learning)

- End Term Theory Examination, End Term Practical Examination

XI. SUGGESTED COS - POS MATRIX FORM

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Course Outcomes (COs)	Programme Outcomes (POs)							Programme Specific Outcomes* (PSOs)		
	PO-1 Basic and Discipline Specific Knowledge	PO-2 Problem Analysis	PO-3 Design/ Development of Solutions	PO-4 Engineering Tools	PO-5 Engineering Practices for Society, Sustainability and Environment	PO-6 Project Management	PO-7 Life Long Learning	PSO-1	PSO-2	PSO-3
CO1	3	2	2	2	1	1	3			
CO2	3	3	3	2	2	2	2			
CO3	3	2	2	1	1	1	1			
CO4	3	3	3	3	3	3	3			
CO5	2	3	3	2	2	2	2			

Legends :- High:03, Medium:02,Low:01, No Mapping: -
*PSOs are to be formulated at institute level

XII. SUGGESTED LEARNING MATERIALS / BOOKS

Sr.No	Author	Title	Publisher with ISBN Number
1	Octave Levenspiel	Chemical Reaction Engineering	Wiley India, New Delhi, 2015 ISBN-978-81-265-1000-9
2	J. M. Smith	Chemical Engineering Kinetics	Mc-Graw Hill New Delhi, 2015 ISBN 007*066574-5
3	H. Scott Fogler	Elements of Chemical Reaction Engineering	Pearson New Delhi, 2015 ISBN 978-81-317-1430-0
4	Srivastav R. P. S.	Elements of Chemical Reaction Engineering	Khanna Publishers, New Delhi, 2015 ISBN 81-7409-083-5

XIII. LEARNING WEBSITES & PORTALS

Sr.No	Link / Portal	Description
1	https://onlinecourses.nptel.ac.in/noc19_ch20/preview	Chemical Reaction Engineering
2	https://nptel.ac.in/courses/103/103/103103153/	Chemical Reaction Engineering
3	https://nptel.ac.in/courses/103/101/103101141/#	Chemical Reaction Engineering
4	https://onlinecourses.nptel.ac.in/noc19_ch20/preview	Chemical Reaction Engineering

Note :

- Teachers are requested to check the creative common license status/financial implications of the suggested online educational resources before use by the students