Chemical Reaction Engineering II - Video course

COURSE OUTLINE

This is a typical second course in the subject of chemical reaction engineering with an emphasis on heterogeneous reaction engineering and nonideal reactors. Catalysis, mechanistic treatment of rate forms and the practical issues of transport limitations, leading finally to design considerations, form the first part. Kinetics and design of reactors for noncatalytic gas-liquid and fluid-solid reactions follows, and the last part of the course deals with the subject of residence time distributions, and how they can be used to characterize and design non-ideal reactors. The course thus consists of the following modules:

1. Catalysis and Kinetics of heterogeneous catalytic reactions
2. Transport effects in catalytic reactors (External and pore diffusion)
3. Catalytic reactor design
4. Multiphase reactors (gas-liquid and fluid-solid reactions)
5. Residence time distributions and nonideal reactors

COURSE DETAIL

Lecture no.	Title	Keywords	Delivered by
1	Introduction to catalysts and catalysis	Catalysts and catalytic reactors, heterogeneous catalyst, activation energy, porous structure, types of catalysts, adsorption	Sanjay Mahajani
2	Steps in catalytic reaction: adsorption, desorption and reaction	Steps in catalysis, adsorption, desorption, surface reaction, types of catalytic reactors, adsorption	Sanjay Mahajani

NP-TEL

NPTEL

http://nptel.iitm.ac.in

Chemical Engineering

Pre-requisites:

Chemical Reaction Engineering -I.

Additional Reading:

1. Sharma, M.M. and Doraiswamy, L.K. Heterogeneous reactions: Analysis, Examples and Reactor Design. Vols. I & II, John Wiley and Sons, NY, 1984.
2. Froment, G.F. and Bischoff, K. B. Chemical Reactor Analysis and Design, II Ed., John Wiley and Sons, NY, 1990.

Coordinators:

Prof. Ganesh A. Viswanathan
Department of Chemical Engineering IIT Bombay

Prof. A.K. Suresh

		isotherm, single site, dual site mechanisms, Langmuir Hinshelwood, Eley Rideal, Rate controlling steps	
3	Derivation of the rate equation	Rate controlling steps, Rate law for hetergeneous reaction, Derivation of rate equation, Catalytic sites, Equilibrium, Site balance	Sanjay Mahajani
4	Heterogenous data analysis for reactor design - I	Deduce mechanism; reactor design	Ganesh Viswanathan
5	Heterogenous data analysis for reactor design - II	Fluidized reactor; Case study: Germanium epitaxial growth	Ganesh Viswanathan
6	Catalyst deactivation and accounting for it in design – I	Deactivation; Rate law; Modes of deactivation	Ganesh Viswanathan
7	Catalyst deactivation and accounting for it in design – II	Poisoning; Fluidized CSTR; Moving bed reactor	Ganesh Viswanathan
8	Synthesize the rate equation	Experimental data, dehydrogenation of cyclohexane, validation, laboratory reactors for catalytic reactions, differential reactors, slurry reactor, least square method	Sanjay Mahajani
9	Introduction to intraparticle	Internal (intraparticle)	Sanjay Mahajani

Department of Chemical EngineeringIIT Bombay

Prof. Sanjay M. Mahajani
Department of Chemical EngineeringIIT Bombay

	diffusion	diffusion, wall effect, tortuosity, porosity, effective diffusivity, constriction, flux, differential balance, types of rate constants and their units, concentration profile inside the catalyst, Thiele modulus	
10	Intraparticle diffusion: Thiele modulus and effectiveness factor Part I	Concentration profile inside the catalyst, effectiveness factor, Derivation of effectiveness factor, Thiele modulus	Sanjay Mahajani
11	Intraparticle diffusion: Thiele modulus and effectiveness factor Part II	Diffusion limited reaction, reactor design, effectiveness factor, spinning basket reactor, apparent order, apparent activation energy, non-isothermal effectiveness factor	Sanjay Mahajani
12	Intraparticle diffusion: Thiele modulus and effectiveness factor Part III	Exothermic reaction, thermal conductivity of catalyst, multiple steady states, endothermic reaction, catalyst geometries, catalyst slab	Sanjay Mahajani
13	Effectiveness factor and Introduction to external mass transfer	Effect of catalyst particle diameter, external mass transfer, boundary layer, mass transfer coefficient, rate controlling	Sanjay Mahajani

		mechanism	
14	External Mass Transfer	External mass transfer coefficient, Reynolds number, Schmidt number, Sherwood number, interfacial area, fixed bed reactor	Sanjay Mahajani
15	Implications to rate data interpretation and design I	Weisz-Prater criterion; Mears'criterion; Packed-bed reactor design	Ganesh Viswanathan
16	Implications to rate data interpretation and design II	Generalized criterion; Network of first order reactions; Vector of effectiveness factors	Ganesh Viswanathan
17	Packed-bed reactor design	Different configurations; Packed-bed reactor design: First order reaction, Second order reaction	Ganesh Viswanathan
18	Fluidized bed reactor design I	Kunii-Levenspiel model: Basic principles	Ganesh Viswanathan
19	Fluidized bed reactor design II	Different regimes; Mass transport in fluidized beds; First order reaction; resistances	Ganesh Viswanathan
20	Gas-liquid reactions-1: Theories of mass transfer into agitated liquids	Mass transfer into agitated liquids; Film theory, Penetration theory	A K Suresh

21	GLR-2: Effect of chemical reaction on mass transfer: the slow reaction regime	Film theory, pseudo-first order, Hatta number, slow reaction regime, kinetic sub-regime, diffusional sub-regime	A K Suresh	
22	GLR-3: Transition to fast reaction, and the Fast reaction regime	Film theory, Enhancement factor; transition to fast reaction, Fast reaction regime	A K Suresh	
23	GLR-4: Fast reaction example; Instantaneous reaction regime	Film theory, second order case; Instantaneous reaction; limiting enhancement; enhancement factor plot	A K Suresh	
24	GLR-5: Transition to Instantaneous reaction; Reaction regimes in surface renewal theories	Film theory, transition from fast to Instantaneous reaction; Surface renewal theories, slow reaction	A K Suresh	
25	GLR-6: Reaction regimes in surface renewal theories (contd..)	Surface renewal theories, transition to fast reaction, fast reaction regime, comparison of surface renewal and film theories, Danckwerts' plot, second order reaction with mass transfer	A K Suresh	
26	GLR-7: Surface renewal theories: Instantaneous reaction and Summing up	Surface renewal theories, Instantaneous reaction, reactor design	A K Suresh	

27	NOT USED		A K Suresh
28	Fluid-solid non-catalytic reactions I	Modes; Basic principles; Progressive-conversion model; Shrinking core model	Ganesh Viswanathan
29	Fluid-solid non-catalytic reactions II	Gas film diffusion control; Ash layer diffusion control; Surface reaction control	Ganesh Viswanathan
30	Fluid-solid non-catalytic reactions III	Other geometries, Combination of resistances; Case study: Dissolution of monodispersed and polydispersed particles	Ganesh Viswanathan
31	Distribution of residence time	Introduction; Non-ideal reactor examples: Gas-liquid CSTR, Packed-bed reactor, CSTR	Ganesh Viswanathan
32	Measurement of residence time distribution	Pulse input; Step input; RTD functions: E and F-curves	Ganesh Viswanathan
33	Residence time distribution function	Properties: Mean, variance, skewness; RTD of ideal reactors: PFR, CSTR.	Ganesh Viswanathan
34	Reactor diagnostics and troubleshooting	RTD of laminar flow reactors; RTD functions: Perfect operation, Bypassing, Dead volume	Ganesh Viswanathan
35	Modeling non-	Combination of	Ganesh

	ideal reactors	reactors: PFR-CSTR in Series; Mixing: Macro- and Micro-mixing	Viswanathan
36	Residence time distribution: Performance of non-ideal reactors	Segregation model; Maximum mixedness model; RTD with multiple reactions	Ganesh Viswanathan
37	Non-ideal Reactors: Tanks-in-series model	Non-ideal reactors, tank-in-series model, one parameter model, axial mixing, variance, E curve	Sanjay Mahajani
38	Non-ideal Reactors: Dispersion model	Dispersion model, closed-closed vessel, open-open vessel, Peclet number, E curve	Sanjay Mahajani
39	Non-ideal Reactors: Dispersion model and introduction to multiparameter models	Dispersion model, Damkohler number, conversion in non-ideal tubular reactor, two parameter model, dead zones, bypass, E curve	Sanjay Mahajani
40	Non-ideal Reactors: Multiparameter models	Tracer experiment, multiparameter model, ideal reactor network, E curve	Sanjay Mahajani

References:

1. H.S. Fogler, Elements of Chemical Reaction Engineering, Fourth Ed., Prentice-Hall, New Jersey (2005).
2. O. Levenspiel, Chemical Reaction Engineering, Third Ed., J. Wiley & Sons, NY (1999).

3. Danckwerts, P.V. Gas-Liquid Reactions, McGraw-Hill, NY (1970)