CONCEPT

Chemical Reactor Design and Catalyst Selection: Kinetics, Reactor Sizing and Deactivation



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Introduction:

Chemical reactor design decisions made on rough rate data, an unchecked reactor type or a catalyst chosen on price alone lead to lost selectivity, hot spots, short catalyst cycles and unplanned change-outs. This Core Concept course equips process and technical services engineers to derive rate laws from plant and pilot data, size and compare batch, CSTR and PFR reactors, control selectivity across multiple reactions, check heat removal against runaway, and select, monitor and regenerate catalysts in fixed, fluidised and trickle bed reactors. Participants build a Reactor Sizing and Catalyst Selection Workbook.

Course Objectives:

- Derive rate laws and Arrhenius parameters from laboratory, pilot or plant data and express reactor results as conversion, yield and selectivity
- Size batch, CSTR and PFR reactors from their design equations and justify the arrangement that meets a conversion target at least volume
- Control selectivity in parallel and series reaction networks through temperature, concentration profile and reactor choice
- Evaluate reactor energy balances and heat removal capacity to recognise the conditions that lead to hot spots and thermal runaway
- Select a catalytic reactor type and catalyst on activity, selectivity, stability and pore diffusion limits, and plan protection against poisoning, sintering and coking
- Monitor reactor and catalyst performance trends and diagnose common catalytic reactor problems in a Reactor Sizing and Catalyst Selection Workbook

Target Audience:

- Process engineers responsible for reactor sizing, debottlenecking and operating targets in petrochemical and chemical plants
- Technical services engineers who track catalyst activity, bed temperatures and run length on refinery and petrochemical reactors
- Catalyst and licensing specialists who evaluate vendor proposals and catalyst change-out options
- Process design engineers who prepare reactor datasheets for new units and revamps
- Process safety engineers who review reactor heat removal and temperature excursion scenarios
- Pilot plant and research engineers who generate kinetic data for scale-up

Course Outline:

Day 1: Reaction Kinetics, Rate Laws and Conversion Measures

- Rate Law Forms: Power-Law, Reversible and Langmuir-Hinshelwood Expressions
- Arrhenius Parameters: Activation Energy and Pre-Exponential Factor from Rate Data
- Integral and Differential Methods for Fitting Pilot and Laboratory Kinetic Data
- Conversion, Yield and Selectivity Definitions on a Reactor Stream Table
- Equilibrium Conversion Limits from Gibbs Energy and Le Chatelier Shifts

Day 2: Ideal Reactor Models: Batch, CSTR and PFR Sizing

- Batch and Semibatch Reactor Design Equation and Cycle Time Build-Up
- CSTR Design Equation, Space Time and Levenspiel Plot Sizing
- PFR Design Equation, Tubular Volume and Pressure Drop Along the Tube
- CSTRs in Series Versus a Single PFR: Volume Comparison at Equal Conversion
- Residence Time Distribution Tracer Tests and Non-Ideal Flow Diagnosis

Day 3: Multiple Reactions, Energy Balances and Heat Removal

- Parallel and Series Reaction Networks: Instantaneous Versus Overall Selectivity
- Selectivity Control by Temperature, Feed Distribution and Reactor Choice
- Non-Isothermal Energy Balance and Adiabatic Temperature Rise Calculation
- Heat Removal Options: Jacket, Internal Coil, Interstage Cooling and Cold-Shot Quench
- Thermal Runaway Awareness: Heat Generation Versus Removal Curves and Hot Spot Triggers

Day 4: Catalytic Reactors, Catalyst Selection and Deactivation

- Fixed Bed, Fluidised Bed and Trickle Bed Reactor Selection Criteria
- Catalyst Selection Matrix: Activity, Selectivity, Stability, Particle Shape and Size
- Pore Diffusion Limits: Thiele Modulus and Effectiveness Factor
- Deactivation Mechanisms: Poisoning, Sintering, Coking and Fouling Signatures
- Regeneration by Coke Burn-Off and Guard Bed Protection Against Poisons

Day 5: Reactor Performance Monitoring, Troubleshooting and Workbook Build

- Performance Monitoring: Weighted Average Bed Temperature, Pressure Drop and Activity Trends
- Troubleshooting Cases: Channelling, Liquid Maldistribution, Hot Spots and Selectivity Loss
- Modelling Exercise: Sizing a CSTR Train and a PFR for a Petrochemical Duty
- Modelling Exercise: Catalyst Shortlist and Cycle Length Estimate for a Hydrogenation Service
- Reactor Sizing and Catalyst Selection Workbook Assembly and Peer Review

Skills You Will Gain:

- Kinetic Data Regression
- Ideal Reactor Sizing
- Residence Time Distribution Analysis
- Selectivity Optimisation
- Reactor Heat Balance Assessment
- Catalyst Deactivation Diagnosis
- Catalyst Vendor Evaluation
- Catalytic Bed Performance Trending

Why Attend This Course:

- Return with a Reactor Sizing and Catalyst Selection Workbook of checked calculations for a petrochemical or chemical duty
- Challenge licensor and catalyst vendor claims on conversion, selectivity and cycle length with your own kinetic and diffusion estimates
- Recognise early signs of hot spots, channelling and catalyst decline before they cost run length or safety margin
- Exchange reactor and catalyst practice with engineers from refining, petrochemicals, fertilisers and specialty chemicals

Conclusion:

Reactor performance decides how much feed becomes saleable product and how long a catalyst charge lasts. The one week move from kinetics, rate laws and conversion measures through batch, CSTR and PFR sizing, multiple reactions, energy balances and heat removal, to fixed, fluidised and trickle bed reactors, catalyst selection, deactivation and regeneration. The final day applies these methods to monitoring and troubleshooting cases and closes with a Reactor Sizing and Catalyst Selection Workbook ready for technical review at work.