Questions for state doctoral exam – field of study: Chemical and Process Engineering
Topic: Reactor and Bioreactor Engineering
Subtopics: Chemical Reactors (1 - 8) and Bioreactors (9 - 16)

1. Basic definition: reaction rate and its variants (component rate, reaction rate based on reactor volume, catalyst weight or number of active centers), stoichiometry, reaction range, reactant conversion, key component, excess, selectivity, product yield.

2. Reaction kinetics, reaction mechanisms, heterogeneous catalysis at one and two active centers (Langmuir-Hinshelwood, Eley-Rideal), Langmuir adsorption isotherm for a multicomponent system. Steady state assumption for intermediates, rate limiting step. Dependence of reaction rate on temperature and reactant concentration, inhibition. Derivation of the reaction mechanism and evaluation of parameters from the measured data. Mechanisms and kinetics of catalyst deactivation.

3. Lateral (parallel) and subsequent (serial) reactions, optimization of the yield of the desired product by means of temperature and residence time in the reactor.

4. Reaction equilibrium. Dependence of equilibrium constant on temperature and pressure, calculation from tabulated data. Expression of equilibrium constant in activities, molar fractions and partial pressures. Combined effect of reaction kinetics and equilibrium on conversion.

5. Mathematical models of tubular flow reactor: mass and enthalpy balances, change of flow velocity along the reactor, piston flow, axial dispersion and heat conduction, Danckwerts boundary conditions, radial gradients, heterogeneous and pseudohomogeneous models with accumulation and steady state, pressure drop . Ideally mixed flow and batch reactor models.

6. Distribution of delay times in flow reactors - distribution function, probability density. Excitement and response method. Description of real devices, axial dispersion coefficient, Péclet's diffusion criterion, cascade of ideally stirred reactors.

7. External mass and heat transfer, transfer coefficients and their calculation from criterion equations. Use of transfer coefficients and transmittance in heterogeneous reactor models. Influence of interfacial surface, flow rate and temperature. Description for the reaction limited by external mass transfer.

8. Internal diffusion in a porous catalyst, volume and Knudsen diffusion, calculation of effective diffusivity, influence of component molar mass, pore size, porosity, curvature, temperature and pressure. Reagent balance within the porous catalyst, dimensionless Thiele modulus, efficiency factor.

9. Cell types, eukaryotic and prokaryotic cells, cell structure, chemical composition of cells, from DNA to protein, cell cycle phase, cell energy acquisition, microbial growth energy.

10. Distribution of enzymes, enzyme reactions, kinetics of enzyme reactions, inhibition of enzymes, influence of pH, ionic strength, temperature.

11. Immobilized enzymes and microbial cells, methods of immobilization, the effect of immobilization on the kinetics of enzyme reactions. Mass transport in systems with immobilized biocatalysts, limiting processes.

12. Kinetics of microbial growth and production of metabolites, models of microbial growth.

13. Cell movement and chemotaxis, mathematical model of chemotaxis in a spatially one-dimensional system. Types of microbial interactions, mathematical models of microbial interactions, competition and the effect of chemotaxis, predator-prey systems.

14. Reactors with enzymes and microbial cells and with enzymes, examples of reactor use, phenomena affecting reactor operation, ideal reactor operation.

15. Mass and heat transfer in bioreactors, oxygen transport and its solubility, kLa.

16. DNA and protein technologies. DNA sequencing, DNA amplification, cDNA libraries, genetic engineering, gene editors.

Recommended literature:

Gilbert Froment, Juray DeWilde, and Kenneth Bischoff: Chemical Reactor Analysis and Design Charles G. Hill: An Introduction to Chemical Engineering Kinetics & Reactor Design
Scott H. Fogler: Elements of Chemical Reaction Engineering
Blanch H.W., Clark, D.S., Biochemical Engineering, Marcel Dekker, New York, 1997.
Alberts B. et al., Molecular biology of the cell, Abingdon, 5th edition, 2008.