COURSES ON CATALYSIS AND RELATED SUBJECTS
IN THE MAIN RUSSIAN UNIVERSITIES

CONTENTS

MOSCOW

MOSCOW STATE UNIVERSITY

CHEMISTRY DEPARTMENT

Specialized courses in catalysis

I. Theoretical foundations of catalysis

Course duration: 36 hours

Lecturer: Professor S. A. Borisenkova

1. Conditions of catalytic reactions passing. Chemical kinetics and catalysis.
2. Areas of catalysis (heterogeneous catalysis; homogeneous catalysis; micro-heterogeneous catalysis).
3. Mechanisms of catalytic action of main catalysts groups (acid-base catalysis; metal-complex catalysis; enzymatic catalysis; catalysis by metals; catalysis by oxides; interphase catalysis; catalysis on membranes; catalysis by transition metal complexes with polymer matrices).
4. Development of theoretical concepts in catalysis.
5. Evolutionary catalysis.

II. Catalytic complexes and systems

Course duration: 36 hours

Lecturer: Professor A. P. Rudenko

1. System approach in kinetics and catalysis.
2. Activated processes. Transient states in catalysis and intermediate surface compounds.
3. Theory of transient state. Quantum-mechanical interpretation of the activation energy according to Eyring and Polany.
4. Theory of the absolute reaction rates.
5. Compensation effect theory.
6. Mechanisms of catalytic action.

III. Methods of catalytic investigation and experimental techniques

Course duration: 56 hours

Lecturer: Associate Professor I. I. Kulakova

1. Kinetic study of catalytic reactions (static method, dynamic method, types of reactors; investigation of catalytic reactions in liquid phase, types of reactors;

methods of evaluation of catalytic reaction rate; basics of mathematical planning and kinetic experiment optimization ; modeling of complex processes kinetics).

2. Specific methods for investigation of reactions and catalysts kinetics (kinetic constants measurement; methods for studying a catalysts surface; application of optical and electron microscopy for investigation of solids; characterization of acid properties of solid catalysts and sorbents surface; study of adsorbate–adsorbent interaction with thermodesorption method; application of spectral methods in studying catalysts, catalytic complexes and reaction products; application of radioactive and stable isotopes in catalytic studies; electrochemical methods in catalytic studies; investigation of kinetics and reaction mechanisms at elevated and low pressure in static and flow systems).

Literature:

1. A. A. Balandin. Multiplet theory of catalysis. Part I, Moscow State University, 1963; part II, Moscow State University, 1964; part III, 1970.
2. A. A. Balandin. Present state of multiplet theory. Moscow, Nauka, 1986.
3. V. I. Kuznetsov. Development of catalytic science. Moscow, Nauka, 1964.
4. G. K. Boreskov. Heterogeneous catalysis. Moscow, Nauka, 1986.
5. G. K. Boreskov. Catalysis. Novosibirsk, Nauka, 1971.
6. O. M. Poltorak. Lectures on heterogeneous catalysis theory. Moscow, Moscow State University, 1968.
7. Modern problems of physical chemistry. Vol. 3, Moscow, Moscow State University, 1963.
8. S. L. Kiperman. Introduction to kinetics of heterogeneous catalytic reactions. Moscow, Nauka, 1964.
9. S. L. Kiperman. Foundations of chemical kinetics in heterogeneous catalysis. Moscow, Khimia, 1974.
10. Henrici Olive G., Olive S. Coordination and catalysis. Moscow, Mir, 1980.
11. Ch. Satterfield. Practical course of heterogeneous catalysis. Moscow, Mir, 1984.
12. A. Nakamura, M. Tsutsui. Principles and application of homogeneous catalysis. Moscow, Mir, 1983.
13. L. Hammet. Basics of physical organic chemistry. Moscow, Mir, 1972.
14. M. I. Shakhparonov. Mechanisms of fast processes in liquids. Moscow, Vyschaya Shkola, 1980.
15. P. Bonchev. Complex formation and catalytic activity. Moscow, Mir, 1975.
16. I. I. Ioffe, L. M. Pismen. Engineering chemistry of heterogeneous catalysis. Leningrad, Khimia, 1972.
17. J. Squires. Practical chemistry. Moscow, Mir, 1971.

18. J. Youngers, S. Satius. Kinetic methods in chemical processes investigation. Leningrad, Khimia, 1972.
19. L. C. Polan, M. Ya. Goldenberg, A. A. Levitsky. Computational methods in chemical kinetics. Moscow, Nauka, 1984.
20. S. Greg, K. Sing. Adsorption, specific surface and porosity. Moscow, Mir, 1970.
21. Experimental methods of catalytic studies. Ed. R. Anderson. Moscow, Mir, 1972.
22. J. Thomas, U. Thomas. Heterogeneous catalysis. Moscow, Mir, 1969.
23. R. E. Eishens, V. Pliskin. – In Catalysis. Catalyst surface investigation. Moscow, IL, 1960.
24. S. R. Morrison. Chemical physics of solid surface. Moscow, Mir, 1980.

Course on chemical kinetics and catalysis for students of a selected physico-chemical group (1996-1997)

Course duration: 64 hours (6th semester)
Lecturer: Professor B. V. Romanovsky
Laboratory of Kinetics and Catalysis

I. Phenomenological kinetics

1. Main notions of chemical kinetics: ordinary and complex reactions, elementary reactions, molecularity of reaction, reaction rate.
2. Direct and reverse problems in chemical kinetics. Kinetic equation, kinetic curve.
3. Phenomenological kinetics of ordinary chemical reactions. Mean life, period of semiconversion.
4. Experimental methods for estimation of reaction rate. Reaction order, ways of its determination. Observed (experimental) rate constant.
5. Kinetics of chemical reactions in static, flow and nongradient reactors.
6. Dependence of chemical reaction rate on temperature. Arrenius equation. Activation energy, preexponential multiplier. Methods for estimation of activation energy, observed (experimental) and actual activation energy. Polythermal kinetics.
7. Mechanism of complex reactions. Principle of independence, principle of detailed equilibrium.
8. Linear-independent reactions, stoichiometric Gibbs rule. Stoichiometric matrix. Stoichiometric basis of complex reaction.
9. Mathematical model of complex chemical reactions. Methods of solving direct kinetic problem for complex reactions.
10. Kinetics of reversible, parallel and consecutive reactions.

11. Limiting stage of complex reaction. Quasistationary approximation, Bodenstein method. Applicability conditions of quasistationary approximation. Quasiequilibrium approximation. Route method.
12. Kinetics of enzymatic reactions. Michaelis-Menthen equation. Concurrent and nonconcurrent inhibition.
13. Kinetics of heterogeneous catalytic reactions. Langmour-Hinshelwood equation. Macrokinetics concept, kinetic and diffusion regions.
14. Chain reactions. Reactions of chain formation, continuation and break. Probability of chain break and continuation. Prestationary and stationary kinetics of nonbranched chain reactions.
15. Branched chain reactions. Reactions of branching, probability of chain branching. Chain and heat explosion. Limiting phenomena in reaction of hydrogen and oxygen.
16. Nonstationary processes. Autocatalytic reactions in closed and open systems. Oscillatory reactions.

II. Chemical kinetics theory

1. Thermal and nonthermal activation of molecules, characteristic intervals of energy and nature of active particles.
2. Types of molecular encounters. Energy exchange in flexible and inflexible encounters. Cross section of chemical reaction, microscopic and macroscopic rate constants.
3. Ordinary theory of encounters: basic postulates. Model of rigid spheres, critical energy. Trautz-Luis equation.
4. Theories of active encounters and bimolecular gaseous reactions. Steric factor.
5. Theory of active encounters: monomolecular reactions. Lindemann scheme, models of Hinshelwood, Kassel and Slayter, RRKM theory.
6. Surface of potential energy, experimental and calculating methods of its construction. Molecular clusters method.
7. Theory of activated complex: basic postulates. Reaction path and reaction coordinate. Statistic-thermodynamic calculation of rate constant, Airing equation. Nonadiabatic reactions.
8. Thermodynamic aspect of activated complex theory, free energy, activation enthalpy and entropy.
9. Theory of activated complex: biomolecular reactions, evaluation of steric factor.
10. Theory of activated complex: mono- and trimolecular reactions.
11. Kinetic isotope effect.
12. Chemical reactions in liquid phase. Cage effect. Influence of solvent. Ionic reactions in solutions.

13. Chemical reaction in imperfect solutions. Broensted-Bierrum equation. Solvation effect, salt effects.
14. Elementary processes in photochemistry. Photoexcitation, photodissociation and predissociation of molecules. Properties of electron-induced molecules, eximers and exiplexes.
15. Photochemical reactions, general laws of photochemistry. Quantum yield.
16. Nonradiating and radiating transitions of electron-induced molecules. Fluorescence and phosphorescence. Fluorescence quenching, Stern-Folmer equation.

III. The basics of catalysis

1. General principles of catalysis. Intermediate compounds in catalysis and principle of energy consistency. Compensation effect. Catalysis and equilibrium.
2. Correlations methods in kinetics and catalysis. Broensted-Polany equation. Linear relations of free energies. Problem of optimal catalyst.
3. Mechanisms of catalytic reactions, stage and united mechanisms. Ion, radical and molecular mechanisms.
4. Mechanisms of acid-basic catalysis, homogeneous general and specific acid catalysis.
5. Homogeneous catalysis with strong acid solutions, Hammet equation. Heterogeneous acid catalysis.
6. Redox homogeneous and heterogeneous catalysis.
7. Catalysis with transition metals complexes. Basolo-Pearson model. Chatt rule.
8. Catalysis with enzymes. Structural organization of enzymes. Adsorption and catalytic centers. Conformation effects. Coenzymes. Mechanisms of enzymatic reactions.

Literature:

1. Lectures
2. N.M. Emmanuel and D.G. Knorre, Course in Chemical Kinetics.
3. I.A. Semiokhin, B.V. Strakhov and A.I. Osipov, Kinetics of Homogeneous Chemical Reactions.
4. P. Etkins, Physical Chemistry, part 2.
5. G.M. Panchenkov and V.P. Lebedev, Chemical Kinetics and Catalysis.
6. E.T. Denisov, Kinetics of Homogeneous Chemical Reactions.
7. G. Airing, S.G. Lin and S.M. Lin, Basics of Chemical Kinetics.
8. O.M. Poltorak, Lectures in Theory of Heterogeneous Catalysis.
9. Physical Chemistry in Question and Answers. Kinetics and Electrochemistry (Editors K.V. Topchieva and N.V. Fedorovich).

10. G.K. Boreskov, Heterogeneous Catalysis.
11. I.V. Beresin and K. Martinek, Basics of Physical Chemistry of Enzymatic Catalysis.

MOSCOW

LUMUMBA RUSSIAN UNIVERSITY OF PEOPLES FRIENDSHIP

DEPARTMENT OF CHEMISTRY

Course "Heterogeneous catalysis"

Course duration: General course for undergraduate students – 36 hours;
Special course for PhD students (Heterogeneous catalysis) – 20 hours

Lecturer: Professor, academician V. M. Gryaznov, Head of the department

1. Definition of catalysis. Classification of catalytic processes. Role of catalysis in industrial processes and environmental safety.
2. Homogeneous catalysis. Kinetics of homogeneous catalysis. Catalysis with acids and bases. Catalysis with complex metal compounds.
3. Heterogeneous catalysis. Catalysis and thermodynamics of chemical reactions. A. A. Balandin multiplet theory of catalysis. Kobosev theory of active ensembles. Thermodynamics of real crystals and catalysis.
4. Catalysis on heterogeneous surfaces. Catalytic poisons and activators. Phenomenon of heterogeneous catalysts modification.
5. Kinetics of heterogeneous catalytic reactions and methods of their investigation. Influence of reagent diffusion on rate and selectivity of heterogeneous catalytic reaction. Hydrogen penetrable membrane catalysts and phenomenon of reactions conjugation over them. Activation energy of heterogeneous catalytic reaction. Principles of mathematical modeling of catalytic processes and reactors.
6. Main types of industrial heterogeneous catalysts (massive, frame and coated metal catalysts; oxide catalysts, zeolite catalysts).
7. Electronic concepts in catalysis.
8. Enzymatic catalysis. Immobilized enzymes and their application.

Literature:

1. A. A. Balandin. Present state of catalytic multiplet theory. Moscow, Nauka, 1986.
2. G. K. Boreskov. Heterogeneous catalysis. Moscow, Nauka, 1986.
3. Ya. I. Gerasimov et al. Physical Chemistry. Vol. 2, Moscow, 1973.
4. O. M. Poltorak. Lectures on heterogeneous catalysis theory. Moscow, Moscow State University, 1968.

Additional literature:

1. V. M. Gryaznov, N. V. Orekhova. Catalysis with noble metals. Dynamic peculiarities. Moscow, 1989.
2. O. V. Krylov, V. F. Kiselev. Adsorption and catalysis over transition metals and their oxides. Moscow, 1981.
3. V. M. Minachev, V. V. Kharlamov. Redox catalysis over zeolites. Moscow, 1990.
4. A. Nakamura, M. Tsutsui. Principles and application of homogeneous catalysis. Moscow, Mir, 1983.
5. O. M. Poltorak, E. S. Chukhray. Physico-chemical principles of heterogeneous catalysis. Moscow, 1971.
6. A. Ya. Rozovsky. Catalysis and reaction medium. Moscow, 1988.
7. Ch. Satterfield. Practical course of heterogeneous catalysis. Moscow, Mir, 1984.

MOSCOW

D. I. MENDELEEV RUSSIAN CHEMICAL TECHNOLOGICAL UNIVERSITY

DEPARTMENT OF GENERAL CHEMICAL TECHNOLOGY

Course "Heterogeneous catalysis and catalytic processes"

Course duration: Lectures – 34 hours, practical course – 20 hours.

Lecturer: Professor V. S. Beskov

1. Principle of catalytic action. Catalysis in industry.
2. Kinetics and mechanism of heterogeneous catalytic reactions. Theory of stationary reaction rates, kinetic models. Catalysts deactivation. Experimental methods of catalysts investigation.
3. Catalyst structure. Processes in porous catalyst granule.
4. Immobilized and pseudofluidized layer of a catalyst. Design of models and analysis of processes in catalyst layer. Reactors for heterogeneous catalytic processes. Choice of industrial reactor and process optimization in it.

Literature:

1. V. S. Beskov, V. Flokk. Modeling of catalytic processes and reactors. Moscow, Khimia, 1991.
2. S. L. Kiperman. Foundations of chemical kinetics in heterogeneous catalysis. Moscow, Khimia, 1974.

MOSCOW

LOMONOSOV MOSCOW ACADEMY OF FINE CHEMICAL TECHNOLOGY

Courses on heterogeneous and homogeneous catalysis

I. Theory of reaction mechanisms and catalysis

Course duration: 52 hours
Lecturer: Professor O. N. Temkin

1. Structure and reactivity of intermediates in noncatalytic and catalytic processes.
2. Nature of elementary stages.
3. Stoichiometric analysis of mechanisms.
4. Mechanism types of complex reactions.
5. Formation of kinetic models of catalytic processes.
6. Methods of hypotheses formulation about the mechanisms of catalytic reactions.
7. Kinetic models of major industrial catalytic processes.

Literature:

1. Reactivity and reaction routes. Ed. G. Klopman. Moscow, Mir, 1977.
2. R. V. Hoffman. Mechanisms of chemical reactions. Moscow, Khimia, 1979.
3. B. Geits, J. Ketsir, G. Shuit. Chemistry of catalytic processes. Moscow, Mir, 1981.
4. G. S. Yablonsky et al. Kinetic models of catalytic reactions. Novosibirsk, Nauka, 1983.

II. Applied catalysis

Course duration: 52 hours
Lecturer: Associate Professor L. G. Bruk
Dr. A. K. Avetisov, Head of Department in Karpov Physical Technical Research Institute

1. Coordination, adsorption and catalysis.
2. Preparation technology of metal complex, oxide and metal catalysts.
3. Regeneration technology of catalysts and formation of reaction nodes.

Literature:

1. I. I. Ioffe, L. M. Pismen. Engineering chemistry of heterogeneous catalysis. Leningrad, Khimia, 1972.
2. Ch. Satterfield. Practical course of heterogeneous catalysis. Moscow, Mir, 1984.
3. Industrial catalysis. Ed. B. Leach, Parts 1 and 2. Moscow, Mir, 1986.
4. O. N. Temkin et al. Acetylene. Chemistry, reaction mechanisms, technology. Moscow, Khimia, 1991.

III. Chemistry and technology of metal complex catalysis

Course duration: 20 hours

Lecturer: Professor O. N. Temkin
Associate Professor L. G. Bruk

1. Principles of chemistry of coordination and metal organic compounds.
2. Activation mechanisms of various molecules.
3. Peculiarities of reaction kinetics in solutions of metal complexes.
4. Mechanisms of catalytic processes.

Literature:

1. O. N. Temkin. Introduction to metal complexes catalysis. Moscow, Moscow Institute of Thin Chemical Technology, 1980.
2. O. N. Temkin. Kinetics of catalytic reactions in solutions of metal complexes. Moscow, Moscow Institute of Thin Chemical Technology, 1980.
3. O. N. Temkin. Chemistry and technology of metal complexes catalysis. (Catalysts and reaction mechanisms.) Moscow, Moscow Institute of Thin Chemical Technology, 1980.
4. O. N. Temkin. Chemistry and technology of metal complexes catalysis. (Chemical catalysts and enzymes. Technological features.) Moscow, Moscow Institute of Thin Chemical Technology, 1980.
5. J. Kolman, L. Higedas, J. Norton, R. Finks. Metal organic chemistry of transition metals. Parts 1, 2. Moscow, Mir, 1989.

ST.-PETERSBURG

ST.-PETERSBURG TECHNOLOGICAL UNIVERSITY

CATALYSTS ENGINEERING DEPARTMENT

Courses on catalysis

I. Theoretical basis of catalysis and catalysts engineering

Course duration: 311 hours (lectures – 90 hours)

Lecturers: Professor E. I. Dobkina
Associate Professor V. I. Deruzhkina

1. Spheres of catalysts application. Kinetics and mechanism of catalytic reactions. Adsorption and catalysis at heterogeneous surfaces.
2. Catalysts interaction with reaction medium. Intermediate compounds. Poisoning mechanism. Structural and energy factors in selection of catalysts. Catalysts preparation. Gibbs' theory of critical germs. Electron state of a crystal and catalyst activity. Fermi level and its role in catalysis.
3. Carrier influence on the catalyst activity. Carriers characterization.
4. General regularities in catalysts selection.
5. Basic principles and technological schemes of catalysts production.
6. Methods for adsorbents and catalysts investigation.

II. Kinetics and mechanism of catalytic reactions

Course duration: 180 hours (lectures – 454 hours)

Lecturer: Professor V. M. Pomerantsev

1. Homogeneous and heterogeneous catalysis. Catalysis by acids and bases. Catalysis by transition metal complexes. Stages of heterogeneous catalytic reactions. Main principles of chemical kinetics. Absolute reaction rates theory. Transient state method. Potential energy surface.
2. Complex reactions. Stationary reactions theory. theory of nonstationary reactions. Chain gas reactions.
3. Adsorption at the ideal homogeneous surface. Theory of real heterogeneous surface of a catalyst.
4. Diffusion kinetics.
5. Kinetics of topochemical reactions.

III. Industrial catalysis

Course duration: 90 hours (lectures – 45 hours)

Lecturers: Professor A. F. Tubolkin

Associate Professor E. A. Vlasov

1. Homogeneous catalysis, advantages and drawbacks, industrial application. Heterogeneous catalysis. Advantages of catalysis on solid catalysts. Classification of catalytic reactors. Kinetic models.
2. Reactors with fixed catalyst layer.
3. Fluidized bed catalysis.
4. The main catalytic industries.

IV. Foundations of engineering and equipment of catalytic industries

Course duration: 247 hours (lectures – 90 hours)

Lecturer: Professor V. E. Soroko

Construction materials of chemical machine building. Corrosion resistance of materials. Choice of material depending on the properties of a medium. Apparatus for liquid-phase processes. Equipment for catalysts drying and calcination. Machines and apparatus for mechanical processes in catalyst production.

Literature:

1. G. K. Boreskov. Heterogeneous catalysis. Moscow, Nauka, 1986.
2. Catalysts engineering. Ed. Prof. I. P. Mukhlenov. Leningrad, Khimia, 1969.
3. Industrial catalysis. Ed. B. Lin. Mir, 1986.
4. G. K. Boreskov. Catalysis. Problems of theory and applications. Novosibirsk, Nauka, 1987.
5. E. B. Stayes. Carriers and coated catalysts. Theory and application. Moscow, Khimia, 1991.
6. Ch. Satterfield. Mass transfer in heterogeneous catalysis. Moscow, Mir, 1984.
7. Ch. Satterfield. Practical course of heterogeneous catalysis. Moscow, Mir, 1984.
8. V. S. Beskov, M. V. Flokk. Modeling of catalytic processes and reactors. Moscow, Khimia, 1986.
9. S. L. Kiperman. Introduction to kinetics of heterogeneous catalytic reactions. Moscow, Nauka, 1964.
10. D. A. Frank-Kamenetsky. Diffusion and heat transfer in chemical kinetics. Moscow, Nauka, 1967.

IVANOVO

IVANOVO STATE CHEMICAL–TECHNOLOGICAL ACADEMY

I. Kinetics and mass transfer in chemical reactions (heterogeneous catalytic reactions)

Course duration: lectures – 51 hours, laboratory – 68 hours, 5 seminars

Lecturer: Professor Yu. G. Shirokov

Catalyst interaction with reaction medium. Kinetic equations. Methods for evaluation the catalysts activity. Mass transfer and heat transfer in heterogeneous catalytic reactions. Diffusion retardation. Influence of catalyst poisoning on the reaction kinetics. Commercial evaluation of catalysts.

II. Catalysts and sorbents

Course duration: lectures – 16 hours, laboratory – 32 hours, students independent work – 42 hours

Lecturer: Professor Yu. G. Shirokov

Mechanism of heterogeneous catalytic reactions. General regularities of catalysts selection. Methods of catalysts and sorbents preparation. Carriers and sorbents. Evaluation of catalysts activity. Development of novel catalysts and catalytic processes. Static and dynamic sorption. Theoretical foundations for preparation of mechanically strong catalysts. Requirements to industrial catalysts. Catalyst productivity. Catalyst life time and regeneration. Present state of catalyst industry in Russia and abroad.

Literature:

1. S. L. Kiperman. Foundations of chemical kinetics in heterogeneous catalysis. Moscow, Khimia, 1979.
2. S. Z. Roginsky. Heterogeneous catalysis. Selected works. Moscow, Nauka, 1979.
3. G. K. Boreskov. Catalysis. Problems of theory and applications. Novosibirsk, Nauka, 1987.
4. G. K. Boreskov. Heterogeneous catalysis. Moscow, Nauka, 1986.
5. Ch. Satterfield. Practical course of heterogeneous catalysis. Moscow, Mir, 1984.
6. Metal catalysts. Ed. D. V. Sokolsky. Nauka, Kaz. SSR, Sib. Otd., 1982.
7. O. A. Malinovskaya, V. S. Beskov, M. G. Slin’ko. Modeling of catalytic processes on porous granules. Novosibirsk, Nauka, 1975.
8. Industrial catalysis. Ed. B. Leach. Mir, 1986.

YAROSLAVL

YAROSLAVL STATE ENGINEERING UNIVERSITY

DEPARTMENT OF GENERAL AND PHYSICAL CHEMISTRY

Courses on catalysis

I. Kinetics and catalysis (part of the course “Physical Chemistry”)

Course duration: 20 hours

Lecturer: Professor E. M. Pliss

II. Kinetics of solid phase reactions

Course duration: 30 hours

Lecturer: Professor, academician G. N. Koshel

III. Kinetics of homogeneous chemical reactions

Course duration: 30 hours

Lecturer: Professor E. M. Pliss

IV. Theoretical foundations of homogeneous and heterogeneous catalysis of organic reactions

Course duration: 30 hours

Lecturer: Professor V. Sh. Feldblum

Literature:

1. G. K. Boreskov. Heterogeneous catalysis. Moscow, Nauka, 1986, 304 p.
2. G. M. Panchenkov, V. P. Lebedev. Chemical kinetic and catalysis. Moscow, Khimia, 1985, 590 p.
3. A. Ya. Rozovsky. Heterogeneous catalytic reactions. Moscow, Nauka, 1980, 323 p.
4. B. Delmon. Kinetics of heterogeneous reactions. Moscow, Mir, 1972, 554 p.
5. A. Nakamura, M. Tsutsui. Principles and application of homogeneous catalysis. Moscow, Mir, 1983, 231 p.
6. S. L. Kiperman. Foundations of chemical kinetics in heterogeneous catalysis. Moscow, Khimia, 1979, 349 p.
7. G. S. Yablonsky, V. I. Bykov, A. N. Gorban’. Kinetic models of catalytic reactions. Novosibirsk, Nauka, 1983, 253 p.

NOVOSIBIRSK

NOVOSIBIRSK STATE UNIVERSITY

Specialized courses in catalysis

I. Catalysis

Course duration: 78 hours
Lecturer: Professor V. A. Likholobov

1. The course is based on the modern concept of the unity of homogeneous, heterogeneous and enzymatic catalysis phenomena.
2. Main causes of catalytic effects, catalyst active site, catalytic cycle. Types of intermediate chemical interactions in catalysis, chemical activation of substances. Peculiarities of catalytic activation of substances with particiaption of gas, liquid and solid catalysts.
3. Factological description of the principles of various catalysts action: acids and bases, metals, metal sulfides, solid organometallic systems, metal clusters, some metal enzymes. Mechanisms of the main processes passing on these catalysts: hydrolysis, isomerization, complete and partial oxidation, hydrogenation, carbonylation, olefin polymerization, reducing oligomerization of carbon monoxide, synthesis of ammonia, hydropurification and reforming, synthesis of methanol, sulfuric acid and some others.
4. Prediction of catalytic action, forecasting the composition of actives sites, methods of their designing. Stages of the development of theoretical concepts in catalysis, modern trends in the methods of catalyst search. Role of computers in these approaches.

Literature:

1. G. K. Boreskov. Heterogeneous Catalysis. Moscow, Nauka, 1986.
2. G. K. Boreskov. Catalysis. Pp. 1, 2. Novosibirsk, Inst. Catalysis Publ., 1971.
3. V. I. Kuznetsov. Development of Catalytic Organic Synthesis. Moscow, Nauka, 1964,
434 p.
4. G. M. Panchenkov, V. P. Lebedev. Chemical Kinetics and Catalysis. Moscow, Khimiya, 1974, 592 p.
5. O. M.Poltorak. Lectures on Heterogeneous Catalysis Theory. Moscow, Moscow State Univ. Publ., 1968, 155 p.
6. I. V. Berezin, K. Martinok. Bases of Physical Chemistry of Enzyme Catalysis. Moscow, Vyschaya Shkola, 1977.
7. G. Henrici-Olive, S. Olive. Coordination and Catalysis. Moscow, Mir, 1980.

8. A. Nakamura, M. Tsutsui. Principles and Applications of Homogeneous Catalysis. Moscow, Mir, 1983.
9. Ch. Masters. Homogeneous Transition-Metal Catalysis. Moscow, Mir, 1983.
10. E. T. Denisov. Kinetics of Homogeneous Catalysed Reactions. Moscow, Vyschaya Shkola, 1978.
11. S. N. Satterfield. Heterogeneous Catalysis in Practice. Moscow, Mir, 1984.
12. I. V. Kozhevnikov. Acid-Base Catalysis. Novosibirsk, Novosibirsk State Univ. Publ., 1991.

Catalysis – seminars:

1. Kinetic Models of Heterogeneous Catalyzed Reactions

Course duration: 80 hours

Lecturer: Dr. V. I. Elokhin

1. Introduction: development of chemical kinetics, definition of the main notions, complexity of the chemical reaction mechanism, the law of acting surfaces for elementary reaction. Physico-chemical requirements to kinetic model as a base for calculation of chemical reactors. Basic principles of ideal and real adsorbed layer. Types of heterogeneity and their influence on kinetic regularities (biographical and induced heterogeneity).
2. Theory of stationary reactions. Hypothesis of quasistationary catalytic reaction. Observed reagents and intermediates, stoichiometric numbers and reaction routes. Route rate. Equation of stages stability. Equation of stationary reactions. Application of the graph theory to stationary reactions with linear mechanism. Structured form of stationary kinetic equation for the reaction of multi-route linear mechanism. Observed order and observed energy of the reaction activation with linear mechanism.
3. Nonstationary kinetic models. Relaxation of the catalytic reactions rate. Types of relaxation, relaxation times, connection of relaxation time and stationary reaction rate, classification of relaxations. Elements of the quality theory of differential equations (related to chemical kinetics). Stability of stationary states. Critical phenomena in chemical kinetics, their interpretation. Estimation of reaction medium effect in kinetic models.
4. Experimental methods of kinetic studies. Static and flow (dynamic) methods, integrated and differential reactors. Models of ideal reactors: ideal mixing and ideal displacing. Methods of studying nonstationary processes. Use of physical methods in kinetic studies.

5. Mass- and heat-transfer in chemical kinetics. Essential laws of mass- and heat-transfer, theory of similarity, criterion dependencies. Regions of process passing in a unit of reaction volume: kinetic, intra- and externally diffusive. Internal diffusion. Model of mass- and heat-transfer of a catalyst granule. Effect of porous structure on the reaction rate. Observed reaction rate, Tile-Zeldovich criterion and degree of usage. External diffusion. Laminar and turbulent modes.
6. Methods of kinetic experiment processing. Initial interpretation of kinetic measurements. Estimation of model parameters, correct formulation of the reverse kinetic problem). Independent and dependent parameters, criteria and algorithms of parameters estimation, fiducial intervals.
7. Practice: 1) PC modeling of typical kinetic dependencies, stationary and nonstationary; 2) Monte-Carlo method for simulation modeling of physico-chemical processes on the catalyst surface.

Literature:

1. G. K. Boreskov. Heterogeneous Catalysis. Moscow, Nauka, 1986.
2. G. S. Yablonskii, V. I. Bykov, A. N. Gorban, and V. I. Elokhin. Kinetic Models of Catalytic Reactions, ***in***: Comprehensive Chemical Kinetics, ed. by R.J.Compton, vol. 32, 1991, p. 396.
3. G.S.Yablonskii, V.I.Elokhin. Kinetic Models of Heteroge neous Catalysis, ***in:*** Perspectives in Catalysis, ed. by J.M.Thomas and K.I.Zamaraev, IUPAC-Blackwell Scientific Publ., 1992, p. 191-249.
4. D.A.Frank-Kamenetskii. Diffusion and Heat Transfer in Chemical Kinetics, N.-Y., Plenum, 1969.
5. O.V.Krylov, B.R.Shub. Far-from-equilibrium Processes in Catalysis, M.: Khimiya, 1990.
6. S.W.Weller. Kinetics of Heterogeneous Catalysed Reactions. Catal. Rev. - Sci. Eng., vol. 34, 1992, p. 227.

2. Kinetics of Homogeneous Catalytic Reactions

Course duration: 16 hours

Lecturer: Professor V. A. Likholobov

1. Methods of rate measurement in solutions. Methods of measurement of fast reactions rates.
2. Influence of a medium on the reaction rate in solutions. Effect of ion force on the rate of reaction between ions and reaction of polar molecules. Sechenov equation.

3. Methods of studying the mechanism of homogeneous catalytic reactions. Kinetic properties of the main types of homogeneous reaction mechanisms (specific and general acid-base catalysis, associative, dissociative, etc.). Application of isotope methods for elucidating the reaction mechanism.
4. Correlative analysis. Description of the influence of the substitute, solvent, reagent nucleophilicity and electrophilicity. Dependence of rate and equilibrium of chemical reactions. Compensation effect. Marcus theory for the reaction of electron and proton transfer.

Literature:

1. E.T.Denisov. Kinetics of Homogeneous Catalyzed Reactions. Moscow, Vyschaya Shkola, 1978.
2. R.W.Hoffmann. Aufklarung von Reactionsmechanismen. Moscow, Khimiya, 1979.

3. Quantum-Chemical Methods in Catalysis Theory

Course duration: 12 hours

Lecturer: Professor G. M. Zhidomirov

1. Place of quantum chemistry in elaboration of catalysis theory. Molecular theory of catalysis.
2. General scheme of quantum-chemical calculation. Atomic basis functions. Nonempirical approach and semi-empirical methods (EHT, ASED, CNDO/2, MINDO/3, MNDO, NDDO/MC), general notion of the density functional method. Molecular orbits of 2-atom molecules, dependence of the 2-atom molecules terms on the inter-atomic distance, influence of electrostatic field. Boundary orbitals, perturbation theory in description of molecules interaction, symmetry limitations in chemical reactions.
3. Simple model approaches to the analysis of molecules activation in catalysis, reactivity indexes method, examples of hydrocarbon molecules activation by acid and base sites.
4. Band and cluster approaches in quantum-chemical studies of heterogeneous catalysts surface, various kinds of cluster approach, “embedding” scheme.
5. Cluster models of Brönsted acid sites (BAS) in aluminosilicates. Experimental methods and theoretical evaluation of BAS force, chemical and structural analysis. Role of NMR and IR methods in BAS studies.
6. Cluster models of Luis acid sites (LAS) of transient oxides of aluminum and zeolites, problem of structure flexibility.

7. Quantum-chemical calculations of interaction of the molecules of NH_3, Py, CO, N_2, H_2O, alcohols, acetylene, ethylene and benzene with BAS in zeolites. Mechanisms of BAS catalysis, problem of structure formation with proton transfer and possible role of synchronous processes.
8. Metastability of zeolites with H-forms, processes of dealuminizing and formation of “more strong” BAS and LAS in zeolites.
9. Cation processes in zeolites demonstrated by an example of zeolites Y and ZSM-5. Formation of metal clusters in zeolite cavities, electron-enriched and electron-deficient states of metal clusters in zeolites, ways of experimental study of such states and theoretical analysis of the reasons of their formation.
10. Selective oxidation site in titano-silicates as an example of catalytically active ion of transition metal located in the lattice position; factor of local structural lability of silicate structure.
11. Selective oxidation site in zeolites ZSM-5 formed at N_2O decomposition. Role of binucleus oxide-hydroxide structures and ways of their formation of extra-lattice structures.
12. Cluster models of structural defects of MgO surface, interaction with H_2, CH_4, H_2O. Homolytic and heterolytic ways of CH_4 activation on the MgO surface modified with chemical additives.
13. Cluster models of various crystallographic planes of the metal with GCK lattice, adsorption positions for the atoms, simple molecules (H_2, CO, NO, H_2O) and fragments at dissociative adsorption of hydrocarbons. Theoretical analysis of the process of hydrocarbons formation from CO and H_2 on the surface of transition metals.
14. Main notions of the structure of metal-complex compounds: valence electrons of transition d-element, neutral and anion ligands, oxidation state, coordination numbers, role of valence cover settlement in chemical activity of the complex. Coordination bond, role of donor-acceptor and dative interaction by the example of coordination of olefins and aromatic ligands. Various mechanisms of molecule activation at coordination. Some typical stages of metal-complex reactions: oxidative coupling (reducing elimination), injection (elimination), dissociative substitution. Catalytic cycle, examples of quantum-chemical calculations of catalytic cycles in metal-complex catalysis. Quantum-chemical calculations of methane activation in metal-complex catalysis.

Literature:

1. S.R.Morrison. Chemical Physics of Surfaces. Moscow, Mir, 1980.

2. V.I.Minkin, B.Ya.Simkin, R.M.Minyaev. Theory of Molecular Structure. Moscow, Vyschaya Shkola, 1979.
3 H.Dunken, V.I.Lygin. Quantenchemie der Adsorption an Festkorperoberflachen. Moscow, Mir, 1980.
4. G. M. Zhidomirov, I. D. Mikheikin. Claster Approximation in Quantum Chemical Investigations of Chemisorption and Surface Structures. INT Ser. Mol. Structure and Chem. Bond, Vol. 9. Moscow, VINITI, 1984.
5. G.Henrici-Olive, S.Olive. Coordination and Catalysis. Moscow, Mir, 1980.
6. I.B.Bersuker. Electronic Structure of Coordination Compounds. Moscow, Khimiya, 1976.

II. Adsorption and Texture of Catalysts

Course duration: 60 hours (lectures – 32 h, seminars – 12 h, practice – 16 h)
Lecturer: Professor V. B. Fenelonov

1. Modern concepts of the structure (texture) and morphology of porous bodies, their classification and modeling based on statistical packing theory, theory of percolation and fractals, etc.; methods of quantitative microscopy; main relations between texture parameters, methods of their estimation and interpretation of the measurements results.
2. Main theories of surface and adsorption phenomena, types of interaction, adsorption thermodynamics, isotherm equations of Gibbs, Langmure, BET, Fauler-Guttenhaim, Hill de Bour, Frenkel-Helsy-Hill and others; adsorption at energetically heterogeneous or fractal surface, peculiarities of adsorption in micropores, at the surface and in the volume of mesopores, regularities of capillary condensation, distribution and redistribution of fluids, modern methods of modeling based on molecular dynamics and Monte-Carlo, methods of experimental study of physical and chemical adsorption, measurements of dispersity, surface and other texture properties.
3. Main properties of porous bodies (heterogeneous catalysts, adsorbents and various ceramics, etc.), typical mechanisms of formation and changing their texture in various conditions (surface, porosity, their distribution and distribution of separate components by size and space, etc.), regularities of colloid chemistry and physics of clusters, peculiarities of mass exchange in porous and dispersed systems (adsorption kinetics and dynamics), use of adsorbents and other porous materials for cleaning and separation of substrates, saving of energy or adsorbed components, damping of fluctuations in concentration, pressure, etc.

Literature:

1. A.W.Adamson. Physical Chemistry of Surface. John Wiley, N.-Y., 1979.
2. M.J.Jaycock, G.D.Parfitt. Chemistry of Interfaces. Ellos Horwood, N.-Y., 1981.
3. D.H.Everett. Basic Principles Colloid Science, Royal Soc. Chem., Kent, 1988.
4. J.K.Rowlinson, B.Widom. Molecular Theory of Capillarity. Oxford Univ. Press, N.-Y., 1989.
5. S.J.Gregg, K.S.W.Sing. Surface Area and Porosity. London, Acad. Press, 1982.
6. V.B. Fenelonov. Porous Carbon Disign. Inst. Catalysis, Novosibirsk, 1995 (in Russian).
7. Characterization of Porous Solids (COPS I-III), eds. K.K.Unger et al. Elsevier, Amsterdam, 1988; 1991; 1994.
8. Preparation of Catalysts. Scientific Bases for the Preparation Heterogeneous Catalysts, ed. by B.Delmon, et al., Elsevier, Amsterdam, 1976; 1979; 1983; 1987; 1991; 1995.

III. Scientific Bases for the Catalysts Preparation

Course duration: 64 hours (lectures – 40 h, seminars – 24 h)
Lecturer: Professor N. A. Pakhomov

1. Problems and objectives of scientific bases for the catalysts preparation. Dependence of the main catalyst properties on preparation conditions. Classification of catalysts by the state of active component and by preparation techniques. Role of catalyst carriers. Requirements to raw materials for catalysts preparation.
2. Physico-chemical bases of the catalysts preparation by precipitation, coating and mechanical mixing techniques.
3. Stage mechanism of hydroxides formation in colloid-chemical precipitation. Basics of the classical theory of crystallization, concepts of the theory of difficultly soluble hydroxides crystallization through the mechanism of directed accumulation. Classification of the levels of hydroxides interaction at coprecipitation.
4. Ways and mechanisms of fixing the predecessors of the active component at the surface of carriers in one- and multi-component catalysts. Types of active component distribution by the carrier granule and ways for its control.
5. Processes passing in thermal treatment of catalysts: thermal decomposition, agglomeration, polymorphous transformations, solid-phase reactions.
6. Factors affecting the depth of interaction between components in the catalysts, prepared by mixing.
7. Basics of the method of the catalyst bulk granulation.

Literature:

1. G.K.Boreskov. Heterogeneous Catalysis. Moscow, Nauka, 1986 (in Russian).
2. V.A.Dzisko. Bases of Methods of Preparation of Catalysts. Novosibirsk, Nauka, 1980
(in Russian).
3. S.N.Satterfield. Heterogeneous Catalysis in Practice. Moscow, Mir, 1984 (in Russian).
4. V.A.Dzisko, A.D.Karnaukhov, J.V.Tarasova. The Physico-Chemical Bases of Synthesis of the Oxide Catalysts. Novosibirsk, Nauka, 1978 (in Russian).
5. O.P.Krivoruchko, R.A.Buyanov. The Development of the Theory of the Low Solubility Hydroxides Crystallization and its Application in the Scientific Bases of Preparation of Catalysts. ***In*** All-Union School on Catalysts. Novosibirsk: Inst. Catalysis, 1981, V.3, p.122-150 (in Russian).
6. Yu.I.Yermakov, V.A.Zakharov, B.N.Kuznetsov. Fixed Complexes on Oxide Carriers in Catalysis. Novosibirsk, Nauka, 1980 (in Russian).
7. Scientific Bases for the Preparation of Catalysts. ***In*** Proceedings of All-Union Meetings. Novosibirsk: Inst. Catalysis. 1984, 1990, 1996 (in Russian).
8. R.A.Buyanov (Ed.). Scientific Bases for the Manufacture of Catalysts. Novosibirsk: Nauka, 1982 (in Russian).
9. G.I.Anderson. Structure of Metallic Catalysts. London-N.Y.- San Francisco: Acad.Press, 1975.
10. Preparation of Catalysts, I, 1975; II, 1979; III, 1983; IV, 1987; V, 1991; VI, 1995., Proc. Intern. Symposiums. Ed. by B. Delmon, P.Grange, P.A.Jacobs and G.Poncelet. Amsterdam: Elsevier.

IV. Physical Methods in Catalyst Studies

1. Fundamentals of EPR and NMR Spectroscopy and their Use in Catalysis

Course duration: 22 hours (lectures – 10 h, practice on recording and analysis of EPR and NMR spectra - 12 h)

Lecturer: Professor E. P. Talsi

1. Main concepts of EPR and NMR spectroscopy (g-factor, chemical shift, constant of superfine splitting, constant of spin-spin interaction, times of spin-spin and spin-lattice relaxation, saturation). Bloch equation for the motion of magnetization vector in magnetic field, also for the case of chemical exchange. Concept of spin Hamiltonian

2. Impulse Fourier spectroscopy. Simple impulse sequences for measuring T_1 and T_2, requirements to duration and intensity of impulses, Fourier transformation, problems in digitizing the free induction drop. Formulae for Overhauser effect. Techniques with polarization transfer: INEPT, DEPT. Review of existing relaxation mechanisms and their contribution to the line width by examples.
3. NMR fine resolution spectroscopy in solids. High-capacity suppression, cross-polarization, magic angle rotation. Principles of analysis of anisotropic EPR and NMR spectra. Examples of application of NMR and EPR spectroscopy to the study of catalyst structure and catalytic reaction mechanism. Practice on registration and analysis of EPR spectra of polycrystalline samples containing V, Cu complexes, as well as ^{1}H and ^{13}C NMR spectra of standard compounds.

Literature (in Russian):

1. A.Carrington, A.D.McLachlan. Introduction to Magnetic Resonance. With Application to Chemistry and Chemical Physics. Moscow, Mir, 1970.
2. A.E.Derome. Modern NMR Techniques for Chemistry Research. Moscow, Mir, 1993.
3. Ch.Slicter. Introduction to the Theory of Magnetic Resonance. Moscow, Mir, 1981.
4. J.E.Wertz, J.R.Bolton. Electron Spin Resonance. Moscow, Mir, 1972.

2. X-ray methods in catalysts study

Course duration: 26 hours (lectures – 14 h, seminars – 12 h)

Lecturer: Professor D. I. Kochubey

1. Fundamentals of the theory of X-ray radiation (radiation, absorption and propagation). Characteristics of the methods oriented to phase analysis, element analysis, morphological analysis of highly dispersed phases, analysis of the charge state and electronic structure. Methods of X-ray diffraction, diffuse X-ray dispersion, small angle dispersion, electron microscopy, EXAFS, XPS and Auger spectroscopy, X-ray emission spectroscopy.
2. Physical basics of these methods, main measured parameters, main experimental techniques, accuracy and sensitivity of the methods, their efficiency.

Literature (in Russian):

1. L.N.Mazalov et al. X-ray Spectra of the Molecules. Novosibirsk, Nauka, 1977.
2. D.I.Kochubey. EXAFS Spectroscopy of Catalysts. Novosibirsk, Nauka, 1992.
3. H.M.Minachev, G.V.Antoshin, E.S.Shpiro. Photoelectron Spectroscopy and its Application in Catalysis. Moscow, Nauka, 1981.
4. Rentgenography of Catalysts. Novosibirsk, Inst. Catalysis Publ., 1977.

3. Optical Spectroscopy in Adsorption and Catalysis

Course duration: 24 hours (lectures – 12 h, seminars – 12 h)
Lecturer: Professor E. A. Paukshtis

1. Optical methods in studying the surface phenomena. Classification of optical methods. Historical review of optical methods application in adsorption and catalysis. The key achievements in adsorption and catalysis based on the use of optical methods.
2. Origin of IR spectra. Methods for registration of IR spectra. Fourier spectroscopy. Main rules of IR spectroscopy (selection rules, notion of characterization, identification of functional groups). Concentration measurements based on IR spectra. Peculiarities of IR spectroscopy of the adsorbed molecules. IR spectroscopy of scattered reflection.
3. Measurement of surface properties on the base of IR spectroscopy data. Method of sounds. Study of the metals and metal cations state. Measurement of acid properties. Measurements of the adsorbed molecules concentration.
4. Mechanistic studies of catalytic reactions. Sample studies of some catalytic processes (hydrocarbons isomerization, bytilamines deamination, methane oxidation, ethylene oxidation).
5. Specific nature of analysing the spectra of catalyst volume (external and internal oscillations, lattice oscillations). Methods for separation the spectra of active component. In situ studies.
6. Other optical methods. Raman spectroscopy. UV-VIS-NIR spectroscopy. Fluorescence.

Literature:

1. G.Hersberg. Infrared and Raman spectra of Polyatomic Molecules. N.-Y, 1945.
2. K.E.Lawson. Infrared Adsorption of Inorganic Substances. N.-Y., Reinold Publ. Corp., 1961.
3. L.H.Little. Infrared Spectra of Adsorbed Species. N.-Y., Academic Press, 1966.
4. M.L.Hair. Infrared Spectroscopy in Surface Chemistry. N.-Y., Dekker, 1967.
5. E. A. Paukshtis. Infrared Spectroscopy for Heterogeneous Acid-Base Catalysis. Novosibirsk, Nauka, 1992 (in Russian).

4. Analytical Chemistry Methods in Catalysis

Course duration: 24 hours (lectures – 12 h, seminars and practice – 12 h)
Lecturer: Professor V. V. Malakhov

1. Characterization of catalyst chemical composition, initial substances and products of catalytic reactions. Element and molecular (phase as well) analysis. Metrology of chemical analysis.
2. Methods of analyzing catalysts and carriers. Chemical and physico-chemical methods: gravimetry, titrimetry, colorimetry, spectrophotometry, electrochemical methods (polarography, potentiometry, ionoselective electrodes as well). Physical methods: optical nuclear spectroscopy, nuclear-absorption spectrophotometry, X-ray spectroscopy (X-ray-fluorescent analysis, microanalysis). Chemical phase analysis of heterogeneous catalysts and carriers. Areas of primary application of various methods of chemical analysis. Special requirements to the methods of chemical analysis. Thermoanalytical methods.
3. Analysis of initial substances and products of catalytic reactions. Main methods of molecular analysis of complex mixtures. Mixtures of organic and inorganic compounds. Chemical, physical and physico-chemical methods of detection, identification, separation and qualitative analysis of compounds: titrimetric, spectral, spectrophotometrical, electrochemical, chromatographic, chromato-mass-spectroscopy. Chromatography as the main method for analyzing the composition of complex mixtures of chemical compounds.

Literature:

1. Analytikum. Leipzig, VEB Verlag fur Grundstoffindustrie, 1971.
2. B.V.Ayvazov. Introduction in Chromatography. Moscow, Vischaya Shkola, 1983 (in Russian).

V. Chemical Engineering in Catalysis

Course duration: 88 hours (lectures – 40 h, seminars – 24 h, computer courses - 24 h)

Lecturer: Dr. S. A. Pokrovskaya

1. Ways of industrial implementation of catalytic processes, types of catalytic reactors.
2. Thermodynamics and kinetics of catalytic reactions.
3. Processes in the catalyst porous granule.
4. Mathematical models of catalytic reactors of various designs, methods of their analysis.
5. Fundamentals of hydrodynamics.
6. Basics of designing and analysis of chemical engineering schemes for industrial implementation of catalytic processes.

7. Review of modern industrial catalytic processes.
8. Computer course:
   - Study of stationary and nonstationary kinetic models of catalytic reactions;
   - Analysis of processes in the catalyst porous granule;
   - Modeling of the processes in the layer of the reactor of of ideal mixing and dislacement; calculation of concentration and temperature fields in the layer, evaluation of the dependence of output characteristics of the process on various parameters of the model, study of transient modes and stability of stationary solutions;
   - Calculation of particular processes in the reactors with the stationary catalyst layer on the base of simplified mathematical models, etc.

Literature:

1. O.Levenspiel. Chemical Reaction Engineering. Moscow, Khimiya, 1969 (in Russian).
2. O.Levenspiel. The Chemical Reactor Omnibook. Oregon State Univ., Corvallis, Oregon, 1993.
3. G.K.Boreskov. Heterogeneous Catalysis. Moscow, Nauka, 1986 (in Russian).
4. Applied Industrial Catalysis. Ed. B.E.Reach. Moscow, Mir, 1986 (in Russian).
5. V.S.Beskov, V.Flock. Modeling of Catalytic Processes and Reactors. Moscow, Khimiya, 1991 (in Russian).
6. D.A.Frank-Kamenezky. Diffusion and Heat Transfer in Chemical Kinetics. Moscow, Nauka, 1987 (in Russian).
7. Mathematical Modeling of Catalytic Reactors. Novosibirsk, Nauka, 1984, 1989 (in Russian).
8. Ch.N.Satterfield. Mass Transfer in Heterogeneous Catalysis. Moscow, Nauka, 1986 (in Russian).
9. R.Aris. Introduction to the Analysis of Chemical Reactors. Leningrad, Khimiya, 1967 (in Russian).
10. General Chemical Engineering. Ed. A.G.Amelin. Moscow, Khimiya, 1977 (in Russian).

VI. Modern Methods for Testing the Catalyst Activity

Course duration: 38 hours (seminars and practice)
Lecturer: Dr. N. N. Bobrov

1. Seminars:

1. Methods for testing the catalytic properties in bench gradientless reactors.
2. Experimental methods for evaluation of catalytic activity as a stationary reaction rate at assigned temperature and composition of the contact reaction mixture.

3. Principles of designing the optimal technologic schemes of the bench catalytic sets.
4. Modern techniques of testing and dosing the gas and steam-gas initial reaction mixtures.
5. Bench catalytic microreactors.
6. Modern techniques of monitoring the compounds and consumption of initial and ultimate reaction mixtures.
7. Automation of catalytic experiments.
8. Practice: model process – deep catalytic oxidation of propane by molecular oxygen at the automated flow-circulation set.

Literature (in Russian):

1. N.N.Bobrov. Experimental Methods of Catalytic Properties Investigations. Novosibirsk, Novosibirsk State Univ. Publ, 1989.
2. N.N.Bobrov, V.V.Arakelyan. Methods and Setups for Industrial Catalyst Activity Testing. Novosibirsk, Inst. Catalysis Publ., 1991.

VII. Computer Applications for Catalytic Studies

Course duration: 60 hours (seminars and practice)
Lecturer: Ing. P. P. Michailenko

1. Computer hardware and software resources.
2. Algorithms and standard programs of mathematical support.
3. Review of methods of numerical solution of chemical problems described by the systems of algebraic, differential equations, equations in partial derivatives.
4. Algorithms and programs of digital processing of stationary and nonstationary kinetic experiments.
5. Programs for evaluation the rate constants and equilibriums of chemicl reactions from experimental data, direct and reverse problems.
6. Methods of processing the graphic information (approximation, smoothing, computer interpolation).
7. Practical application of programming systems.
8. Text editors.
9. Stages of program preparation for execution.
10. Use of graphic stacks.

Literature:

1. E.B.Lazarevich, G.F.Choroshavina. Hardware and Software for Professional PC. Minsk, Vyschaya Shkola, 1991 (in Russian).