

National Academy of Sciences of Ukraine
V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry

PROGRAM

for passing the entrance exams to the postgraduate studies
for studying at the third (educational and scientific) level of higher
education

Doctor of Philosophy (PhD)

in the specialty **E3 Chemistry**,
specialization in petrochemicals and coal chemistry

Kyiv - 2025

Approved by the Academic
Council
Institute of Bioorganic Chemistry
and Naftochemistry V.P. Kukhar
NAS of Ukraine
from 08 May 2025,
Protocol No. 6

Explanatory note

The purpose of the entrance examination for postgraduate studies in the specialty E3 Chemistry (specialization "Petrochemistry and Coal Chemistry") is to determine the level of theoretical knowledge and practical skills of applicants acquired during their studies at the educational degree / specialist / master's level in order to form a rating list and competitive selection of applicants for higher education of the degree of Doctor of Philosophy in the specialty E3 Chemistry within the license volume of the Institute.

Form of professional entrance test

The professional entrance exam is held in two stages. Written - applicants answer the questions of the exam ticket in writing on paper with the seal of the Institute. The written stage lasts 60 minutes. Oral - an interview on the questions of the exam paper and research proposal.

Structure of the exam ticket

The professional entrance exam ticket contains 3 theoretical questions. The questions in the tickets are formed on the basis of this program.

Requirements for the applicant's answer

The questions assess the applicant's knowledge of the basic professional disciplines that are necessary for the correct expression of certain concepts, as well as for understanding a wide range of theoretical and practical tasks, and possession of skills required for professional activities within the program. The correctness of the tasks is assessed in accordance with the criteria for assessing knowledge.

criteria

The assessment of the applicant's response to the postgraduate program is based on the level of his or her preparedness for research and experimental activities in the field of petrochemistry and coal chemistry.

Each question of the ticket and research proposal is evaluated on a 100-point scale. The total score is determined as the arithmetic mean of the sum of the scores for all questions.

Scale of evaluation: national and ECTS

Sum of points for all types of learning activities	ECTS evaluation	Score on the national scale
		for the exam, practice, differentiated test
90 - 100	A	excellent
82-89	B	well
74-81	C	
64-73	D	satisfactorily
60-63	E	
35-59	FX	unsatisfactory with the possibility of reassembly

0-34	F	unsatisfactory with mandatory re-study of the discipline
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90-100 - "excellent". The applicant presents the program material in a reasoned and complete manner. In his answers, he relies on the research of scientists, uses the methods of comparative analysis, generalization, gives examples, proofs. Consciously, accurately, and fully presents the program material in writing; highlights the main points. Shows a creative approach to revealing the essence of phenomena. Skillfully combines the acquired knowledge, skills, abilities with practice. Excellent performance of the task with only a small number of errors

74-89 - "good". The entrant shows knowledge of the course content. Gives examples when reproducing the program material, but lacks a creative approach to solving the problem. Shows knowledge of the course content, but does not fully reveal the essence of the phenomena. Correctly uses knowledge, skills, abilities only in standard situations.

60-73 - "satisfactory". The applicant makes mistakes in the answers and has difficulties in eliminating them. The answers to the questions are not complete. Has difficulties in applying the acquired knowledge, skills and abilities in practice. In general, the program material is partially mastered.

0-59 - "unsatisfactory". Has difficulty in explaining the content of basic concepts. Makes a significant number of mistakes in the reproduction of program material. Has a poor command of basic concepts, reveals the essence of phenomena, concepts at the level of reproduction. Cannot combine the acquired knowledge with practice. Answers to questions are fragmentary, do not reflect the essence of the problem.

Program content

Section 1.

PETROCHEMICALS

1. Elements of theoretical foundations of petrochemical synthesis

Chemical reaction at the molecular level. Stable substances and intermediates. Material balance of chemical reactions. Stoichiometric analysis. Basic concepts of chemical kinetics. Kinetic model of a chemical reaction. Construction of kinetic models of reactions involving stable substances. Experimental setups for studying the laws of chemical reactions: ideal batch reactor; continuous reactors. The course of simple reactions in continuous reactors. First-order reaction. Irreversible second-order reaction involving two reagents. Equilibrium reaction. Kinetics, composition of products and selectivity of complex reactions. Integral method of analysis of kinetic curves. Selection of conditions for simple reactions.

2. Raw materials and starting materials of basic organic and petrochemical synthesis.

Basic organic and petrochemical synthesis industry, its main features and development prospects. Main types of products: , monomers, plasticizers and auxiliary substances, synthetic fuels and oils, , solvents, pesticides.

3. Starting substances. Alkanes, their technical properties and application.

Separation of lower alkanes from natural and associated gases. Calorific value, pour point, anti-detonation properties. Deparaffinization of oil fractions. Ways of using *n-paraffin* hydrocarbons. Isomerization of paraffins.

4. Alkenes, their technical properties and applications.

Theory of pyrolysis reactions. Technology of hydrocarbon pyrolysis, equipment and schemes of pyrolysis and gas separation, directions of process development. Thermal cracking of alkanes. Characterization of alkene fractions, their purification, processing of butylene and amylene fractions. Acid polymerization of alkenes and the products obtained. Organometallic synthesis of alkenes and its products. Disproportionation and metathesis of alkenes.

5. Aromatic hydrocarbons, their technical properties and applications.

Aromatic hydrocarbons of pyrolysis. Theoretical foundations and technology of reforming processes, products obtained. Separation of aromatization products and their purification. Characterization of aromatic hydrocarbon fractions. Isomerization of polymethylbenzene and their separation. Preparation of benzene and naphthalene by dealkylation processes. Preparation of benzene and *para*-substituted dialkyl benzene by disproportionation of the corresponding monoalkyl benzene.

6. Cycloalkane hydrocarbons, their technical properties and applications.

Cycloalkanes as constituents of all oils and oil fractions, structure of the main classes of cycloalkane hydrocarbons. Solid cycloalkanes. Adamantane. Technical properties: calorific value, anti-detonation properties and viscosity characteristics. Ability to oxidize.

7. Diene hydrocarbons.

Diene hydrocarbons with isolated and conjugated double bonds. The most important representatives of dienes with conjugated bonds: the ability to polymerize and copolymerize, to add sulfur oxide, hydrogen, halogens and halogenated hydrocarbons. Methods of obtaining diene hydrocarbons, the main ways of their application in industry.

8. Acetylene, its technical properties and applications.

Production of acetylene from calcium carbide and its purification. Theoretical foundations and methods of acetylene production from hydrocarbons. Technology of acetylene production and separation.

9. Carbon monoxide and synthesis gas, their technical properties and applications.

Theoretical foundations and methods of hydrocarbon conversion. Technology of synthesis gas production and its purification. Production of concentrated carbon monoxide.

10. Halogenation processes.

Halogenation processes.

Classification of reactions, their energy characteristics. Halogenating agents. Labor protection in the process of halogenation.

Chlorination of alkane hydrocarbons and their chlorine derivatives. Process theory and methods of chlorination. Products of liquid-phase chlorination, selection of parameters, types of reaction apparatus and process technology. Products of gas-phase chlorination, selection of parameters, types of reaction apparatus.

Chlorination of alkenes. Products and technology of substitutional chlorination of alkenes. Theory and products of additive chlorination of alkenes. Selection of parameters. Types of reaction apparatus and process technology. Processes of alkene chlorination, their theoretical basis and technology.

Chlorination of acetylene. Products and technology of additive chlorination of acetylene. Theory and technology of synthesis of vinyl chloride from acetylene.

Chlorination of aromatic compounds. Theoretical foundations and technology of chlorination into the aromatic core. Side-chain chlorination and additive chlorination, theory

and technology of these processes. Products obtained by chlorination of aromatic compounds.

The reaction of chlorinated hydrocarbon derivatives, combined and combined processes. Technology for the synthesis of vinyl chloride from ethylene, other applications of combined and combined processes.

Chlorination of other organic compounds. Theoretical basis, products and technology of chlorination of alcohols, carbonyl compounds, carboxylic acids, acid amides. Synthesis of phosgene.

Fluoridation processes. Fluoridation with elemental fluorine and metal fluorides, theory and technology of the process. Fluoridation with hydrogen fluoride, theoretical basis of the process. Technology of freon production. Organofluorine monomers and methods of their preparation.

11. Catalytic splitting of hydrocarbons.

Catalytic cracking: raw materials, purpose, catalysts, conditions of implementation, technology, main reactions, products. Cracking parameters and their impact on product distribution. Evolution of views on the mechanism of cracking: β - and α -decomposition. Fundamentals of J. Ohl's theory.

Hydrocracking: raw materials, purpose, catalysts, reaction conditions, technology, process parameters, products, main reactions. Hydrogenolysis. Mechanism of hydrocracking.

12. Processes of hydrolysis, hydration, dehydration, esterification and amidation

Classification of reactions. Hydrolyzing agents and catalysts. Hydrolysis and alkaline dehydrochlorination of chlorine derivatives, theory of these reactions, products and types of reactors. Technology of epichlorohydrin production.

Esterification, process theory and main products. Types of reactors and technology of esterification with carboxylic acids, acid anhydrides and chlorohydrates. Amidation reaction. Dehydration, hydrolysis and esterification of amides. Hydrolysis of nitriles. Technology for the preparation of methyl methacrylate. Isocyanates, carbamates and dithiocarbamates. Production of melamine.

Sulfuric acid hydration of alkenes. Theory of synthesis of sulfates from alcohols and alkenes, influence and choice of parameters. Surfactants such as alkyl sulfates, properties and applications, technology of their production. Hydrolysis of alkyl sulfates and products of sulfuric acid hydration. Types of reactors and production technology.

Direct hydration and dehydration processes. Theory of direct dehydration of alkenes, selection of conditions. Technology of ethanol production. Hydration of acetylene, theoretical foundations, methods and reaction equipment. Dehydration reaction with the formation of esters and saturated substances, process methods and products. Dehydration of carboxylic acids, acetic anhydride and ketene.

13. Alkylation processes.

Classification of reactions and their energy. Alkylating agents.

Alkylation by carbon atom. Theory of alkylation reactions of aromatic hydrocarbons, selection of conditions. Products and methods of alkylation, reaction apparatus. Technology of alkylbenzene production. Alkylation of phenols, choice of conditions. Alkylphenols and technology of their production. Chemistry and technology of alkylation of isoalkanes: purpose of the process, catalysts, environmental aspects, promising (solid) alkylation catalysts.

Alkylation by oxygen, sulfur, and nitrogen atoms. The theory of these reactions and the products obtained. Selection of conditions and types of reactors. Technology of amine synthesis.

Processes of β -oxyalkylation and other reactions of α -oxides. Chemistry and theoretical basis of the oxyethylation reaction, selection of conditions. Ethylene oxide and propylene

oxide processing products, nonionic surfactants. Types of reactors and technology of oxyalkylation processes. Other syntheses based on α -oxides.

Vinylization processes. Chemistry and theoretical basis of the process. Technology of vinyl acetate production. Acetylene oligomers and their synthesis. Vinylation of amides and carbazole.

Alkylation by atoms of other elements. Direct synthesis of organochlorosilanes, reactors and process technology. Organosilicon monomers and other products. Theoretical basis and technology of synthesis of aluminum trialkyls, their application. Production of tetraethyl lead.

14. Sulphurization and nitration processes

Sulfation of aromatic compounds, process theory, sulfating agents. Selection of conditions and types of reactors. Sulfonation products, surfactants such as alkylarylsulfonates, technology of their production.

Sulfonation of alkanes, chemistry and theoretical foundations of sulfochlorination and sulfoxidation reactions. Surfactants such as alkyl sulfonates and their production technology.

Nitration. Chemistry and theoretical foundations of nitration of aromatic compounds, technology of synthesis of nitro compounds. Nitration of alkenes and acetylenes. Chemistry and technology of alkene nitration. Nitroalkanes.

15. Oxidation processes

Classification of reactions, oxidizing agents. Energy characteristics of reactions. Labor protection in oxidation processes.

Homogeneous oxidation processes. Scientific and engineering fundamentals of homogeneous oxidation processes, mechanism, kinetics and catalysis, process selectivity, selection of conditions and reactors. Liquid-phase oxidation of *n-butane* and gasoline. Technology for the production of synthetic fatty acids. Oxidation of cycloalkanes, basic laws of the process, products obtained. Technology of oxidation of cyclohexane and production of adipic acid. Cyclic ketones and aliphatic dicarboxylic acids. Oxidation of aldehydes, basic laws of the process and products. Production of acetic acid. Technology of combined production of acetic acid and acetic anhydride. Oxidation of hydrocarbons to hydroperoxides, basic laws of the process. Technology of hydroperoxides production. Acid cleavage of alkylbenzene hydroperoxides, theory and methods of reactions. Technology of cumol method of phenol and acetone synthesis. Other methods of phenol production and their comparison. Oxidation of side chains of aromatic compounds and carboxylic acids, basic reaction laws and products. Technology for the preparation of dimethyl terephthalate. Other methods for the preparation of aromatic polycarboxylic acids.

Heterogeneous catalytic oxidation processes, their mechanism, kinetics and catalysis, selectivity, choice of conditions and type of reaction apparatus. Oxidation of alkenes at the saturated carbon atom, basic laws of the process and the products obtained. The oxidative ammonolysis reaction, its theoretical basis, regularities and products. Technology of acrylonitrile production. Hydrocyanic acid. Vapor-phase oxidation of aromatic compounds into acid anhydrides, basic laws of the process and products. Technology of ethylene oxide production, comparison of methods of its production.

Oxidation of alkenes with metal complex catalysts. Epoxidation reaction, its scientific basis and regularities. Combined syntheses based on epoxidation with alkenes, their technology. Oxidation of alkenes with a palladium catalyst, theoretical foundations and regularities of the process. The products obtained and their production technology.

16. Dehydration and hydrogenation processes.

Classification of reactions, their thermodynamics. Mechanisms, catalysis and kinetics of reactions. Fundamentals of selection of hydrogenation and dehydrogenation parameters.

Dehydration processes. Dehydration and oxidative dehydration of alcohols. Basic laws of the process and the products obtained. Technology of formaldehyde production. Dehydrogenation of alkyl benzene, chemistry and methods of obtaining styrene and its homologues. Technology of styrene production. Dehydration of paraffins, basic laws of the process. Comparison of methods for the production of divinyl and isoprene. Technology of two-stage production of butadiene and isoprene. One-step process and its regularities. Technology of separation of mixtures and isolation of dienes. Processes of oxidative dehydrogenation of alkanes.

Hydrogenation processes. Chemistry and basic laws of hydrogenation reactions. Hydrogenation of hydrocarbons by double, triple and aromatic bonds. Aromatic hydrogen redistribution reactions. Hydrogenation and selective hydrogenation of alcohols, carbonyl compounds, nitriles, nitro compounds. Reaction of hydroammonolysis. Destructive hydrogenation. Technology of hydrogenation processes. Liquid-phase hydrogenation, its parameters and types of reactors. Technology of obtaining higher alcohols from acids. Gas-phase hydrogenation, its parameters and types of reactors. Technology of hydrogenation of benzene into cyclohexane. General features of hydrogenation technology.

17. Syntheses based on carbon monoxide.

Classification of reactions. Syntheses from carbon monoxide and hydrogen, their conditions and products. Theoretical basis and technology of methanol production.

Oxosynthesis, its chemistry and theoretical foundations, and the products obtained. Selection of conditions and schemes of aldehyde oxosynthesis reaction units. Process technology.

Carboxylation processes, chemistry and theoretical basis of the reaction. Carboxylation of alcohols and esters. Preparation of formic acid and its esters.

Condensation on the carbonyl group. Classification of reactions, their theoretical basis.

18. Acid-catalytic processes.

Condensation of carbonyl compounds with aromatic compounds, chemistry and reaction products. Technology of synthesis of DDT and diphenylpropane. Chloromethylation reaction. Synthesis of acetals and the Prince reaction. Chemistry and technology of isoprene production from butylene. Condensation of carbonyl compounds with nitrogenous bases, chemistry and reaction products. Synthesis of oximes and their rearrangement into lactams. Technology of caprolactam production, other methods of its production.

19. Basic catalytic processes.

Chemistry of aldol condensation, products obtained. Selection of reaction conditions and types of reactors. Production technology of 2-ethylhexanol and pentaerythritol. Synthesis of cyanhydrides and vinyl pyridines. Alkynol synthesis, chemistry and process technology, products obtained. Alkylation of toluene with methanol at the methyl group.

20. Metathesis reaction.

Metathesis of alkenes: catalysts, mechanisms. Main types of metathesis reactions. Industrial processes.

21. Cluster catalysis

Cluster catalysis: concept of metal clusters, examples of catalytic mechanisms.

22. Alternative raw materials for petrochemical synthesis

Methods of processing coal into hydrocarbon feedstock (thermal dissolution, liquefaction, destructive hydrogenation). Coal gasification. Semi-coking and coking. Coke tar is a source of aromatic raw materials. Coal is an alternative to oil and natural gas as a raw material for the petrochemical industry. Use of carbon monoxide in the production of fuels and petrochemical feedstocks. The Fischer-Tropsch process. Modern understanding of the mechanism of the Fischer-Tropsch process. Methanol is a fuel and raw material for petrochemical synthesis. Conversion of methanol to hydrocarbons. Simple methyl esters - additive to gasoline.

Biological resources are potential raw materials for organic and petrochemical synthesis.

23. Biofuels

Biodiesel fuel. The initial raw materials. Chemistry of technological processes. Biobenzines. Feedstocks of biofuels. Gasoline formulations. Pros and cons of using biofuels.

Section 2: Coal chemistry

1.Introduction

Solid fuels are a source of heat and electricity and chemical raw materials. Brief history of the development of chemical fuel technology. The most important deposits of fossil . Resources of fossil fuels in Ukraine and around the world. Production and consumption of various types of fossil fuels in Ukraine and other countries.

Prospects for the development of mining and thermal processing of various types of fossil fuels in Ukraine. The main directions and methods of processing fossil fuels to produce high-quality fuels and chemical raw materials.

a. Chemistry of solid fossil fuels (SFC)

General taxonomy of different HCS and their defining features (peat, lignite, coal, anthracite, sapropels, bogs, oil shale). Stages of development THC (peat, lignite,). The origin of THC. Carbonaceous components. Origin of petrographic components. Origin of humus coal and sapropels. Mixed coal. Striped coal.

Known methods of classification of fossil coals (Potonier, Zhemchuzhnikova, Ginzburg, Stadnikova, Gruner, Stops, Karavayeva, etc.). Characterization of TGC according to their technical analysis. Moisture, mineral components and ash content of coal. Yield of volatile substances from THC. Characterization of solid non-volatile residue. Total sulfur and types of sulfur compounds in coal. Conditional and true organic (combustible) weight of coal. The relationship between technical analysis data and the chemical nature, maturity and composition of fossil fuels.

Characterization of THC by elemental analysis. The relationship between elemental analysis data and the chemical nature of THC. Classification of coal by elemental composition. Elemental composition and calorific value of THC.

Interaction of THC with various solvents and . Effect on THC of various organic solvents (benzene, anthracene oils, pyridine, etc.) and chemical reagents (mineral acids, alkalis, halides, etc.). Group chemical composition of different types of THC. Humic acids. Mountain waxes. Bitumen. Coal thermal bitumen.

Molecular structure of THC. Physical and physicochemical research methods (X-ray diffraction analysis, electron and optical microscopy, , EPR, NMR, dielcometry). Study of physical, mechanical, thermal and electrophysical properties. Possibilities of using the methods of naval chemistry. Study of the chemistry and mechanism of thermochemical transformations of coal. Modern ideas about the molecular structure of substances of different types of THC. Molecular structure and supramolecular organization of natural coal. Chemical bonds in coal.

There are known models of the coal macromolecule (Stadnikov, Kasatokin, Given, Van Crevelen, Weiser, Solomon, Lazarov, Shinn, etc.). Two-phase model of coal structure. The nature of interactions between phases (Marzec). A model of a self-associated multimer with a three-dimensional structure (Gagarin, Skripchenko, Krichko). The model of vitrified organic mass of coal (OMW) as a "labile polyconjugated supersaturated structure of predominantly non-aromatic character" (Rusyanova).

Scientific and industrial classifications of TGC. International classification of coal and lignite. Preparation of solid fuels for processing and quality control. Theoretical foundations of enrichment of TGC, their desulfurization.

b. Theoretical foundations of the thermal destruction of THC

Patterns of pyrolysis of solid fuels under isothermal and non-isothermal conditions. Influence of temperature and heating time on the degree of decomposition of THC. Influence on the process of thermal destruction of fuels of their nature, heating rate, particle size, pressure, composition of the gas medium. Two main stages of thermal treatment of fuels: heating of the fuel mass and a process that includes physical and chemical changes in the organic mass of the fuel

Methods for studying fast (10^{-1} , $10^{(-4)s}$) reactions and processes of destructive pyrolysis of organic matter of fuels with heating rates several orders of magnitude higher than those used for these purposes in industry. High-speed process of fuel decomposition.

Homogeneous and heterogeneous pyrolysis reactions of solid fuels. Qualitative and quantitative yield of products of thermal destruction of fuels as a result of chemical reactions and physical changes in the reaction medium. Determination of macrokinetic characteristics of pyrolysis of fuels in isothermal and non-isothermal conditions. Chain and radical chain mechanisms of the process of destruction and compaction of carbon mass. Autocatalysis in the process of pyrolysis of pitch materials.

Modern methods of studying the mechanism and kinetics of the process of destruction of organic substances of solid fuels. Determination of the kinetic characteristics of solid fuels decomposition by the derivatographic method in the low-thermal regime

c. Theoretical basis of the process of fuel gasification and conversion of hydrocarbon gases

Chemical equilibrium of the main reactions of carbon with gases. The kinetic method of interpreting chemical equilibria. Calculation of the equilibrium gas composition in the process of interaction of carbon with gases. Chemical equilibrium in imperfect gas mixtures.

Mechanism of carbon-gas reaction and hydrocarbon gas conversion reactions. Reverse, sequential and parallel-serial reactions of the process of interaction of carbon with gases and conversion of hydrocarbon gases. Scheme of the mechanism of reaction of carbon with CO_2 , H_2 , O , O_2 . Chemical adsorption. Formation and decomposition of a solid surface complex. Inhibitory effect of reaction products. Chain mechanism of reactions of carbon with gases. Kinetic equations based on the concepts of the mechanism of reactions of carbon with gases.

Basic diffusion-kinetic theories of combustion and gasification of solid fuels. Share participation of individual reactions in the total process. Dependence of the total process rate on chemical and physical factors. Determination of the main kinetic characteristics of reactions of carbon with gases. Derivation of kinetic equations taking into account the change in the volume of the gas phase during the reaction for reverse, sequential and parallel-serial reactions of carbon with gases. Kinetic method for determination of equilibrium constants of reactions of carbon with gases.

Calculation of the reaction zone in isothermal conditions. Calculation of the reaction zone in non-isothermal conditions. Types of non-isothermicity. Thermal regime of endothermic and exothermic reactions. System of equations for determining the concentration, temperature of gas and solid phase in the reaction zone. Calculation of the reaction of carbon with gases in non-stationary and non-isothermal conditions.

d. Technology for thermochemical destruction of THC without air access

Influence of the heating method on the yield and quality of products of thermal processing of fuels and their use. Coke residue (semi-coke), primary resin, gas, and resin water.

Features of oil shale processing technology. Chemical products of oil shale processing. Thermal processing of oil shale with a solid coolant. Features of the technology of thermal destruction of peat and methods of its direct use.

Energy technology methods of fuel utilization. Necessary conditions for connecting power plants with industrial furnaces for thermal processing of fuels. High intensity of the process. Process control. Production of high-calorie gas and high-quality low-component liquid products. Energy technology methods of oil shale thermal treatment. Integrated energy and technological use of fuels under the new structure of the fuel balance. Chemical products of thermal processing of lignite and peat and their characteristics as raw materials for synthesis.

The use of coal, peat, oil shale and their products in . Humic fertilizers, herbicides, etc.

Semi-coking and coking. Basic technologies. Influence of heating rate, temperature and type of coal. Known methods of semi-coking and coking of hard coal. Processes occurring during the coking of baking coal and coal . Composition of coal . Plastic state as a result of thermal destruction of coal. Swelling and bursting pressure. Sintering, transformation of semi-cokes into coke. Shrinkage and cracking. Emission of gaseous products at different stages of the coke formation process. Sintering, sintering and coking capacity of hard coal and methods of their determination. Influence of various factors on the coking process. Assessment of coke quality. Modern technology of coke production. Ways to expand the raw material base of coking.

Chemical products of semi-coking and coking of coal. Condensation and capture. Extraction of crude benzene. Distillation, crystallization, and adsorption processes. Production of concentrated ammonia and ammonium sulfate. Coal tar. Methods of its processing.

e. Residue-free gasification of fuels

Gasification of fuels as a method of residue-free utilization of organic mass of fuels. Raw materials for gas production (solid and liquid fuels, natural gases, associated gases and gases of oil production and refining). Main ways of development of solid fuels gasification. Intensity of the process. Energy efficiency. Analysis of shortcomings and opportunities for intensification and increase of economic efficiency of gas production from solid fuels. Physical and chemical basis of the process. Autothermal and allothermal processes.

Characterization of the gas formation process in a dust flare, in a fluidized bed and in a dense fuel layer. Disadvantages of modern industrial methods of gas production. The need to include the gas generating process in the energy and technological scheme.

Gasification of steam and gas products formed during the thermal decomposition of . Methods for the production of air, steam-air, water and steam-oxygen gases from pulverized, fine-grained and lumpy fuels.

Characterization of liquid fuels used for gasification. Production of gases from liquid fuels for the synthesis of alcohols and ammonia. Production of olefins and acetylene hydrocarbons. Gasification of liquid fuels under high pressure. Main indicators of fuel gasification.

f. Destructive hydrogenation of fuels and synthesis of hydrocarbons from hydrogen and carbon monoxide

Features and purpose of destructive hydrogenation processes. Chemical basis of the process. Assessment of coal suitability for hydrogenation. Catalysts and technological parameters of destructive hydrogenation. Stepwise destructive hydrogenation of resins and oil residues. Liquid-phase and vapor-phase hydrogenation. Yield and characterization of hydrogenation products. Preparation of chemical products by hydrogenation of fuels. Joint hydrogenation of coal and oil. Industrial hydrogenation equipment.

Hydrogenation of individual substances. New promising directions of destructive hydrogenation of THC and their economic feasibility.

Physical and chemical basis of the process of hydrocarbon synthesis from CO and H₂. Requirements for the gas entering the synthesis. Catalysts of the synthesis process. Mechanism

of action of catalysts. Schematic diagram of synthesis at atmospheric and medium pressure. Characterization of synthesis products. Methods of processing synthesis products.

g. Other methods of processing fossil fuels

Extraction of THC with organic solvents. Yield, composition and properties of bitumen depending on the type of raw material and extraction conditions. Catalytic extraction. Mechanism of the process. Catalysts.

Oxidation of THC. Types of oxidizing agents, influence of oxidation conditions on the composition and yield of products. The use of THC oxidation products.

h. Technology of carbon graphite materials

Properties of carbon-based materials (physical, electrical, magnetic, mechanical, and chemical) and their use. Electrodes of metallurgical, electrochemical and chemical industries. Fire-resistant products. Electric coal products (shields, lighting coal). Antifriction materials. Carbon fibers and fabrics. Glass carbon. Use of graphite for synthesis of artificial diamonds.

Raw materials (fillers and binders). Technology of carbon graphite materials. Hardening of carbon graphite materials. Grinding and dispersion of carbon materials. Technology of preparation of masses. Mixing of masses. Pressing of masses. Firing of carbon graphite materials. Production of carbon fabrics and fibers. Production of glassy carbon. Prospects for the development of technology and industry. Materials based on carbon.

i. Environmental protection in solid fuel processing

Legislative measures in Ukraine to protect nature. The main sources of air, water and soil pollution at chemical fuel and carbon processing enterprises. Prospects of transition to drainless technological processes. Pipeless, waste-free technology.

Basic literature

1. Bratychak M.M., Grinishin O.B. Oil and Gas Technology. - Л.: Lviv Polytechnic, 2017.
2. Bratychak M.M. Fundamentals of industrial petrochemistry. - Л.: Lviv Polytechnic, 2008.
3. Saranchuk V.I., Ilyashov M.O., Oshovsky V.V., Biletsky V.S. Fundamentals of chemistry and physics of combustible minerals - Donetsk: Eastern Publishing House, 2008. 640 p.
4. Bratychak M.M., Pyshiev S.V., Rudkevych M.I. Chemistry and technology of coal processing. - Lviv: Beskyd Bit Publishing House. - 2006. - 272 p.
5. Pikh Z.G. Theory of chemical processes of organic synthesis. Textbook - Lviv: Lviv Polytechnic National University Press. 2002. -396 c. 2.

Additional literature
to section 1 - petrochemicals

1. V.V. Humenetsky Processes and equipment of oil refineries. - Л.: Lviv Polytechnic, 2003.
2. Pikh Z. Chemical Reaction Engineering. Mathematical description, modeling, optimization. - Lviv. 370 p.
3. Melnyk S.R., Melnyk Y.R., Pikh Z.G. Design and calculation of technological processes of organic synthesis. Lviv: Lviv Polytechnic National University Press, 2006. 448 p. 4.
4. Pikh Z.G., Melnyk Y.R., Melnyk S.R., Catalysis in Chemistry and Technology - Lviv. 2016. -286 c.

5. S.V.Boichenko, A.V.Yakovleva, O.O.Vovk, M.M.Radomska, L.M.Charniak, I.O.Shkilniuk Fundamentals of chemistry. - National aviation university, 2019.
6. S. Boichenko, O. Aksionov, P. Topilnytskyi, A. Pushak, K. Lejda Selected aspects of providing the chemmotological reliability of the engineering. - National aviation university, 2019.
7. Wienckowska J., Bratyczak M., Topilnicki P. Catalytic adsorption desulfurization of gases. - Oficyna Wydawnicza Politechniki Wroclawskiej.
8. O. Machinsky, P. Topilnitsky Hydrocracking. - Л.: Lviv Polytechnic, 2011.
9. Patryliak L.K. Catalytic cracking: practice and theory, development of research in Ukraine (Review). Catalysis and Petrochemistry, 2001, No. 9-10, pp. 14-25.
10. Patrylyak L.K., Ionin V.O. Alkylation of isobutane with butenes (Review). Catalysis and Petrochemistry, 2007, No. 15, pp. 26-37.

Additional literature
to section II - Coal chemistry

1. Koveria A. S. Physics and chemistry of combustible minerals: Lecture notes. Part I. - Dnipropetrovs'k: NMetAU, 2010. - 52 p.
2. Koveria A. S. Physics and chemistry of combustible minerals: Lecture notes. Part II. - Dnipropetrovs'k: NMetAU, 2010. - 50 p.
3. Bansal R.C., Goyal M. Activated carbon adsorption: Taylor & Francis Group, 2005. - 472 p.
4. Tamarkina Yu.V., Kucherenko V.A., Shendrik T.G. Alkaline activation of coals and carbon-base materials // Solid Fuel Chem. - 2014. - Vol.48. - No.4. - P.251-259.
5. Ovsienko I.V., Vovchenko L.L., Matsui L.Y.. Carbon materials and intercalated compounds based on them. Study guide. Scientific and Production Enterprise "Publishing House "Naukova Dumka" of NAS of Ukraine", 2009, 129 pp.
6. Saranchuk W. I, Shendrik T. G, Simonova W. W., Komraus J. L., Popiel E. S. Iron Compounds in the Ukrainian Saline Coals and Their Transformation During Hydrogenation //Erdol und Kohle.- 1994. - 47.- p. 385-388.
7. Tamarkina Y. V., Shendrik T. G., Krzton A., Kucherenko V. A., Reactivity and structural modification of coals in HNO₃ - Ac₂O system // Fuel Processing Technology, 77-78 (2002), p. 9-15.

The supplementary list of references is indicative and does not exclude the applicants' own initiatives in their selection and use