Summaries

UDC 544.452.2

**Root L.O., Smorygina K.S., Zvyagintseva E.S., Ilyin A.P.
CATALYTIC EFFECT OF CHROMIUM (III) OXIDE ADDITIVES
ON ALUMINUM NANOPOWDER COMBUSTION PROCESS
IN THE AIR**

The authors studied the effect of chromium (III) oxide additives on aluminum nanopowder combustion process in the air and parameters of its chemical activity. It was determined that the maximum oxidation rate grew at increase of the test additive content in the mixture and achiever maximum (24,15 wt. %/min) for the mix of aluminum nanopowder with 1,6 mole % Cr_2O_3. It was ascertained that chromium (III) oxide additives (0,1...1,6 mole %) stimulate the increase of aluminum nitride yield decreasing the content of unburnt aluminum. The authors made a conclusion on catalytic effect of chromium (III) oxide additives on oxidation processes of aluminum nanopowder.

UDC 546.3:537.39:544.77.023.523

**Korshunov A.V.
FEATURES OF DISPERSE COMPOSITION AND MORPHOLOGY
OF PARTICLES OF THE METAL POWDERS PRODUCED
BY THE METHOD OF WIRES ELECTRIC EXPLOSION**

The author studied the disperse composition and morphology of particles of electroexplosive powders of Al, Cu, Fe, Ni, Mo, W metals using the complex of methods including scanning and transmission electronic microscopy, low-temperature argon adsorption and dynamic light scattering. The article demonstrates the features of applying the methods to the samples with multimodal particle diameter distribution. The authors ascertain the dependence of diameter distribution function type on metal density and electric explosion conditions. The authors explained the formation of different size particles at electric explosion based on the overcooling effect of molten metal small volumes on the base of morphological and structural differences of nanoscale range particles with the diameter less than 50...80 nm determined experimentally and having mainly polyhedral shape and spherical particles of micron range as well as on the base of thermodynamic calculations.

UDC 546.3:537.39:544.778.4:539.26:537.533.35

**Korshunov A.V.
SIZE DEPENDENCE OF PARTICLE STRUCTURE
PARAMETERS OF ELECTROEXPLOSIVE METAL POWDERS**

The author studies the structure of oxide shell and particle metal core of electroexplosive powders of Al, Cu, Fe, Ni, Mo, W metals using the techniques of X-ray diffraction and high-resolution transmission electron microscopy. The influence of oxide shell state and its phase composition on protective function relative to metal particle oxidation at storing is analyzed. It is shown that in case of high values of molar volume ratio of surface crystal oxide and metal the oxide shell does not form continuous contact with metal and does not prevent full oxidation of nanoscale range particles. It is ascertained that the parameter of metal particle elementary cell with the diameter of 20 nm and more is not a dimension-dependent magnitude and takes the values common for solid state metals within the measurement accuracy. It is shown that size dependence occurs in features of structure faults of different size range particles. The author proposes the explanation of the observed dependence which considers the difference in temperature conditions of powder particles formation.

UDC 546.82:539.374.6:544.65

**Bozhko P.V., Korshunov A.V.,
Grabovetskaya G.P., Stepanova E.N.
THE INFLUENCE OF Zr−1 % Nb ALLOY STRUCTURE
ON ITS ELECTROCHEMICAL BEHAVIOR**

Using the cyclic voltammetry method the authors study electrochemical behavior of Zr−1 % Nb alloy with coarse-grain ($d=6\ \mu m$) and submicrocrystalline structure ($d\approx0,6$ and $0,15\ \mu m$) obtained at severe plastic deformation, in H_2SO_4, HCl, NaOH solutions, artificial sea water, physiological solution. It is shown that the alloy structure influence on its electrochemical characteristics occurs to a greater extent in H_2SO_4 solutions owing to higher conversion rate of the material with submicrocrystalline structure into a passive state. Based on thermodynamic calculations of equilibrium activities of metal−solution interaction products as well as on the basis of anodic process parameter values the authors explain Cl^- ion activate influence on high velocity of anodic oxidation of Zr in comparison with Ti.

UDC 544.43

**Stepashina E.V., Mustafina S.A.
FORMING MATHEMATICAL MODEL OF CATALYTIC
PROCESSES WITH VARIABLE REACTION VOLUME BASED
ON THEORETICAL−GRAPH APPROACH**

Based on graph theory the properties of solving chemical process kinetic model were proved. The algorithm for specifying the chemical reaction mechanism was developed on the base of the method for analyzing the direct link graph with error propagation. The numerical algorithm is tested on the catalytic process of α-methylstyrene dimerization.

UDC 544.72.31.17

**Gonchikov V.Ch., Gubaydulina T.A.,
Kaminskaya O.V., Apkaryan A.S.
FILTER MATERIAL FOR PURIFYING WATER FROM IRON,
MANGANESE AND HYDROGEN SULPHIDE**

The authors obtained a new filter material for water purification from iron, manganese and hydrogen sulphide. It contains as a base the local granular material of natural origin − the burnt rock of Kiselevsk coal deposit «Dalnie gory» in Kemerovo region. The laboratory researches and field tests of the filter material were carried out at different water types. The conclusion is made that oxide and hydroxide complex obtained at the burnt rock surface allows removing from water not only iron and manganese but hydrogen sulphide as well.

UDC 622.778:621.318.2

**Sofronov V.L., Buynovsky A.S., Makaseev Yu.N.,
Makaseev A.Yu., Dogaev V.V.
MAGNETIC SEPARATION OF SLAGS OF REM-Fe(Co)-B
AND REM-Fe ALLOYS PRODUCTION**

The article introduces the results of investigation of applying magnetic separation in processing production wastes of manufacturing REM-Fe (Co)-B and REM-Fe magnetic alloys by fluoric technology. The authors show the possibility of obtaining magnetic fraction in the form of REM-containing concentrate at REM extraction to 60 wt. % from residual content of metal fluoride reduction melting in slags.

UDC 691.4

Safonova T.V., Vereshchagin V.I., Bayandina E.V.
PROCESSING CHARACTERISTICS AND SINTERING
OF CLAY RAW MATERIAL IN SOUTH BAIKAL REGION

The article demonstrates the dependence of processing characteristics of polymineral clay raw material in South Baikal region on the amount and type of clay minerals. These rocks plasticity grows at increase of clay mineral content in the raw material. Sensitivity coefficient to raw material drying depends on clay particle content and it is mainly determined by montmorillonite occurrence. The article introduces the dependence of strength development intensity at various stages of clay raw material burning on mineral composition.

UDC 691.327.333

Lotov V.A., Sudarev E.A.
THE INFLUENCE OF SODIUM CHLORIDE AND CALCIUM
CARBONATE ON RHEOLOGICAL CHARACTERISTICS
OF SYNTHETIC FOAMING AGENTS
IN MANUFACTURING FOAM CONCRETE

The authors consider the influence of inorganic salts on the main rheological characteristics of synthetic foaming agents by the example of NaCl and $CaCO_3$. Optimal salt consumption and optimal mass fraction of foaming agent in water solution are determined. Application of NaCl and $CaCO_3$ allows obtaining persistent foam concrete mass. It is shown that foam concrete obtained on the basis of this mass has high strength properties and uniform-pore structure with the predominant closed porosity.

UDC 66.021.1

Balyasnikov A.V., Zaripova L.F., Pishchulin V.P.,
Svarovsky A.Ya.
MODELING THE MIXING PROCESS BY THE JET METHOD
OF LIQUID RADIOACTIVE WASTE IN CYLINDER RESERVOIRS

The authors consider the process of liquid radioactive wastes (LRW) mixing in cylinder reservoirs under tangent position of nozzles. The process modeling is carried out on the basis of the similarity theory. The authors define the constructive characteristics of mixing devices; the solution velocity characteristics while flowing from mixing devices; the conditions of particles weighing in weak-salt LRW for defining the time of mixing by the jet method.

UDC 544.653.22

Ustinova E.M., Gorchakov E.V., Kolpakova N.A.
THE RESEARCH OF COMPOSITION OF BINARY
ELECTROLYTIC INDIUM–PLATINUM DEPOSIT

The authors studied the composition of binary electrolytic indium-platinum deposit and proposed the method for calculating potential displacement value of electronegative component (indium) from electrolytic deposit with platinum. The comparison of calculated data obtained when using Pauling equation with the experimental data obtained at the deposit electro-oxidation allows estimating the phase composition of intermetallic compounds formed at the electrode. It is shown that the formation of five intermetallic compounds is observed at indium platinum ratio from 5000:1 and higher. At indium platinum ratio higher than 10000:1 the formation of one intermetallic compound.

UDC 544.653.22

Shekhovtsova N.S., Glyzina T.S.
USING THE STEP–BY–STEP METHOD OF MATHEMATICAL
RESOLUTION FOR ESTIMATING THE COMPOSITION
OF ELECTROLYTIC DEPOSIT Pt–Bi

Using the step by step method of mathematical separation of overlapping signals the authors separated multicomponent signals obtained at electro-oxidation of binary deposits Pt–Bi from graphite electrode surface by the stripping voltammetry technique. The authors compared the calculated and experimentally determined potential displacement values of bismuth selective electro-oxidation peaks from intermetallic compound with platinum.

UDC 771.534.2:771.534.13

Gudymovich E.N., Vanifatyeva E.Yu.
PHOTOETCHING OF SILICON DIOXIDE FILMS
IN DONOR–ACCEPTOR COMPOSITIONS

The article introduces the experimental results in photo activated etching of SiO_2 dielectric layers used in microelectronic planar technique. It is shown that the compositions containing proton donors and acceptors and fluorine-containing compounds support high velocity of silicon dioxide etching owing to fluorine ion release from solvate shell and their activation at UV irradiation.

UDC 542.61

Tosmaganbetova K.S., Dosmagambetova S.S., Tashenov A.K.
THE INFLUENCE OF ACCOMPANYING ELEMENTS
ON SILVER EXTRACTION WITH THIOSEMICARBAZIDE
IN STEARIC ACID MELT

The authors studied some factors influence on extraction extent of cations of copper (II), zinc (II), lead (II) accompanying silver cation (I) in polymetallic ores with thiosemicarbazide in stearic acid melt. Optimal conditions of their quantitative extraction are determined. The differences in values of pH solutions at optimal extraction conditions may be used for separating these metals cations from silver cation. The results are proved by artificial mixture analysis.

UDC 542.61

Tosmaganbetova K.S., Dosmagambetova S.S., Tashenov A.K.
THE INFLUENCE OF ACCOMPANYING ELEMENTS
ON SILVER SPECTROSCOPIC DETERMINATION
WITH THIOSEMICARBAZIDE IN STEARIC ACID MELT

The authors obtained the spectra of diffusive reflection and adsorption of copper (II), zinc (II), lead (II) compounds in thiosemicarbazid melt in stearic acid. The spectra are characterized by proper parameters different from those of original reagents and silver compounds (I) spectra. Based on spectral characteristics of the samples obtained by extraction of water solutions containing ions of silver (I) and copper (II), zinc (II), lead (II) in different ratios and the analysis of artificial mixtures containing simultaneously all the elements studied it is shown that the accompanying metals ions to the ratio 1:10 do not influence on spectroscopic determination of silver (I) in solid extracts.

UDC 661.721.41:544.478−03:544.18

Kravtsov A.V., Popok E.V., Yuryev E.M.
MATHEMATICAL MODELING OF METHANOL SYNTHESIS
BY QUANTUM–CHEMICAL COMPUTATIONAL TECHNIQUES

The authors studied the methanol synthesis mechanism on the surface of low-temperature zinc-copper catalysts. The rates of the mechanism different stages were calculated by the quantum-chemical techniques. It was proved that hydrogen surface adsorption is the limiting state of the process. Hydrogen adsorption velocity for low-temperature contacts promoted by boron and zirconium was computed. Based on the values obtained the authors formed the process modeling system and carried out the adequacy test of this system.

UDC 66.048.3

Samborskaya M.A., Kravtsov A.V., Volf A.V.
THE ANALYSIS OF POLYSTATIONARITY
OF OIL AND OIL PRODUCT FRACTIONATION

Multiplicity analysis is a key stage in chemical engineering design and control system development. The authors developed the method for analyzing multiplicity based on distillation mathematical models. The proposed algorithm for model conversion to obtain analytical dependencies of output variables of the project, design and control parameters enables to analyze input-output multiplicity due to various factors. Input multiplicity analysis for crude distillation unit was implemented. The existence of equal mole fractions was shown for a number of components under different input conditions. The recommendations on selection of the key components and the range of process variables were given to increase the efficiency of the design calculations.

Dolganov I.M., Kirgina M.V., Ivashkina E.N.,
Ivanchina E.D., Dolganova I.O.
**OPTIMIZATION OF HIGHER ALKANE DEHYDROGENATION
INSTRUMENTATION USING THE MATHEMATICAL
SIMULATION TECHNIQUE**

The authors propose a new method for increasing operating efficiency of the reactor block for paraffin dehydrogenation using the mathematical model considering the interaction of the processes occurring in chemical-engineering system apparatus. The numerical estimation of the influence of raw material chemical composition, process conditions and catalyst deactivation degree on operating efficiency of chemical-engineering sheet devices of dehydrogenation industrial plant is carried out.

Sharova E.S., Faleev S.A., Ivanchina E.D.,
Poluboyartsev D.S., Kravtsov A.V.
**STUDYING THE COMPOSITION AND THE PROPERTIES
OF Pt–CATALYSTS OF BENZENE REFORMING
INDUSTRIAL PROCESS**

The mechanism of forming coke on Подробно изучен Pt-contact surface in reforming benzenes was studied in details. Differential-thermal and X-ray structure analyses of industrial catalysts samples were carried out. The possibility of hydrogenating amorphous coke deposits when regulating the process main technological parameters was determined. The necessity of continuous monitoring of industrial plants for increasing their operation level was proved.

Gorda E.O., Chekantsev N.V.,
Ivanchina E.D., Gyngazova M.S.
**ESTIMATING THE RECONSTRUCTION EFFICIENCY
OF A ONE–PASS CIRCUIT OF L–35–11/300 DEVICE USING
THE MATHEMATICAL MODEL**

The article considers the variants of reconstruction of a one-pass circuit for isomerization device using the mathematical model. The authors estimate the economic effect and payback period at implementation of different variants – with unconverted component recycle, with the preliminary deisopentanisation of raw materials and using the combined variant.

Shulikin S.N., Shulikina M.S., Marin S.S.
**THERMODYNAMIC COMPATIBILITY OF SOLVENTS
AND KINETICS OF THEIR EVAPORATION AT HEAT
TREATMENT OF INSULATING IMPREGNATING COMPOUNDS**

The article considers the issues of solvent thermodynamic compatibility with insulating impregnating compounds. The interaction between solvent capacity of polymeric film organic solvents and their strength is determined. The authors obtained experimentally the evaporation intensity kinetic curves of the solvent of alkyd-melamine varnish ML-92 with different viscosity and under different modes of heat treatment.

Zhdaneev O.V.
CHROMATOGRAPHY OF THE VARIABLE GEOMETRY

The author describes for the first time the theory of chromatographic system with the variable geometry column and optimal profiles of distributing chromatographic column parameters. The results of modeling allow concluding that these changes correspond in their effects to the methods for programming temperature and flow and lift some fundamental restrictions. The column profiles proposed in the article allow increasing considerably the resolution ability of chromatographic system and reducing the time for analysis.

Zhdaneev O.V.
**CHROMATOGRAPHY OF THE VARIABLE GEOMETRY IN THE
CASE OF RECTANGULAR CHROMATOGRAPHIC COLUMNS**

The author describes the theory of chromatographic system with the rectangular column of the variable geometry. The results of modeling allow concluding that the use of the column rectangular profile allows preserving all the main advantages of moduling the chromatographic system geometry, opening simultaneously the way to industrial application of the proposed technique.

Noskova G.N., Zakharova E.A., Chernov V.I.,
Zaichko A.V., Elesova E.E. Kabakaev A.S.
**PROPERTIES AND APPLICATION
OF GOLD–CARBON–BEARING COMPOSITE ELECTRODES
IN ELECTROCHEMICAL ANALYSIS TECHNIQUE**

The authors studied the properties of composite solid carbon electrodes of industrial polyethylene concentrate of technical carbon and ensemble of golden micro/nanoelectrodes arranged irregularly on their substrate. The concentrate parameters influencing the analytical characteristics of electrodes were determined. The electrodes are simple in production and possess high sensitivity and stability during the long operation time (not less than 14 days). The electrode in the form of golden microelectrode ensemble may be used for determining arsenic, copper, selenium, mercury on the level of 10^{-4} mg/l by the stripping voltammetry method; iron and chromium are determined by the method of the direct voltammetry on the level of 10^{-3} mg/l.

Shumar S.V.
**POTENTIOMETRIC DETERMINATION OF SILVER USING
THE PROCESS MATHEMATICAL MODEL**

The author proposes the technique for quantitative determination of silver ions by the method of potentiometric precipitation titration with the computer processing of titration curves by partial linearization. The use of the process mathematical model and the post-processing of the experimental data allowed decreasing by three orders a lower boundary in the range of determining silver ions, defining the product of precipitation solubility and the equivalence point with high accuracy. The medicines «Argosulphan» and «Protargol» were analyzed by the proposed technique.

Kambalina M.G., Pikula N.P.
**ATOMIC ADSORPTION DETERMINATION
OF SILICON CONTENT IN NATURAL WATERS**

The article shows the possibility of determining silicon content in natural and underground waters of different mineralization by the atomic adsorption method with Zeeman correction of background nonselective adsorption. This method high selectivity allows determining silicon content without preliminary sample preparation even in high-mineralized samples of underground waters (in particular, in formation waters).

Galanov S.I., Sidorova O.I., Litvak E.A., Kosyreva K.A.
**MANGANIFEROUS CATALYSTS FOR PROCESSING
PASSING OIL GASES INTO OLEFINS**

The article considered the variants of processing the passing oil gases into liquid hydrocarbon fuels. The authors studied the oxidative transformations of C_1–C_4-hydrocarbons into olefins on the oxide manganiferous catalysts in periodic mode. The two-stage process may be considered as the promising direction in processing passing oil gas. The first stage is the olefins synthesis from C_1–C_4-hydrocarbons; the second stage is the conversion of unsaturated hydrocarbons into engine fuels.

UDC 544.4

Stankevich V.S., Nesyn G.V., Romanenko S.V.
STUDYING THE KINETIC LAWS OF HEXENE
POLYMERIZATION ON HETEROGENIC MICROSPHERE
CATALYST IN UNSTEADY CONDITIONS

The authors obtained the kinetic equations of hexene polymeriza-
tion in unsteady conditions, calculated experimentally the constants of
these equations. It was shown that the kinetics of hexene polymeriza-
tion on heterogenic microsphere catalyst depends on the chemical
process area.

UDC 536.658+541.183

Dmitrieva Z.T., Bondaletov V.G., Troyan A.A.
THE METHOD FOR DETERMINING SPECIFIC SURFACE
OF POLYMER ADSORBENTS

The authors proposed the method for determining specific surfa-
ce of polymer adsorbents based on the measurement of their equili-
brium adsorption capacity at hydrocarbon adsorption from gas phase.
The applicability of the method for determining the specific surface of
polymer adsorbents was studied in comparison with the methods for
calculating the same adsorbents specific surface based on the integral
heat of hydrocarbon adsorption from liquid phase and isothermas of
low-temperature nitrogen adsorption on their surface. The specific
surface values determined by the adsorbent capacity and by nitrogen
adsorption isotherma conform best of all to each other. The authors
discussed the reason of differences in specific surface values obtained
by three independent techniques.

UDC 547.8.3.665.61

Gerasimova N.N., Sagachenko T.A., Ayurova A.M.
LOW–MOLECULAR NITROGEN–CONTAINING BASES
OF HIGHLY PARAFFINIC CRUDE

Low-molecular nitrogen-containing bases of highly paraffinic
and sweet crude oil from Paleozoic deposits of West Siberia have be-
en studied. It was shown that the content of these compounds in the
test oil was lower than that in coeval low- and medium-paraffinic
sweet oils occurring in the region. The structural-group composition of
strong bases in highly paraffinic oil is characterized by a set of compo-
unds typical for the West Siberian crudes.