

## AN ALTERNATIVE TECHNOLOGY FOR CATALYTICAL PROCESSES. THE AEROSOL NANOCATALYSIS (p. 4-11)

Marat Glikin

The reasons of searching for alternative chemical catalytic technologies were analyzed in the paper. Oxidation of organic components with a complex molecule at high temperature leads to precipitation of carbon and some reaction products on the catalyst supports and in their pores, which reduces the efficiency of catalysis and requires its replacement. In aerosol nanocatalysis technology, reactants and continuously comminuted catalyst particles are involved in chemical interaction. It was experimentally shown that catalyst aerosol, even low-activity  $\text{Fe}_2\text{O}_3$ , only  $0.3 \text{ g/m}^3$  of the reactor is enough in the oxidation process. This is two orders of magnitude less than during the catalysis on the support. Moreover, there is no need for expensive support. This technology will lead to increased reaction rate by 104–106 times, reduced catalyst consumption by the same value, decreased reaction temperature by 100–200 °C; increased selectivity, reduced reactor volume by 10–100 times. Currently, about 40 reactions of the environmental focus were carried out in a laboratory using spray nanocatalysis. Target syntheses, which are of interest to the industry: natural gas conversion, catalytic cracking of vacuum gas oil on different catalysts, oxydechlorination, oxydehydrochlorination, vinylolation, ammonia oxidation for nitric acid production, disposal of acid tars and coke production waste, etc. were also investigated. Each process showed high economic effect.

**Keywords:** catalyst, nanoparticle, chemical technology, efficiency, heterogeneous catalysis, aerosol nanocatalysis.

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## REGULARITIES OF OBTAINING AND PROPERTIES OF THE HYDROXYAPATITE FILLED POROUS COMPOSITES BASED ON POLYVINYLPIRROLIDONE (p. 12-17)

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New hydroxyapatite-filled porous composites based on methacrylic esters and polyvinylpyrrolidone, which can be used in bone regeneration processes were synthesized. The influence of the polymer-monomer composition structure, nature and amount of filler, silver nitrate on the polymerization rate was studied. It was found that with the increase in the amount of polyvinylpyrrolidone in composition, the polymerization rate rises, and the induction period is practically absent. The polymerization rate of compositions of hydrophobic glycidyl methacrylate is significantly higher than in the case of 2-hydroxyethyl methacrylate. Compositions that contain hydroxyapatite in an amount of more than 70 wt. % have lower reactivity compared to the compositions without filler. Adding silver nitrate to the composition reduces the polymerization rate.

The influence of the foam stabilizer nature, hydroxyapatite amount on properties of composites was examined. The porous structure of the material is formed with the content of hydroxyapatite in the original composition of at least 25 wt. %. The highest porosity is observed when using glycerol in an amount of 50 wt. %.

Silver nanoparticles in the form of polyhedra with different sizes in the composite structure were obtained by restoring silver nitrate by tertiary nitrogen of polyvinylpyrrolidone. Formation of silver in this reaction is confirmed by UV spectroscopy and chemical analysis of the products of interaction between  $\text{AgNO}_3$  and polyvinylpyrrolidone. Synthesized silver-containing composites are characterized by bactericidal and fungicidal properties, in particular regarding the bacteria *Escherichia coli*, *Staphylococcus aureus* and *Aspergillus niger*.

**Keywords:** porous hydrogels, polyvinylpyrrolidone, silver nanoparticles, hydroxyapatite, bactericidal and fungicidal properties.

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## OBTAINING OF NANODISPersed FERRIFEROUS PIGMENTS USING CONTACT NONEQUILIBRIUM PLASMA (p. 17-21)

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The paper shows the efficiency of using a contact nonequilibrium low-temperature plasma for producing nanodispersed pigments of different colours. The influence of the initial pH, treatment time and electrical parameters of the plasma-chemical synthesis on the main technological properties of the pigments was determined. Colour characteristics of the obtained products were studied. Their phase composition was analyzed. According to the data on the dependence of the phase composition of the products formed by the oxidation of iron hydroxide (II) on the synthesis parameters, the system diagram was created to display predominant areas of each phase formation in the pH plasma treatment time coordinates.

The main trends in changing the phase composition of the solid phase from the synthesis conditions were determined during the studies.

It was found that the final product of iron hydroxide (II) oxidizing depending on the synthesis parameters can be oxyhydroxide of iron (III -a) – modification, magnetite or iron hydroxide (II).

A phase composition of the obtained product depends largely on the solution's pH. With increasing the pH from 6 to 10 under the same synthesis parameters, such sequence of phase formation is indicated: Fe(OH)<sub>2</sub> – a – FeOOH – Fe<sub>3</sub>O<sub>4</sub>. With the further increase of the solution's pH, Fe<sub>3</sub>O<sub>4</sub> is formed.

**Keywords:** pigments, magnetite, goethite, obtaining, contact nonequilibrium low-temperature plasma.

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## DENSITY FUNCTIONAL THEORY IN INVESTIGATION OF PSEUDO-IMMUNOLOGICAL SPECIFICITY OF THE “ARTIFICIAL RECEPTOR” AGAINST MELAMINE (p. 22-26)

Kateryna Muzyka

In this paper, computational approach for pseudo-immunological specificity investigation of acrylamido-2-methyl-1-propanesul-

fonic acid (AMPSPA), acrylic acid and itaconic acid to a molecule of melamine was developed based on DFT-calculations at the level of theory *Rw97XD / 6-31G (d)*. It should be noted that improving of the ligand-selectivity of "artificial receptor" is an important step in order to achieve sensors with high selectivity. The results of computational experiments show that among the considered monomers AMPSPA is most suitable for further synthesis of "artificial receptor" for melamine, as formed the strongest complex with melamine. Conducted theoretical research can be the basis for developing a sensor for melamine, which due to the presence of "artificial receptor" of AMPSPA will provide a high selectivity of detection.

**Keywords:** artificial receptor, molecular imprinting, melamine, density functional theory, pseudo-immunological specificity.

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#### EXPERIMENTAL DETERMINATION OF POSSIBLE DIFFUSION MODELS DURING PERVAPORATION PROCESS IN POLYMER MEMBRANES (p. 26-31)

Inessa Burtina, Otar Gachechiladze

Some parameters that are influenced by the solvent molecule diffusion in the polymer membrane body were experimentally studied using a pervaporation process. The time dependencies of these parameters during the pervaporation were obtained. It was shown that the mechanism of the solvent molecule diffusion in the polymer membrane consists of two components: a diffusion through the thermal activation of the system and a diffusion occurring through the free volume. Moreover, the rate of thermally activated diffusion is much larger and is observed in the beginning of the pervaporation process. Whereas, a diffusion using the free-volume model begins to manifest itself in the middle of the process and passes more slowly, but it is the source of transferring the majority of solvent molecules. These results make it possible to interpret diffusion models in polymer membranes.

**Keywords:** polymer, membrane, pervaporation, thermal activation, free volume, diffusion, voids, jump, technology.

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#### QUANTUM-CHEMICAL RESEARCH OF THE REACTION MECHANISM OF [4+2]-CYCLOADDITION OF 2,3-DIMETHYLBUTA-1,3-DIENE AND ALLYLMETHACRYLATE (p. 32-36)

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The mechanism of the [4+2]-cycloaddition reaction of 2,3-dimethylbuta-1,3-diene and allyl methacrylate was studied by the quantum-chemical modelling using a semi-empirical programme of MOPAC2009 by the RM1 method. The quantum-chemical calculations allowed analyzing the qualitative sides of the reaction.

It was found that the interaction of 2,3-dimethylbuta-1,3-diene and allyl methacrylate has a stepwise mechanism with the formation of an intermediate with an open electron shell, not a synchronous mechanism with a closed electron shell. The end product molecule – allyl-1,3,4-trimethylcyclohex-3-encarboxylate has a semi-armchair form in which a carboxylate group is in the endo-position to a cyclohexene ring. The molecule structure also indicates that the interaction of 2,3-dimethylbuta-1,3-diene and allyl methacrylate is agreed by the stepwise mechanism with a disrotatory cycle closure in the second step.

The compliance of the experimental data with the activation parameters obtained by means of the quantum-chemical calculations of this reaction confirms the proposed mechanism.

**Keywords:** 2,3-Dimethylbuta-1,3-diene, Allyl methacrylate, allyl-1,3,4-trimethylcyclohex-3encarboxylate, MOPAC2009, RM1.

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### DETERMINATION OF ELASTIC CONSTANTS OF ANISOTROPIC HEAVY PETROLEUM PRODUCT USING MOLECULAR DYNAMICS SIMULATION (p. 37-44)

Maksym Stetsenko

For the purpose of experimental verification of the assumption that the elastic properties of heavy petroleum can be characterized by a matrix of elasticity for a transversely isotropic medium, molecular dynamics simulation studies were performed. It is shown that the main structural elements of heavy petroleum are some saturated hydrocarbons, resin-solvated asphaltenes and self-associated asphaltenes. The obtained numerical results of the Young's modulus, shear modulus and Poisson's ratio in a wide temperature range for these compounds suggest that their elastic properties are closer in nature to the properties of solids, rather than amorphous entities. The method presented for determining the elasticity of a complex material in this paper can be found convenient and sufficiently accurate. This is so, since by analyzing the molecular composition of a complex compound and defining the main structural elements of it, properties of each of them can be estimated separately, in a first place, and then a general result can be derived for a substance as a whole.

Numerical results obtained in this research may be useful for those who are interested in heavy petroleum fractions rheology, and those who perform numerical studies in petroleum hydrodynamics and acoustics.

**Keywords:** normal paraffin, resin, asphaltene, molecular dynamics, force field, elastic constants.

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### DEVELOPMENT OF AROMATIC COMPOSITIONS FROM SALVIA SCLAREA ESSENTIAL OIL FOR ENCAPSULATION BY GUM ARABIC (p. 45-51)

Natalia Chepel

This article presents the development of aromatic compositions from *Salvia sclarea* essential oil for their encapsulation depending on the adsorption properties of gum arabic with regard to organic classes of aromatic compounds. The dynamics of aromatic compounds adsorption in applying the gum arabic has shown the low selectivity for the organic class of terpenes and the high selectivity for the organic classes of oxygen derivatives of terpenes. The separation of *Salvia sclarea* essential oil into its fractions with the low terpenes content and the difference of aromatic properties were performed by vacuum rectification using the complex approach. The mathematical modeling for the development of aromatic compositions from *Salvia sclarea* essential oil was used. The development of aromatic compositions from *Salvia sclarea* essential oil depending on the adsorption properties of gum arabic has allowed to find out the mass ratios of its fractions for the aromatic composition "Sweet Sage" – 2fraction: 3fraction: 4fraction=1.34 – 1.45:2.05-2.15:86.32 – 86.76: 3.78 – 4.98 and for the aromatic composition "Muscat Harmony" – 2fraction: 3fraction: 4fraction=0.76 – 0.81:10.78 – 10.85:17.43 – 17.56:43.22 – 43.67. The first fraction of *Salvia sclarea* essential oil with high

terpenes content has not been used in the development of aromatic compositions.

**Keywords:** aromatic compositions, *Salvia sclarea* essential oil, gum arabic, flavourings.

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## OXIDATION OF ISOMERIC HYDROXYTOLUENES WITH OZONE IN ACETIC ANHYDRIDE (p. 52-56)

Andrey Galstyan

The reaction of ozone with isomeric hydroxytoluenes in acetic anhydride medium to obtain corresponding aromatic alcohols and aldehydes was investigated. It was shown that in the research conditions, acetic anhydride acts as both solvent and acylating agent. The main reaction products are aliphatic peroxides (80–90 %), corresponding acetoxybenzylacetates (7–14 %) and acetoxybenzaldiacetates (3–6 %) were identified among the oxidation products by the methyl group of substrates. A scheme for the liquid-phase oxidation of acetoxytoluenes with ozone in acetic anhydride, which explains the obtained experimental data was proposed.

During the studies, the concentration of methylbenzenes and their conversion products in the solution was determined by gas-liquid chromatography at chromatograph with a flame ionization detector. The content of peroxide compounds was determined by iodometric titration. The rate constants of the reaction of ozone with methylbenzenes were calculated using the method, described in the work [3].

The obtained experimental data are the basis for developing environmentally friendly methods of synthesis of hydroxybenzyl alcohols and hydroxybenzaldehydes.

**Keywords:** oxidation, acylation, ozonolysis, selectivity, ozone, acetoxytoluene, sulfuric acid, peroxide, acetoxybenzylacetate, acetoxybenzaldiacetate.

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## INVESTIGATION OF THE SURFACE LAYER OF DIMETHYL ETHER/TRIETHYLENE GLYCOL SOLUTIONS (p. 56-62)

Vitaly Zhelezny, Tatyana Sevastianova

Method for calculating density and concentrations profiles of dimethyl ether (DME) solutions in triethylene glycol (TEG) was proposed in the paper. The thickness values of the surface layer of solutions were determined, and its structure was studied. The method for determining the effective surface concentration of the solution was proposed. The studies were performed in the framework of the gradient theory using the Peng-Robinson equation of state in single-fluid approximation with a modified procedure for determining the SE coefficients.

The studies were conducted in order to determine the effective composition of the surface layer of the solution. It is this solution composition rather than of the bulk liquid phase composition that must be taken into account when interpreting the experimental data on the saturated vapor pressure and surface tension of solutions.

As a result, it was found that the effective thickness of the surface layer of the solution increases with a decrease in the DME amount in solution, and as approaching the critical temperature tends to infinity. Herewith, surface layer of the studied solutions is composed of two sublayers. DME partial molar density profiles have a maximum. This means that the surface layer of the solution is enriched with this component. Analysis of the results has shown that the difference between the component concentrations in the surface layer and in the bulk liquid phase of the solution increases with temperature. The results are of fundamental importance in both the experimental investigation of the solution properties, and thermodynamic modeling of phase equilibria of solutions and forecasting their surface tension.

**Keywords:** gradient theory, single-fluid approximation, density profile, effective composition of surface layer.

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