ABSTRACT AND REFERENCES

TECHNOLOGY OF ORGANIC AND INORGANIC SUBSTANCES

DOI: 10.15587/1729-4061.2017.99022

STUDY OF KINETIC PARAMETERS FOR THE CATALYTIC CRACKING PROCESS IN Y TYPE AEROSOL CATALYST (p. 4-8)

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At present, in the petroleum refining industry, catalytic cracking is carried out on the heterogeneous zeolite-containing or aluminosilicate supported catalyst. A well-known deficiency of supported catalyst is the blockage of pores by coke. A aerosol nanocatalysis technology is proposed as the solution to this problem. The basic principle of this technology is complete exclusion of the use of a support from the industrial practice. In this case, the catalyst particles in the process of chemical transformation reach nano dimensions due to the mechanochemical treatment of particles. As a result, we observed an increase in the reaction rate, a decrease in the concentration of catalyst and the time of contact, as well as a rise in productivity by the basic component.

The basic principle of the aerosol nanocatalysis technology makes it possible to successfully repeatedly return the catalyst to the reactor. It is established that the use of zeolite-containing catalysts (type Y) in the form of aerosol does not decrease productivity of the process of catalytic cracking of vacuum gas oil. In this case, an increase in the reaction rate and selectivity is observed. It was found that the temperature and the oscillation frequency make it possible to control the progress of chemical transformation under conditions of AnC technology. The process of catalytic cracking under conditions of AnC technology could be proposed for the implementation either in parallel to the acting installations or as the independently operated unit for small-scale refineries.

Keywords: catalytic cracking, vacuum gas oil, aerosol nanocatalysis, vibrating bed, gasoline and diesel fraction.

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DOI: 10.15587/1729-4061.2017.99580

DEVELOPMENT OF COMPOSITIONS OF UREA GREASES ON AMINOAMIDES OF FATTY ACIDS (p. 9-14)

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In the interaction between stearic acid and diamines of different structure we synthesized amino amides. The composition and chemical structure were defined by the spectrometric methods of analysis. We demonstrated the possibility of applying the nitrogen-containing surface-active substances of plant origin as components of dispersed phase of urea thixotropic plastic systems. It was found that urea – a product of the interaction between amino amides of stearic acid and isocyanate – is an effective thickener of petroleum oils. The obtained urea greases are characterized by high levels of thermal, mechanical and colloidal stability.

A prospect to saturate the market of lubricants with urea greases produced in Ukraine, using the components obtained from available bio raw materials, predetermined the research into creating balanced lubricating compositions of optimal formulation with correctly chosen basic oils, additives, and fillers.

We developed a polyfunctional packet of oleo-additives consisting of sulphur-containing ethyl ester of higher fatty acids of rapeseed oil and the product of condensation of phosphatide concentrate with ethanolamine. It was found that the introduction of these products to the composition of grease on diurea improves its tribological characteristics and anti-oxidation properties, increases the level of biodegradation. Considering the given indicators, the new urea grease is better than some known commercially available analogous products.

Keywords: urea grease, amino amide, isocyanate, packet of oleo-additives, tribological characteristics, biodegradation.

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DOI: 10.15587/1729-4061.2017.101015

RESEARCH INTO FATTY ACID COMPOSITION OF PROBIOTIC CONSORTIUMS WITH THE INCLUSION OF PROPIONIC ACID BACTERIA (p. 15-20)

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We studied fatty acid composition of the bacterial leaven of bifidobacteria and propionic acid bacteria that were grown together, and in a monoculture on the lactose medium with the addition of soybean serum in the amount of 3 %. The polyunsaturated fatty acids cannot be synthesized de novo in the organism of mammals. For this reason, searching for the new sources of polyunsaturated fatty acids is a relevant problem of biotechnology. Microorganisms appear to be a promising raw material. They are capable of synthesizing and accumulating in the cells up to 70 % lipids, including free fatty acids. In the course of the accumulation of biomass of the examined strains it was revealed that the propionic acid bacteria enter symbiotic relations with bifidobacteria. In the consortium, density of the population of both types of microorganisms was larger than that in a monoculture. We employed the dynamic method of gas chromatography in experimental studies using a flame-ionization detector. The results obtained allowed us to establish that the bacterial leaven B.longum-Ya3 and P.shermanii-PS4 differed from other samples by the high content of unsaturated fatty acids. In this leaven, the amount of linoleic acid was the largest and made up 23.99 % of the total sum of fatty acids.

The data received confirm the expediency of using the probiotic bacteria for constructing the effective biologically active additives that contain essential fatty acids.

Keywords: propionic acid bacteria, bifidobacteria, saturated fatty acids, unsaturated fatty acids.

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DOI: 10.15587/1729-4061.2017.99787

EXAMINING THE EPOXIDATION PROCESS OF SOYBEAN OIL BY PERACETIC ACID (p. 21-28)

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The main principle of green chemistry is the use of renewable, ecological raw materials, which will contribute to subsequent biodegradation and reduction of toxicity of the product in the production of polymers. Vegetable oil (VO) is the cheapest and most common biological raw material, the use of which has such advantages as low toxicity and natural biodegradation.

We analyzed experimental dependences of the consumption of reagents and the accumulation of epoxide in the interaction between a solution of soybean oil (SO) in toluene and the epoxidizing systems H_2O_2/acetic acid (AA)/KU-2×8 and H_2O_2/acetic anhydride (AAn)/KU-2×8.

It was established that the use in the process of epoxidation of soybean oil of the specified systems makes it possible to achieve high values of selectivity of epoxidation by double bonds. The resulting values of selectivities in the epoxidation process by double bonds and by the consumption of peroxide when studying the epoxidizing system H_2O_2/AAn/KU-2×8 are higher. The advantages of using the specified epoxidizing system include a reduction in the total volume and mass of the reaction mixture. Obtaining the epoxidized soybean oil with a low resulting value of bromine number provides subsequent good thermal and oxidative stability of materials on its base.

We calculated the values of rate constants of the epoxidation reaction of SO at different temperatures. By using the methods of IR and Raman spectroscopic studies, we demonstrated structural changes in raw materials and confirmed the progress of the epoxidation reaction. The developed technique for recalculating the values of bromine, iodine numbers of products of the epoxidation reaction, unsaturation and epoxy number, selectivity of the process in the epoxidation of mixtures of unsaturated compounds allows comparing the results of research. The use of the specified technique also makes it possible to draw unambiguous comparative conclusions about the effectiveness of reagents consumption and the selectivity of reaction. In this case, there is a possibility to improve the technology of obtaining the epoxidized compounds. The calculation formulas obtained were applied to analyze the progress of the epoxidation process of soybean oil.

Keywords: epoxidized vegetable oils, oxirane oxygen content, epoxy number, kinetic studies, IR spectroscopy, Raman spectroscopy.

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DOI: 10.15587/1729-4061.2017.99341

REGULATION OF PROPERTIES OF EBONITE COMPOSITIONS AND VULCANIZED ANTICORROSIVE COATINGS USING A FTORLON FILLER (p. 29-35)

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Ebonite compositions, which are oligo-butadienes-based, are widely used for gumming the chemical equipment and instruments that are operated in aggressive media. For the ebonite compositions with anti-corrosion purposes, of scientific and practical interest was to explore the possibility of using as a filler of chemically resistant polymeric materials, which include the ftorlon powder F-2M. We examined the effect of a ftorlon filler on the rheological properties of ebonite compositions based on 1.2-oligo-butadiene. Results of the study revealed that the compositions on the base of oligo-butadiene, filled with a ftorlon powder, are the weakly structured systems with a pseudo plastic nature of the flow. Fluctuation grids of the compositions filled with ftorlon are easily destroyed under the action of uniform shear and temperature. In order to resolve this issue and to ensure the developed coagulation structure, the compositions need to be introduced with structure-forming additives, in particular aerosil (up to 5 % by weight).

We determined the dependence of strength of a vulcanizate on the sulfur content and the duration of vulcanization of coatings, which is important in order to regulate the properties and technological process of obtaining the chemically resistant coatings with improved properties. As a result of vulcanization of the examined compositions, it is possible to receive coatings with high strength (up to 27 MPa at tearing) and adhesion (9.8–10.2 MPa at tearing) without the use of specialized primers and adhesives. We explored the ohmic-capacitive characteristics and demonstrated chemical resistance of the vulcanized coatings in the 20 % solutions of sulfuric and hydrochloric acids.

Keywords: ebonite compositions, ftorlon filler, vulcanization of coating, electrical capacitance, chemical resistance.

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DOI: 10.15587/1729-4061.2017.99755

MODELING THE HETEROGENEOUS CATALYTIC RECOVERY PROCESSES OF ALDEHYDES AND KETONES (p. 36-43)

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Mathematical models of the recovery reactions of cyclohexanone and anise aldehyde with subsequent esterification by the Meerwein-Ponndorf-Verley mechanism are constructed. Experimental research was conducted into recovery reactions of aldehydes and ketones in order to find the optimal catalyst for the recovery reaction of cyclohexanone and to establish the limiting stage in the recovery process of anise aldehyde. We analyzed the activity of three catalysts, in the presence of which the recovery reaction of cyclohexanone proceeded, and selected for further calculations and studies the most active zeolite – SnMgAl(CO_3). By using the MathCad 15.0 programming environment, we solved the inverse problem of chemical kinetics for the examined reactions. It was found that the value of rate constant of the recovery reaction of cyclohexanone in the presence of zeolite SnMgAl(CO_3) is the largest and reaches 0.2544 s^{-1}, in other words, this is the most effective catalyst. As far as the recovery reaction of

aldehyde anise is concerned, it was established that the first stage of this reaction (anise aldehyde recovery) proceeds slower than the second stage (anise alcohol esterification) and it is the limiting stage of the reaction. Results obtained in the course of experimental research might be used to solve the direct and inverse problems of chemical kinetics.

Keywords: Meerwein-Ponndorf-Verley mechanism, inverse problem of kinetics, rate constant, heterogeneous catalysis, zeolites.

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DOI: 10.15587/1729-4061.2017.102182

DEVELOPMENT OF A BOOTSTRAP-MODEL FOR DETERMINING THE RELEASE OF MEDICINAL PREPARATIONS IN THE HUMAN ORGANISM (p. 43-49)

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We developed a bootstrap-model for evaluating the release kinetics of medicines in the organism and its computer realization. The model is based on the interpolation of experimental data for the release at pH 1.2; 4.5 and 6.8 by the linear and cubic splines and the use in the simulation of dissolution in the organism by passing the zones with the indicated pH values. The profile of the release is considered to be a random process, realized in separate points of time.

In order to perform the bootstrap-simulation of a pseudo-profile of the release in the organism, we generated a spline-pseudo-profile of dissolution at pH 1.2 (imitation of stomach); by using it, we determined mass of the released preparation in 2 hours. Employing the data obtained, we built a spline-pseudo-profile of dissolution at pH 4.5 (duodenum), which matches a residual amount of the preparation. Next, in a similar way, we constructed a spline-pseudo-profile, corresponding to a residual quantity of the preparation, and determined the release at pH 6.8 (small intestine).

The method devised is demonstrated on the example of the simulation of the release kinetics of the preparation Trizipin Long in the organism based on results of the release kinetics in vitro. The model makes it possible to estimate the mean profile, spread and confidence interval of the release. It is established according to results of the simulation that the release of the preparation Trizipin Long from a tablet of mass 1000 mg in the organism in 14 hours makes up on average 870 mg and, with a probability of 0.95, could be within the range from 788 to 946 mg.

The advantage of the developed approach is its universality, as the method is not linked to any particular physical model of the dissolution and the release.

Keywords: bootstrap-simulation, spline, interpolation, profile of the release in vivo, Trizipin-Long, distribution function.

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DOI: 10.15587/1729-4061.2017.101032

STUDY OF CHANGE IN THE DEFORMATION-STRENGTH PROPERTIES OF NANOMODIFIED FINE-GRAINED CONCRETES OVER TIME (p. 50-54)

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We examined a change over time of such properties of fine-grained concrete as strength at compression and deformation under the action of an external load. The studies were conducted for the possibility of determining the physicomechanical properties of concretes, required to calculate the ferroconcrete structures, first of all monolithic, at different age of their fabrication. We established a relation between the rates of formation of the deformation properties and the strength at compression of fine-grained concrete. It is found that the strength of fine-grained concrete and its deformations under the action of an external load depend on the composition of concrete and the presence in it of the surface-active substances that form micelles. The existence of micelles ensures the catalysis of synthesis reactions of hydro silicate during the hardening of cement. This leads to the acceleration of formation of compressive strength and the deformative properties of concrete. An increase in the content of the given surface-active substances to a specific magnitude, which depends on the type of the used cement and the composition of concrete, leads to an increase in the strength of concretes and the rate of its formation. The magnitudes of strength of the obtained concrete and the rate of its formation also depend on the type of the utilized cement and the composition of concrete. At the same time, the optimum content of these surface-active substances, which ensures maximum magnitude of the initial modulus of elasticity of concrete prior to the age of concrete of 28 days, has not been practically established. The value of initial modulus of elasticity of concrete at this age is proportional to its content of the surface-active substances that form micelles.

The studies conducted make it possible to determine the methods of control over the strength and deformativeness of fine-grained concretes for shortening the time of constructing the monolithic and the duration of hardening of the prefabricated ferroconcrete structures.

Keywords: fine-grained concrete, nano-modifier, modulus of elasticity, micellar catalysis, surface-active substances.

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DOI: 10.15587/1729-4061.2017.101071

USAGE OF MOTHER LIQUOR RECYCLING FOR THE OBTAINING OF Fe(VI) COMPOUNDS (p. 55-59)

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In order to improve the indexes of ferrates(VI) synthesis and reduce production costs of the target product, we studied the recycling features of spent mother liquor. It is shown that the composition of mother liquors depends on the method of obtaining Fe(VI) compounds. Low-temperature salting-out is offered as the main technological decision for recycling. The solubility of K_2FeO_4 and some ballast salts (KCl, KNO_3, K_2SO_4), which accumulate during the synthesis of ferrate in the mother liquor and when OH^- ions are in large excess has been studied. It is shown that the solubility of the target product decreases with increasing concentration of potassium hydroxide and is ~0.7 g/l in 14.3 M KOH at 20 °C. The influence of temperature and concentration of potassium hydroxide on the solubility of ballast salts has been studied and it is found out that for the effective removal of impurities it is necessary to maintain temperature within the range 0–10 °C at C (KOH)=14 M.

It has been established that the electrochemical synthesis of crystalline K_2FeO_4 based on the transpassive dissolution of Fe in the concentrated NaOH solution is impractical, as profitable recycling of the spent mother liquor is practically impossible.

It has been determined that with the hypochlorite method of obtaining ferrates(VI), the least amount of impurities enters the system when FeO(OH) is used as the initial Fe-containing precursor. At the same time, the least amount of OH^- anions is also used for the formation of 1 mole of the target product. Therefore, the recycling of the mother liquor for synthesis based on FeO(OH) is the simplest and the most profitable.

Keywords: obtaining of Fe(VI) compounds, hypochlorite, electrosynthesis, recycling, mother liquor.

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DOI: 10.15587/1729-4061.2017.100982

STUDY OF THERMAL DEHYDRATION OF SODIUM ORTHOPHOSPHATE MONOSUBSTITUTED
(p. 60-66)

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Depending on the conditions of conducting the synthesis, it is possible to obtain polymeric phosphates of different composition and structure. The mixtures of polyphosphates, employed in the production of technological lubricants, are expedient to synthesize by the high-temperature dehydration of sodium orthophosphate monosubstituted. The temperature ranges, over which the thermochemical transformations of sodium orthophosphate monosubstituted with the formation of polyphosphates proceed, are established by the thermogravimetric method. The composition of polyphosphates is determined using the X-ray phase analysis. Quantitative composition of the mixtures of polyphosphates is determined by applying the original method of eluent ion-exchange chromatography. It is established that the basic products of thermal dehydration of sodium orthophosphate monosubstituted in the range of temperatures 200–650 °C are $Na_3P_3O_9$, $Na_2H_2P_2O_7$ and $Na_6P_6O_{18}$. Thermochemical transformations of NaH_2PO_4 into $Na_6P_6O_{18}$ at temperature 650 °C are accompanied by the side reactions of formation of $Na_3H_2P_3O_{10}$. We proposed the chemical scheme of the high-temperature dehydration of sodium orthophosphate monosubstituted. Kinetics of the isothermal process of obtaining the polymeric phosphates from sodium orthophosphate monosubstituted at different temperatures is examined.

We established quantitative composition of the mixtures of inorganic polymeric phosphates depending on the duration of isothermal process of dehydration. The possibility of obtaining a salt mixture of polymeric phosphates of the assigned qualitative and quantitative composition is demonstrated. We proposed to use the mixture: 76 % $Na_6P_6O_{18}$, 8 % $Na_2H_2P_2O_7$, 8 % $Na_3H_2P_3O_{10}$, 8 % NaH_2PO_4, obtained at 650 °C, as the basic phosphate component of technological lubricants for the hot rolling of pipes.

Keywords: polymeric phosphates, high-temperature dehydration, sodium orthophosphate monosubstituted, chemical scheme.

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