ABSTRACT AND REFERENCES

TECHNOLOGY OF ORGANIC AND INORGANIC SUBSTANSE

TRANSPORT PROCESSES IN POLYMER MEMBRANES. PART 4 (p. 4-11)

Inessa Burtna, Otar Gachechiladze

This paper is the fourth in a series of scientific papers on the transport of solvent molecules in polymer membranes. The objectives on realizing the basic properties of the polymer membrane - "semi-permeability" – determining thermodynamic and kinetic parameters of the system solvent-polymer membrane during the passage of small solvent molecules through the membrane body are clearly stated in the paper. It is shown that the thermodynamic conditions, required for dissolving any solvent in the given membrane can be determined and predicted. Things stand worse with describing the kinetic processes of solvent molecules motion in the macromolecular structure of the polymer membrane. The basic problem, which is that the thermodynamic system solvent-membrane and all the processes, occurring in the system, are not perfect and so they cannot be described by classical laws such as Henry's or Fick's laws, is defined. In this paper, the authors have made an attempt to determine the main kinetic parameters using the results of sorption and desorption of various solvents in the membranes, differing by the macromolecular lattice stiffness. These results correlate well with the structural feature of membranes, as well as properties of solvents. The method of representing bulk diffusion processes as a combination of several individual diffusion parts of the membrane, which are suitable for applying classical diffusion laws and determining their numerical values, is noteworthy.

Keywords: membrane, solvent, dissolution rates, swelling, diffusion, the classical laws, sorption, desorption

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NITROGEN FERTILIZERS CAPSULATION WITH CHICKEN MANURE SUSPENSION IN THE FLUIDIZED BED DEVICE (p. 11-15)

Ruslan Ostroha, Mykola Yukhymenko

Despite the widespread use of nitrogen fertilizers in the cultivation of crops, they have an increased solubility of nutrients, which leads to disruption of the biological rhythm of plant growth and fertilizer overuse. In the paper, it is proposed to cover mineral granules with organic coating in the form of chicken manure. A fluidized bed device should be considered as the most efficient device for mineral granules capsulation. To study this process, the experimental device is proposed and the method of carrying out experiments is developed. Temperature conditions of urea granules capsulation by the chicken manure suspension are established experimentally and the optimal operating mode of the process is determined. The mathematical description of the granule size distribution during capsulation, and the results of analytical calculations and their comparison with the experimental data, is given. This allows predicting the change of the average diameter of granules during capsulation in the fluidized bed.

Keywords: capsulation, fluidized bed, suspension, chicken manure, temperature mode, distribution function.

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MODEL OF CONTINUOUS NITRATION OF BENZENE IN PERFECT MIXING REACTOR (p. 16-22)

Serhiy Kondratov, Mokhammed Al Khamadani

A dynamic mathematical model for the continuous nitration of benzene with a mixture of sulfuric and nitric acids in the perfect mixing reactor, taking into account chemical and physico-chemical processes, allowing to simulate processes in the industrial nitration reactor, was developed. It was found that the model has only one steady state, indicating the reactor stability. The steady state with increasing the spent acid module and reducing the residence time shifted towards reducing the degree of benzene and temperature conversion.

Based on the computer simulation method of constructing the tolerance range of input variables (module and concentration of spent acid, residence time, reduced heat transfer), ensuring that the output variables (temperature and conversion degree) are in the normative specified value ranges, was developed. For a series of module values and the spent acid concentration the values of the minimum residence time were determined, the equations connecting the upper and lower boundaries of the heat transfer with the residence time in the nitration reactor were obtained.

The obtained results can be used for solving problems related to the design of reactors and control systems of benzene nitration process.

Keywords: benzene, continuous nitration, mathematical model, stationary states, heat transfer, interval estimation

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COOLIGOMERIZATION OF C_9 FRACTION UNSATURATED HYDROCARBONS INITIATED BY PEROXIDES (p. 23-28)

Bohdan Dzinyak

Today one of the ways of efficient use of ethylene production by-products, namely liquid pyrolysis products (LPP) of petroleum fractions is obtaining cooligomers - petropolymeric resins (PPR), used as substitutes for natural products in various industries. One method of industrial obtaining of PPR is cooligomerization of unsaturated hydrocarbons, contained in LPP fractions, initiated by organic peroxides. But at the same time, to obtain PPR with a satisfactory yield, considerable reaction time, increased concentration and dosed supply of initiator are needed. For increasing the PPR yield, it is expedient to raise the process temperature that requires using heat-resistant initiators, among which silicon peroxide compounds are of great interest.

As a result of experimental studies, cooligomers from C_9 fraction hydrocarbons of diesel fuel LPP using a number of heat-resistant organosilicon peroxides are obtained. The basic regularities of cooligomerization of C_9 fraction unsaturated hydrocarbons, initiated by organosilicon peroxides are determined, the influence of the main factors (temperature, reaction time, nature and concentration of initiator) on the yield and physicochemical characteristics of the obtained cooligomers is defined. The relationship between the structure of peroxides and their effectiveness in the cooligomerization reaction is shown. The efficiency of using tris-tert-butylperoxy-vinylsilane, which provides increased raw materials hydrocarbons conversion and PPR yield is proved. Based on statistical analysis of the obtained results, regression equations are constructed and optimal technological parameters, which allow to obtain PPR with high yield, low color index and high bromine number value are selected.

The obtained results are of practical interest in refining pyrolysis by-products for obtaining petropolymeric resins.

Keywords: liquid pyrolysis products, fraction, hydrocarbons, initiator, peroxide, petropolymeric resin, cooligomerization

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ANALYSIS OF POSSIBILITY OF HYDROMETALLURGICAL PROCESSING OF LEAD-CONTAINING SLUDGES (p. 28-31)

Viktoria Kosenko, Olga Kubyakina

The main world trends of obtaining lead by processing lead-containing dust were studied, the main advantages and disadvantages of these methods were defined. The composition of coarse and fine dust, which is formed during lead raw material smelting and essential elements, which are lost with them, was given. It was found that the low-temperature processes, i.e. sludge processing using hydrometallurgical methods are the most promising for fusible and toxic lead. The method, which consists of two stages of sludge processing: hydrometallurgical and pyrometallurgical, was proposed. A thermodynamic analysis of the process under study was carried out, the results of which showed that conducting the process of lead-containing sludge processing according to the given technology improves the cost-effectiveness of the process by reducing costs for equipment and electric heating.

Keywords: lead dust, battery scrap, roraty kiln, sodium carbonate, lead-containing sludge.

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MONTE-CARLO METHOD APPLICATION IN SIMULATIONS OF ELECTRON PROCESSES AT IMPACTS OF ATOMS WITH THE SURFACE (p. 32-37)

Michael Grankin, Anatoliy Kargin

High-efficient energy accommodation of heterogeneous chemical reaction of hydrogen atom recombination by electron subsystem ZnS, ZnS, CdS-Ag, exposed to ionizing radiation is investigated. It is shown that the effect of ionizing radiation on ZnS, ZnS, CdS-Ag increases the reaction heat accommodation rate on the electronic channel by several orders. A model of the mechanism of the heterogeneous recombination of atoms on ZnS, ZnS, CdS-Ag, with the participation of metastable electronic states, generated by ionizing radiation is developed. Numerical and mathematical simulation of the surface processes using the Monte Carlo method is performed. It is found that the electron channel of accommodation may be the main channel for the H atoms recombination energy accommodation on the considered samples if they are exposed to ionizing radiation. The regions of activation and relaxation catalysis of the H atoms recombination reaction on the ZnS, ZnS, CdS-Ag are defined. The considered problem of exothermic reaction energy accommodation is of a general nature and carries information about the surface and physicochemical processes on it that is important for the physics and technology of semiconductors, catalysis and plasma chemistry.

Keywords: Monte Carlo method, mathematical simulation, algorithm, accommodation, surface, ZnS, UV radiation, hydrogen, chemical reaction.

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IMPROVEMENT OF CATALYTIC ACTIVITY OF ACTIVATED BENTONITE CLAY BY TREATMENT WITH CETYLTRIMETHYLAMMONIUM BROMIDE (p. 38-42)

Taras Voronchak, Irena Nykulyshyn, Zorian Pikh, Anna Rypka, Zoriana Gnativ

It was found that treatment of activated bentonite clay (ABC) with cetyltrimethylammonium bromide (CTAB) allows to reduce the average particle size due to the partial stratification of sheet aluminum silicate. Thus, the available specific surface area increases, and, therefore, the number of active centers, which can be involved in chemical reactions grows. Using the activated bentonite clay during cooligomerizing the mixture, which models the composition of C_9 fraction of liquid pyrolysis products of diesel fuel in the raw state and after treatment with surfactant showed that the surfactant catalyst treatment allows to increase significantly the cooligomer yield.

However, the positive effect of this treatment is observed only when the CTAB/ABC ratio value is less than 0.2, and 0.1 can be considered as the optimum ratio. When using too many surfactants, the cooligomer yield falls despite the increase in the available specific surface area and becomes equal to zero at the CTAB/ABC ratio ≥ 0,3. This phenomenon is most likely caused by deactivation of active centers of catalyst by the surfactant residues, molecules of which are able to react with the indicated centers.

This technique can be used for improving the catalytic activity of other catalysts of clay nature, which can be used not only in cooligomerization processes, but also in other reactions, which use acid-base catalysis.

Keywords: activated bentonite clay, catalysis, cooligomerization, surfactant, particle size, ζ-potential.

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DETERMINATION OF THE MASS-TRANSFER COEFFICIENT IN DESIGNING HETEROGENOUS CATALYTIC PROCESSES (p. 42-45)

Anna Ponomarenko, Valery Ved

Description of mass-transfer heterogeneous catalytic processes based on the experimental data, obtained when studying the thermocatalytic benzene vapor destruction reaction on the solid catalyst of the $Co_3O_4/\alpha\text{-}Al_2O_3$ system is performed. The dependences of mass-transfer coefficient on such parameters as the phase contact time, the surface concentration of the catalytically active component on the carrier, and the initial hydrocarbon concentration in the gas flow are described. A method for calculating mass-transfer coefficient of heterogeneous catalytic conversion of gaseous impurities, which includes all the above parameters is proposed. Temperature dependences of mass-transfer coefficient of the studied process obtained based on the proposed method and experimental data, on the phase contact time, the surface concentration of the catalytically active component on the carrier, and the value of the initial benzene vapor concentration in the gas flow are built. The adequacy of the obtained mathematical dependence is confirmed by computational methods that allows to use it for intensifying the mass-transfer processes during heterogeneous catalytic reactions in catalytic converters.

Keywords: mass transfer, mass transfer, catalysis, hydrocarbon destruction, heterogeneous catalytic process, removal of gaseous impurities.

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NUMERICAL STUDY OF THE NITROGEN OXIDES ADSORPTION AND STORAGE (p. 46-49)

Svitlana Prymyska, Yuri Beznosyk, Wladimir Reshetilowski

Adsorption of nitrogen oxides in the micropores of solid sorbent becomes an alternative to storage of compressed gas for the next decades. Thus, the effectiveness of the method of nitrogen oxides concentration in the zeolite micropores is experimentally investigated. The model of mass transfer in the adsorber is presented as non-equilibrium. The formulated mathematical problem is a system of three equations: the kinetic equation, the equilibrium equation and the continuity equation. Solution of the mathematical model was achieved using the finite difference method. Comparison and agreement of the numerical results of the developed model with experimental data was performed, the agreement is within 10–12 %. When modeling numerical calculations, the complex of temperatures of 298-318 K and pressure of 0.15-3.5 MPa in the adsorber was covered. Based on the obtained data it was concluded that storage of nitrogen oxides in the adsorber, filled with zeolite is an efficient method of concentrating nitrogen oxides (twice more efficiently compared with the conventional gas compression). Mathematical model adequately describes the concentration process, it is amenable to direct solution and can be used in practice to optimize the operation of adsorber and forecast its basic performance features. This technology also allows to reduce the operating pressure that is a very important economic and technological factor in implementing the process at the industrial level.

Keywords: nitrogen oxides, modeling, adsorption, storage, zeolites

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MATHEMATICAL MODEL OF ADJUSTMENT STRETCHING SHOE LEATHER MATERIAL WITH MINERAL FILLING (p. 50-56)

Oksana Kozar, Viktor Konoval, Boguslaw Wozniak, Andriy Olenich

Shoe shape stability is one of the most important indicators of quality which depends primarily on the deformation properties of the skin, its stretching. It is possible to increase shoe shape stability using the technological process of adjustment operations of stretching the skin to optimal values , which are necessary for the production of high quality footwear.

Ductility index influences the percentage of leather waste in the performance of recover and last operations , i.e. material resource saving and cost of shoes. We present a mathematical model of stretching adjustment of the skin with mineral content to accurately calculate the area of parts of the work piece in this paper. The proposed concept of stretching adjustment method involves iterative process of skins preliminary tensile elongation with fixation of each cycle. The physical model of the process has been built, including hydration operations, stretching, drying in a stretched state and relieve of tension. By means of mathematical analysis and the theory of sets, the dependence of the residual elongation size of the researched skins on the degree of hydration of the skin, stretching the size and number of repeated stretching has been found.

Implementation of the correction stretching process of shoe leather will reduce the material and energy resources while improving the competitiveness of shoes.

Keywords: leather, shoes, natural minerals, formation, residual deformation, shape stability, quality.

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