XIX МЕЖДУНАРОДНАЯ НАУЧНАЯ КОНФЕРЕНЦИЯ «ФИЗИКО-ХИМИЧЕСКИЕ ПРОЦЕССЫ В АТОМНЫХ СИСТЕМАХ»

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2024

3-5 декабря

ТЕХНИЧЕСКАЯ ПРОГРАММА

РОСАТОМ

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НИЯУ МИФИ

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Technical Program and Abstracts

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The book of abstracts and poster presentations at the XIX International Scientific Conference “Physical and Chemical Processes in Atomic Systems” is devoted to the separation of isotopes that are in demand for nuclear energy, medicine and other applications as well as the separation of liquids and gases and by membrane technology.
The conference is held in accordance with “The plan of scientific and technical conferences, meetings, seminars, and schools by the enterprises and organizations of the State Atomic Energy Corporation ROSATOM in 2024”. It is dedicated to the 300th anniversary of the Russian Academy of Sciences.

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TECHNICAL PROGRAM

December 3, 2024
Hotel Intourist-Kolomenskoe

9:30 – 10:00	Registration of participants	
10:00 – 10:20	Opening ceremony	V.E. Cherkovets *Scientific Director SRC RF TRINITI, Professor* G.D. Zasukhina-Petryanova *The Vavilov Institute of General Genetics RAS, Chief Researcher* K.I. Ilin *SNC RF TRINITI, Director* A.K. Budyka *Rosatom, Scientific Secretary*
10:20 – 10:45	Features of disperse systems in gas phase: theory and experiment	V.A. Zagaynov *Dept. of General Physics, NRNU MEPhI*
10:45 – 11:05	FlowVision: numerical modeling of physical and chemical processes in nuclear industry problems	S.V. Zhluktov *TESIS*
11:05 – 11:30	Waves in gas centrifuges	S.V. Bogovalov *Dept. Molecular Physics, NRNU MEPhI*
11:30 – 12:00	Coffee Break	
12:00 – 12:25	Generalization of the Q-cascade theory to include material losses and gains	Zeng Shi *Dept. Engineering Physics, Tsinghua University, Beijing, P.R.China*

12:25 – 12:50	An efficient method for calculating muti-component square cascades	Quanxin Xie *Research Institute of Physical and Chemical Engineering of Nuclear Industry Tianjin, P.R.China*
12:50 – 13:15	Production of highly enriched isotope 10B by laser separation in combination with conventional enrichment methods	V.B. Laptev *Department of laser spectroscopy, Institute of spectroscopy of RAS*
13:15 – 14:15	Lunch Break	
14:15 – 14:40	Prediction of the selectivity of gas separation membranes	A.O. Malakhov *A.V.Topchiev Institute of Petrochemical Synthesis RAS*
14:40 – 15:05	Gas separation properties of membranes based on polyethyrimides of copolymer structure	A.V. Varezhkin *Institute of Materials for Modern Energy and Nanotechnology Mendeleev University of Chemical Technology of Russia*
15:05 – 15:30	Demonstration of efficiency of detritization of NPP unbalance water by the isotopic exchange method in the system H2 – H2O	M.B. Rosenkevich *Dept. Technologies of isotope separation and Hydrogen Energetic, Mendeleev University of Chemical Technology of Russia*
15:30 – 16:00	Coffee Break	
16:00 – 16:40	A retrospective of isotope separation technologies. Little-known facts and myths in the history of gas centrifuge development	G.M. Skorynin *Veteran of the nuclear industry*
16:40 – 17:05	Isotope technologies in medicine and industry, key products of State Atomic Energy Corporation Rosatom	O. Valzdorf *Head of the Marketing Department JSC Isotope*
17:05 – 18:00	Poster Session (Conference Hall Moskvorechie)	

December 4, 2024
Hotel Intourist-Kolomenskoe

10:00 – 10:30	Technological processes with laser irradiation of gaseous and condensed media	A.F. Glova *SRC RF TRINITI*
10:30 – 11:00	Using a weak longitudinal magnetic field to form an extended tubular plasma in argon at low pressure	A.V. Petryakov *SRC RF TRINITI*
11:00 – 11:30	Charging of dust particles in humid air plasmas created by an external source of gas ionization	A.V. Filippov *SRC RF TRINITI*
11:30 – 12:00	The main regularities of radiation corrosion of iron. current state, problems and prospects	N.I. Trushkin *SRC RF TRINITI*
12:00 – 12:30	Coffee Break	
12:30 – 13:00	Comparative analysis of promising antitumor drugs for prostate cancer therapy in in vitro experiments	D.Y. Chuvilin *Deputy Head of Kurchatov Complex of Physical and Chemical Technologies, National Research Center "Kurchatov Institute"*
13:00 – 13:25	Structural factors determining the relationship between thermal conductivity, electrical conductivity and elastic modulus of carbon fibers	V.M. Samoilov *JSC Research Institute for Graphite-Based Structural Materials "NIIgrafit"*
13:30 – 14:30	Lunch Break	

14:30 – 14:55	Synthesis of SiC/SiC composite materials by electroforming, impregnation and pyrolysis methods	M.A. Sokolov *National Research Center "Kurchatov Institute"*
14:55 – 15:20	Optical properties of thermal-radiation-modified polytetrafluoroethylene films irradiated by accelerated xenon ions	A.S. Smolyanskii *Laboratory of Functional Nanocomposites, Department of Kinetics and Catalysis, N.N. Semenov Federal Research Center for Chemical Physics*
15:20 – 15:50	Coffee Break	
15:50 – 16:15	Features of recombination processes of photoexcited charge carriers in porous anodic aluminum oxide	E.A. Konstantinova *Physics Department M.V. Lomonosov Moscow State University*
16:15 – 16:40	Oil spill removal with nonwoven materials produced by melt electrospinning	S.N. Malakhov *National Research Center "Kurchatov Institute*"
16:40 – 18:00	Continuation of Poster Session	

December 5, 2024
Hotel Intourist-Kolomenskoe

10:00 – 10:30	Biomedical applications of nanofiber materials	T.H. Tenchurin *National Research Center "Kurchatov Institute"*
10:30 – 11:00	Aerosol filtration in high-tech applications	V.A. Kirsh *A.N. Frumkin Institute of Physical Chemistry and Electrochemistry*
11:00 – 11:30	"Nuclear winter" and other aerosol climate disasters	A.S. GinzburgA. M. *Obukhov Institute of Atmospheric Physics*
11:30 – 12:00	Current state of small systems thermodynamics	Yu.K. Tovbin *A.N. Frumkin Institute of Physical Chemistry and Electrochemistry*
12:00 – 12:30	Coffee Break	
12:30 – 12:45	Hydrodynamic theory of mixed type fiber filter	R.F. Mardanov *Kazan Federal University*
12:45 – 13:00	Comprehensive assessment of the effectiveness of the NEVA filter material for its use in the manufacture of respirators intended for the use of atomic energy	L.E. Nazarova *LLC "Respiratory Complex"*
13:00 – 13:15	Flow models of nanofibers and nanoparticles at low Knudsen numbers	Sh.Kh. Zaripov *Kazan Federal University*
13:15 – 13:30	Dry aerosol printer for forming micro-sized objects on various substrates	V.V. Ivanov *Moscow Institute of Physics and Technology*
13:30 – 14:30	Lunch Break	

14:30 – 14:45	Numerical methods and phase transitions in the equations of aggregation-fragmentation of substances	R.R. Dyachenko *HSE University and Skolkovo Institute of Science and Technology* *Marchuk Institute of Numerical Mathematics, RAS*
14:45 – 15:00	Aerosol synthesis of single-walled carbon nanotubes	A.G. Nasibulin *Skolkovo Institute of Science and Technology*
15:00 – 15:15	Cold sonoluminescence of cavitation bubbles in water	V.V. Maksimenko *Dept. of General Physics, NRNU MEPhI*
15:15 – 15:30	Chemical processes in atmospheric haze	A.N. Ermakov *V.L. Talrose institute for energy problems of chemical physics*
15:30 – 16:00	Evaluation of the effectiveness of personal respiratory protective equipment (PPE) considering the behavior of bioaerosols containing pathogen-containing viruses	D. A. Pripachkin *NRNU MEPhI*
16:00 – 16:30	Experience in implementing scientific and practical approaches to the study of radioactive aerosols in the nanometer range	M.E. Vasyanovich *Institute of Industrial Ecology UB RAS*
16:30 – 17:50	Continuation of Poster Session	
17:50 – 18:00	Award for the best poster presentation	
18:00	Closing Ceremony	

ABSTRACTS

ORAL PRESENTATIONS

FEATURES OF DISPERSE SYSTEMS IN GAS PHASE: THEORY AND EXPERIMENT

V.A. Zagaynov[1], S.V. Kharakos[2]

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The history of the study of dispersed systems in the gas phase has more than 100 years. Nevertheless, both the description of the processes that take place in it and the measurement of the dispersed composition of these systems remain a rather difficult problem that has not been completely solved. Numerous model approaches have been created in the field of theory, which gave an adequate description in the limited conditions of reality, at the same time, no general theory has been created. The most adequate approach was proposed by Smolukhovsky in 1917, but his equation did not determine the efficiency coefficients of collision and evaporation of particles, information about which could be obtained from the theory of kinetics and dynamics of collisions. After that, there were approaches by Szillard, Farkas, Frenkel, Zeldovich and many other researchers, which were valid only for limited conditions of formation of the dispersed phase. A.A. Lushnikov proposed the theory of sol-gel transition, which at that time was a significantly new effect in the theory of dispersed systems. At the same time, a general approach to solving the problem of the formation of a dispersed phase has not yet been proposed. A similar situation exists in the field of experiment. For a range of sizes from tens of micrometers to 0.2 microns, optical particle detection methods work quite well. In the range of sizes from 3 nm to 0.2 microns, methods of electrical mobility and a diffusion dynamic method with all their disadvantages and limitations have been developed. However, reliable methods for measuring the particle size spectrum in the gas phase do not yet exist for the size range from molecular to 3 nm. At the same time, these problems remain extremely relevant in various fields of human activity – medicine, energy, climatology, meteorology and others.

FLOWVISION: NUMERICAL SIMULATION OF PHYSICAL AND CHEMICAL PROCESSES FOR PROBLEMS IN NUCLEAR INDUSTRY

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The FlowVision software is used in nuclear industry since 2002. The software sequentially integrates the partial differential equations constituting the mathematical model of the problem solved. The following processes are simulated: fluid and gas motion, described by the full Navier-Stokes equations, flows with contact surfaces, flows with particles, flows in porous media, heat transfer including conjugate heat transfer, mass transfer with chemical reactions, turbulence, processes on solid surfaces, radiation. The processes are toggled on and off depending on the particular problem. Numerical integration of the governing equations is performed using an implicit method. Pressure-velocity splitting approach is implemented for integration of the Navier-Stokes equations. The method enables moving and contact boundaries in the computational domain. The boundaries are treated within the Euler paradigm (the grid does not move). The method allows time integration of the governing equations with steps exceeding the explicit time step by orders of magnitude. FlowVision automatically builds Cartesian adaptive locally refined grids. Initial cells of a grid are hexahedral. A cell crossed by a curvelinear or complex boundary transforms into a polyhedral in a natural way – it is truncated by the boundary. The equations are approximated by a high-order scheme both in hexahedral and polyhedral cells. In regions of high gradients, dynamic adaptation is performed according to the specified adaptation criteria. Presentation describes the models implemented in the FlowVision software: turbulence models, models of turbulent heat transfer, radiation models, mass transfer models, models related to particles flows and porous media, models for simulation of oxidation of nuclear graphites.

Keywords: turbulence, heat and mass transfer, chemical reactions, particles flow, graphite oxidation

WAVES IN GAS CENTRIFUGES

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We present studies of waves in gas in centrifugal fields of gas centrifuges. We have obtained a full spectrum of waves consisting of five modes. The connection of these waves with buoyancy waves in a gravitational field is discussed. There are common features and significant differences. Of particular interest are the purely acoustic waves that we discovered, propagating strictly along the rotation axis. The energy density of these waves is concentrated near the rotor walls. These waves have the lowest attenuation compared to all other types of waves. Estimates of the attenuation decrement of these waves are given. The possible influence of these waves on the dynamics of gas and on the process of separation of binary isotope mixtures in gas centrifuges is discussed.

Keywords: waves, separation of isotopes, gas centrifuges

GENERALIZATION OF THE Q-CASCADE THEORY TO INCLUDE MATERIAL LOSSES AND GAINS

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Material losses and gains can hardly avoided in isotope separation cascades because of chemical reactions of process gas with its contacting materials or/and thermal decomposition of process gas. The well-known Q-cascade model was generalized to be able to deal with the situations with both material losses and gains. To verify the correctness of the generalization, three test cases were investigated in separation of natural uranium to produce an LEU of 5% ^{235}U, in which UF_6 incur material losses, generating the light impurity HF. Without taking any measures to control the HF concentration, HF would accumulate at the product end of cascade and endanger the cascade safe operation. The HF concentration can be controlled by two approaches, one using a carrier gas and another removing HF to suppress the HF concentration in the product down to the required level. The results showed that using carrier gas needed a large quantity of it and increased the relative total flow of cascade, whereas removing HF required a technology with a strong capability of HF elimination. The results demonstrate the applicability of the theory in the study of separation cascades, but further improvements are necessary in order to solve more complicated practical cases such as multiple feeds and withdrawals.

Keywords: Isotope separation, Multicomponent, Cascade, Q-cascade theory, Material losses and gains

AN EFFICIENT METHOD FOR CALCULATING MUTI-COMPONENT SQUARE CASCADES

Quanxin Xie, Liming Wang, Chengye Liu

Research Institute of Physical and Chemical Engineering of Nuclear Industry, Tianjin 300180, P.R.China

The stationary mass transfer of a multi-component isotopic mixture in a square cascade is usually calculated by using numerical iteration methods. A " quasi-linearization" method, in which the normalization condition of component concentrations is used to accelerate the convergence process, is presented in this pater. It is not necessary for this method to use a weight factor that appears in some numerical iteration methods and affects the iteration convergence. The method possesses considerable high convergence rate.

ПРОИЗВОДСТВО ВЫСОКООБОГАЩЕННОГО ИЗОТОПА ^{10}B МЕТОДОМ ЛАЗЕРНОГО РАЗДЕЛЕНИЯ В КОМБИНАЦИИ С ТРАДИЦИОННЫМИ МЕТОДАМИ ОБОГАЩЕНИЯ

В.Б. Лаптев, Г.Н. Макаров, А.Н. Петин, С.В. Пигульский, Е.А. Рябов

Отдел лазерной спектроскопии ФГБУН Институт спектроскопии РАН, Москва, Троицк, 108840 Россия

Изотоп бор-10 (^{10}B) широко используется в атомной энергетике в системах управления и защиты (СУЗ) ядерных реакторов, а также в системах регулирования тепловыделения и аварийного охлаждения реакторов (в форме борной кислоты). В процессе эксплуатации элементов СУЗ, содержащих изотоп ^{10}B, происходит его постепенное выгорание, что обусловливает необходимость их регулярной замены. Несмотря на чрезвычайную стратегическую важность бора-10 для отечественной промышленности и энергетики, в России ^{10}B практически не производится в промышленных объемах и существующие потребности в данном материале удовлетворяются в основном за счет импортных поставок.

Проведен сравнительный научно-технический анализ наиболее перспективных традиционных способов обогащения изотопа бора-10 и лазерного метода разделения изотопов, основанного на эффекте изотопически селективной ИК многофотонной диссоциации (МФД) борсодержащих молекул под действием резонансного излучения импульсного CO_2-лазера. Предложены различные варианты реализации лазерного метода, как в чистом виде, так и в комбинации с традиционными технологиями. Сделан вывод, что использование лазерного метода в любом варианте приведет к существенному снижению капитальных и текущих затрат при производстве ^{10}B в промышленном масштабе и, соответственно, к уменьшению себестоимости продукции.

Ключевые слова: обогащение изотопа бор-10, традиционные методы обогащения, изотопически селективная ИК многофотонная диссоциация молекул, сравнительный анализ

PREDICTION OF THE SELECTIVITY OF GAS SEPARATION MEMBRANES

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Polymeric membranes are used to separate nitrogen from air, carbon dioxide from natural gas, C_{2+} hydrocarbons from natural gas, for separation of olefins and paraffins. For most of the polymers studied, permeability measurements were performed in single gas conditions. However, experimental data accumulated over the years show that measurements of permeabilities of pure gases cannot serve as a reliable basis for characterizing membranes in mixed-gas conditions. The so-called ideal selectivity α_{12}, calculated by the ratio of the permeabilities for pure gases 1 and 2 can differ rather significantly from the actual, mixed-gas selectivity α_{12}^{mix}.

Theoretically, the description of gas mixture permeation based on irreversible thermodynamics results in a system of differential equations for component fluxes that include sorption and diffusion coupling effects. These equations can only be solved using numerical methods. As a practical matter, it is highly desirable to have simple analytical methods for estimating membrane selectivity in the mixed-gas conditions.

A simple explicit expression for mixed gas selectivity was derived using the so-called linear transport model, which is a linearized version of the original differential flux equations. The input parameters for the model are the single gas transport parameters. Testing the linear model using experimental data for the separation of hydrocarbons (*n*-butane/methane, *n*-butane/*i*-butane, propylene/propane) revealed an acceptable fit. A comparison of the model with recent experimental data on the separation of CO_2-containing mixtures using microporous polymers is also presented.

Acknowledgements: The author acknowledge the financial support of the State Program of TIPS RAS.
Keywords: membranes, selectivity, permeability, model, coupling

DEMONSTRATION OF THE EFFICIENCY OF NPP DEBALANCE WATER DETRITIATION BY THE ChIE IN THE $H_2 – H_2O$ SYSTEM METHOD

Yu.S. Pak, A.N. Bukin, S.A. Marunich, V.S. Moseeva, M.B. Rozenkevich

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In 2020, a paper was published [1], where the options for removing tritium from NPP debalance water to a concentration corresponding to the Radiation Protection Standard (RPS) of Russia were considered. In 2024, in accordance with the research project of VNIIAES JSC, an experimental test of the detritiation efficiency of real debalance water from the Leningradskaya and Balakovskaya NPPs was carried out at Mendeleev University. For this purpose, a modified separation installation operating to the technology of countercurrent catalytic chemical isotope exchange (ChIE) of hydrogen with water was used. The main characteristics of the unit: the column diameter is 62 mm, the height of separation part is 4.8 m, the operating temperature is 55^{0}°C, the pressure is 0.1 MPa. The column is packing with a mixed bed of RCTU-3SM hydrophobic catalyst and stainless still spiral packing. An TPE electrolyzer with a capacity of 1 m^3 of hydrogen per hour is used as a unit for converting the water flow from the column to hydrogen. Tritiated water from the NPP, with a tritium concentration of 10^5 Bq/kg and flow of 0.4 kg/h was fed to the electrolyzer. An equal flow of distilled water of natural isotopic composition was fed to irrigate the column. Continuous operation of the separation column continued until the tritium concentration in the electrolyzer water reached 10^6 Bq/kg. In accordance with the task, the target function of the column operation was the concentration of tritium in hydrogen at the outlet of the column. During the entire period of the installation operation, tritium concentration did not exceed 50 Bq/m^3 at the level of 1900 Bq/m^3 permitted in the RPS. Thus, the work performed demonstrated the high efficiency of using ChIE technology for detritiation of unbalanced waters.

[1] M.B. Rozenkevich et al. Atomic–Hydrogen Energy and Tritium Purification of NPP Discharges Based on WWER Generation 3+ Reactors// Nanotechnologies in Russia, 2020, Vol. 15 Nos. 3–6, pp. 362–367,

GAS SEPARATION PROPERTIES OF MEMBRANES BASED ON POLYETHYRIMIDES OF COPOLYMER STRUCTURE

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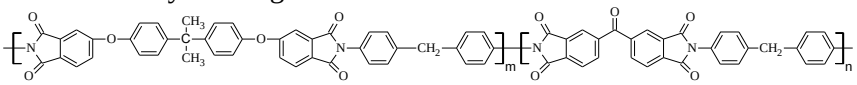
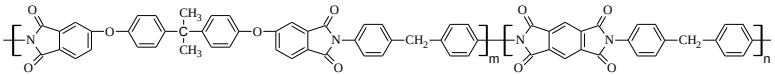
The purpose of the study is to develop a polymer membrane material for the separation of hydrogen and helium from gas mixtures. 2 lines of polyethyrimides of copolymer structure have been synthesized: a line with laboratory labeling MAB



and MAP



The MAB line was synthesized by polycondensation of 4,4-diaminodiphenylmethane (MDA) with a mixture of bisphenol-A (BFADA) dianhydrides and 3,3,4,4-benzophenonetracarboxylic acid (BFDA). The MAP line was synthesized by polycondensation of MDA with a mixture of pyromellitic acid dianhydrides (PMDA) and BFADA.

It was found that at a concentration of rigid-chain BFADA and BFDA above 30%, the synthesized polymer loses solubility, which makes it unsuitable for the manufacture of membranes by converting the polymer into a viscous state through a solution. To study the gas separation properties, polymer films were cast in which the content of hard-chain dianhydride did not exceed 30% mol.

The polymer MAB 90/10 showed the same selectivity in the separation of H_2/N_2 gas vapor with respect to the industrial polymer Ultem1000, but at the same time its hydrogen permeability is 2.5-2.8 times higher.

Acknowledgements The study was carried out within the framework of the scientific program of the National Center for Physics and Mathematics (project 8 “Physics of Hydrogen Isotopes”, direction 8.1 “Research in the field of interaction of hydrogen with solids”.

Keywords: membrane, polyetherimide, hydrogen, helium, permeability.

RETROSPECTIVE OF ISOTOPE SEPARATION TECHNOLOGIES. LITTLE-KNOWN FACTS AND MYTHS IN THE HISTORY OF GAS CENTRIFUGES

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Many famous scientists and designers participated in the creation of isotope theory and the development of separation methods. Some of them devoted most of their creative lives to this topic, while others' contributions were limited to individual episodes, which often remain forgotten for a number of reasons. This report examines the origins of the main concepts and methods of isotope separation. Based on an analysis of primary sources, little-known and forgotten episodes in the lives of outstanding scientists associated with their contributions to the emergence and development of isotope technologies were identified. The main focus of this report is on the milestones in the creation of gas centrifuges, which have ensured Russia's technological leadership in the world market for uranium enrichment and the separation of stable isotopes. An attempt was made to clarify the authorship of technical solutions, the priority of which (so far) has not been agreed upon. One of the goals of the report is to debunk the myths that are abundantly circulating in the media regarding the history of isotope separation technologies.

Keywords: history, isotopes, separation technologies, centrifuges, priorities of creation

TECHNOLOGICAL PROCESSES WITH LASER IRRADIATION OF GASEOUS AND CONDENSED MEDIA

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The results of work on laser technologies are presented, including the influence of the aggregate state of the irradiated medium on the mechanism and efficiency of laser processing of materials.
The speed of remote laser cutting and drilling of metals in the presence of a hydrocarbon flame increases at a radiation intensity of more than 10^5 W/cm^2. The growth occurs due to the brightening of the radiation propagation channel in the flame and the change of the mechanism of melt removal under the action of gravity to the mechanism of removal under the action of a vapor recoil pulse.
The method of applying coatings during laser ablation of particles in a gas-dust medium jet allows to reduce the radiation intensity compared to the ablation of a solid target. The adhesion of the coating to the anode substrate is affected by the negative charge of the particles of the medium by the electrons of the plasma of the auxiliary glow discharge.
Diamond coatings were synthesized on inserts of a turning tool made of WC-Co8 hard alloy when irradiated with a plasma jet of an optical plasmatron. The characteristics of the coatings were measured, and the temperature of electrons in the plasma jet was determined.
The results of work on removing paraffin film from the surface of water using radiation from a pulse-periodic CO_2-laser can be used to clean reservoirs from oil product films.
It is shown that the efficiency of metal cutting in water in the absence of a water and gas jet is almost an order of magnitude lower than in air.
With pulsed laser heating of fuel element shell simulators, the critical heat flux for the first boiling crisis in water increases compared to stationary heating.
The possibility of fast drilling of thin holes in ceramics and metal with millisecond pulses is demonstrated.
It is established that the type of filler affects the speed of laser welding of tapes made of polymer composite materials.

Keywords: laser, radiation intensity, processing efficiency

USING A WEAK LONGITUDINAL MAGNETIC FIELD TO FORM AN EXTENDED TUBULAR PLASMA IN ARGON AT LOW PRESSURE

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The results of experimental studies on the formation and subsequent evolution of extended (l = 300 mm) and thin-walled ($\Delta r \approx 10$ mm) tubular ($2r \approx 110$ mm) plasma in a weak longitudinal magnetic field ($B = 175$ Gs) without the use of a thermionic cathode are presented. The cylindrical chamber in which the tubular plasma was formed was pumped with high purity argon (99.998%) at an average velocity of about 1 m/s at a pressure of $P = 10^{-3}$-10^{-2} Torr. Two methods of creating seed electrons initiating the development of ionization avalanches were used. A difference inherent to these methods has been established in the dynamics of breakdown, completing in the formation of a tubular discharge. In the first of them, a pulsed discharge preceding the high voltage supply of the main discharge created gas preionization in a small area around the sectioned cathodes. In the second method, seed electrons were created in the entire working area of the discharge chamber by an RF discharge with a frequency of 85 kHz and duration of about one second. High-speed shooting with a 4-frame ICCD camera allowed us to establish the dynamics of tubular discharge formation at all its stages. Measurements of the longitudinal and radial discharge current were carried out. The results obtained showed the possibility of spatial isolation of an extended tubular plasma from the close located metal wall of the discharge chamber by using a weak longitudinal magnetic field ($B \approx 0.02$ T).

Keywords:low pressure gas, tubular plasma, preionization, seed electrons, plasma filament, longitudinal magnetic field.

CHARGING OF DUST PARTICLES IN HUMID AIR PLASMAS CREATED BY AN EXTERNAL SOURCE OF GAS IONIZATION

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The paper is devoted to study the charging of micron-sized dust particles in humid air plasmas at different volume rates of gas bulk ionization by an external ionization source, such as a beam of fast electrons with an energy of more than 100 keV. The plasma composition far from the dust particle was determined based on the kinetic model of ion-molecular processes described in detail in [1]. These data served as boundary conditions on the outer boundary of the computational cell. The charging of dust particles was described based on 56 non-stationary balance equations for electrons, negative and positive ions, including hydrated ions containing up to 12 water molecules. The kinetic model of ion-molecular processes included more than 600 reactions, including 9 channels of ionization of humid air molecules under the action of a beam of fast electrons, processes of charge exchange and conversion of ions, processes of recombination of electrons and positive ions, recombination of positive and negative ions, processes of electron attachment.
It has been established that despite the negligibly small number density of electrons far from a dust particle in undisturbed plasma, the charge of dust particles is determined precisely by the electron flux when the gas ionization rate exceeds the critical value. This leads to fairly high values of the dust particle charge. Studies have been conducted on the effect of the ionization rate and gas composition, including air humidity, on the dust particle charge.

[1] A.V. Filippov, et al., J. Exp. Theor. Phys. **125**, 246–267 (2017).

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Keywords: drift-diffusion approach, dusty plasma, micron sized particles, e-beam ionization, ion-molecular processes

THE MAIN REGULARITIES OF RADIATION CORROSION OF IRON. CURRENT STATE, PROBLEMS AND PROSPECTS

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The paper presents the summary results of experimental and theoretical studies of iron corrosion under extreme conditions of radiation exposure of the material. Currently, structural iron-based alloys are widely used in long-term storage systems for radioactive waste. Experimental data on the effect of ionizing radiation intensity, absorbed dose, composition and temperature of the irradiated plasma-forming medium on the rate and nature of corrosion are presented. It has been established that the rate of radiation corrosion of iron depends on both the intensity and the dose of the absorbed energy of radioactive radiation. The crucial role of plasma chemical processes involving long-lived active particles generated by high-energy ionizing radiation in the kinetics and mechanism of radiation corrosion is shown, and the contribution of short-lived plasma components to the corrosion process is established. The results of the analysis of the elemental composition, chemical state and crystal structure of the formed corrosion products, as well as the thickness of the oxidized iron layer, depending on the properties of ionizing radiation and plasma-forming corrosive medium, are presented. It was found that the composition of the products of radiation plasma chemical corrosion of iron in a humid air environment differs significantly from the composition of natural iron oxide formed during open storage of iron samples in air and consisting mainly of a mixture of magnetite Fe3O4 and maghemite γ-Fe2O3. The results of modeling of the effect of the composition of a plasma-forming gas medium on the velocity, kinetics and mechanism of radiation corrosion of iron are presented. It is shown that the current understanding of the mechanism of radiation corrosion is far from complete and does not meet the increasing needs of the nuclear industry. The directions of further experimental and theoretical studies of radiation corrosion are outlined.

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Keywords: iron, corrosion, plasma, radiation, humidity.

СРАВНИТЕЛЬНЫЙ АНАЛИЗ ПЕРСПЕКТИВНЫХ ПРОТИВООПУХОЛЕВЫХ ПРЕПАРАТОВ ДЛЯ ТЕРАПИИ РАКА ПРЕДСТАТЕЛЬНОЙ ЖЕЛЕЗЫ В ЭКСПЕРИМЕНТАХ *IN VITRO*

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Простат-специфический мембранный антиген (PSMA) является перспективной мишенью для диагностики и таргетной терапии рака предстательной железы (РПЖ). Экспрессия PSMA в клетках простаты при РПЖ на порядки превосходит его экспрессию в других тканях и неизменённых клетках предстательной железы. Это даёт возможность напрямую, через таргетные молекулы к PSMA, доставить необходимую дозу радиоактивного вещества в злокачественные клетки. Окружающие здоровые ткани при этом практически не затрагиваются.

Многочисленные исследования свидетельствуют о том, что таргетные к PSMA молекулы отличаются оптимальными химическими характеристиками для комплексообразования с различными радионуклидами. Это объясняет активное использование PSMA-молекул в качестве таргетного носителя для диагностических и терапевтических радионуклидов.

В настоящей работе с целью разработки отечественного препарата для терапии РПЖ было исследовано 3 новых PSMA-молекулы: PSMA-BQ7876 [1], PSMA-D1 и PSMA-D2 [разработка НИЦ «Курчатовский институт»]. Исследования выполнены методом прямого сравнительного анализа с препаратом на основе молекулы PSMA-617, выбранного в качестве фармацевтического прототипа. Проведена оценка специфичности и цитотоксической активности PSMA-комплексов относительно опухолевых клеток (эксперименты *in vitro*): гиперэкспрессирующих PSMA-антиген (культуры клеток 22RV1) и с низкой экспрессией PSMA (культуры клеток PC3).

1. ПСМА-таргетное соединение и его комплекс с радионуклидами для тераностики опухолей, экспрессирующих ПСМА. Патент RU (11) 2 803 734 C1. 05.10.2022. Авторы Толмачев В.М., Орлова А. М., , Сейтова К. и др

СТРУКТУРНЫЕ ФАКТОРЫ, ОПРЕДЕЛЯЮЩИЕ ВЗАИМОСВЯЗЬ ТЕПЛОПРОВОДНОСТИ, ЭЛЕКТРОПРОВОДНОСТИ И МОДУЛЯ УПРУГОСТИ УГЛЕРОДНЫХ ВОЛОКОН.

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Рассмотрены основные свойства структурные модели углеродных волокон (УВ) на основе различных прекурсоров. Дан анализ структурных факторов, определяющих модуль упругости, теплопроводность и электропроводность УВ. Приведены корреляционные зависимости теплопроводности УВ от их модуля упругости и электропроводности. Осуждается возможность прогнозирования продольной теплопроводности УВ на основании данных о модуле упругости и электропроводности.

СИНТЕЗ КОМПОЗИТНЫХ SiC/SiC МАТЕРИАЛОВ МЕТОДОМ ЭЛЕКТРОФОРМОВАНИЯ, ПРОПИТКИ И ПИРОЛИЗА

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Композиты на основе карбида кремния при высоких температурах обладают высокой прочностью, химической и радиационной стойкостью. Возможность получать карбидокремниевую керамику методом пиролиза полимерного прекурсора позволяет получать изделия различных форм и использовать их в различных областях. Некоторые керамические изделия состоят из матрицы и армирующего каркаса из карбидокремниевых волокон.

В докладе представлен новый способ создания SiC/SiC композита. Каркас создают методом электроформования из раствора поликарбосилана в хлороформе. Регулирование интенсивности процесса отверждения (сшивки) нетканого материала позволяет добиться частичного оплавления полимерного мата на стадии пиролиза и образования кораллоподобной 3D структуры из карбидокремниевой керамики, пригодной для использования в качестве армирующего каркаса. В частности, при использовании в качестве приемного устройства графитового барабана, получен образец в форме цилиндрической оболочки. Предложенный способ получения карбидокремневых каркасов, технологически значительно проще и экономически выгоднее существующих методов, основанных на плетении карбидокремниевых волокон вокруг трубчатой подложки. Полученный каркас пропитали раствором полимерного прекурсора и подвергли пиролизу (PIP process). Нетканый материал, керамический мат и композитная цилиндрическая оболочка изучены методами электронной микроскопии и элементного анализа.

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Keywords: карбид кремния, кремнийорганические полимеры, электроформование.

OPTICAL PROPERTIES OF THERMAL-RADIATION-MODIFIED POLYTETRAFLUOROETHYLENE FILMS IRRADIATED BY ACCELERATED XENON IONS

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By means of the methods of optical spectroscopy and diffuse and specular reflection spectroscopy, Fourier-IR spectroscopy and atomic force microscopy as well as GEANT4 modelling, radiation-induced changes in the optical properties of thermoradiation-modified Polytetrafluoroethylene (TRM-PTFE) films irradiated with accelerated xenon ion flows with an energy of 1 MeV/nucleon in the fluence range from 10^8 to 10^{11} cm^{-2} at the U-400 heavy ion accelerator in the Flerov Laboratory of Nuclear Reactions at the Joint Nuclear Research Institute (Dubna, Moscow Region, Russian Federation) were studied for the first time.

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Keywords: Polytetrafluoroethylene, Xe ion irradiation, optical transmittance, reflectance, atomic force microscopy

FEATURES OF RECOMBINATION PROCESSES OF PHOTOEXCITED CHARGE CARRIERS IN POROUS ANODIC ALUMINUM OXIDE

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Porous anodic aluminum oxide (PAAO) is an ensemble of vertically oriented nanotubes, so it can be used as membrane filters, matrices for creating various nanocomposites, as templates for creating nanostructures of various chemical compositions. It is important to obtain PAOA with low photoluminescence (PL) intensity by varying the synthesis conditions. Thus, the aluminum oxide matrix itself will not contribute to the processes of radiative recombination of photoexcited charge carriers, that is, the luminescence will be exclusively due to the luminescence of the test analyte in pores. The PAOA samples were formed by the electrochemical method in electrolytes based on different acids - sulfuric and selenium and at different synthesis parameters. The samples were divided into 2 parts: the original and with the applied analyte - rhodamine dye. It was found that all PAOA films have an amorphous structure. The samples formed in the electrolyte based on selenic acid have the required properties: the original films do not luminesce, PAOA with the dye are characterized by intense rhodamine PL. It was found that the main type of defects in the PAOA structures synthesized in sulfuric acid are oxygen vacancies responsible for radiative recombination processes. In PAOA films obtained in selenic acid, oxygen vacancies in low concentrations and oxygen radicals (non-radiative centers) in high concentrations were registered.

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Keywords: porous anodic aluminum oxide, photoluminescence, defects

OIL SPILL REMOVAL WITH NONWOVEN MATERIALS PRODUCED BY MELT ELECTROSPINNING

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Nonwoven micro- and nanofibrous materials produced by electrospinning have found their application for solving various tasks, from filtration to medicine. One of the areas where nonwovens are currently being used on an industrial scale is the removal of liquid hydrocarbons: both during various technological operations and during the cleanup of oil spills caused by man-made disasters. Thus, there is a need for effective sorbents for rapid oil spill removal from the water surface. Nonwoven polymeric materials with low density, high porosity (up to 95% and sometimes more), high hydrophobicity and relatively low cost are well suited for the role of sorbents.

The work shows the possibility of obtaining nonwoven materials with an average fiber diameter of 1-10 μm from melts of a number of commodity polymers (polyolefins, polyamides, polystyrene, polylactic acid and their blends). The structure of polymers and its changes in the process of electrospinning and post-treatment of fibers (e.g., annealing) were characterized using IR spectroscopy and X-ray diffraction analysis. It is shown that the obtained materials are characterized by high hydrophobicity and rapid oil absorption, which allows their application as effective hydrocarbon sorbents. It is established that the sorption capacity of nonwoven fabrics for motor oil reaches 100 g/g, and the sorbed oil can be almost completely removed from the materials (residual content - less than 5%), which allows their multiple reuse with an efficiency of up to 60% of the original.

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Keywords: electrospinning, nonwoven materials, polymer melts, oil spill

БИОМЕДИЦИНСКОЕ ПРИМЕНЕНИЕ НАНОВОЛОКНИСТЫХ МАТЕРИАЛОВ

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Развитие нанотехлогий производит революцию во многих отраслях начиная от электроники и медицины до производства строительных материалов и очистки воздуха. Ключевым типом наноматериалов являются нановолокна размером около 100 нм. Нановолокнистые материалы привлекают к себе внимание благодаря высокой удельной поверхности, пористости, уникальным физико-механическим свойствам. Стоит отметить, что многие природные материалы имеют волокнистое строение с иерархической структурой, включающей, нанофибриллы и нановолокна. Например, шелк паука и шелкопряда, шкуры крупного рогатого скота, рыбья чешуя, волосы, рога, копыта, панцири ракообразных, древесина, бамбук, пшеничная солома, лен и др. Среди различных способов получения нановолокон метод электроформования (electrospinning) остается наиболее простым и универсальным, позволяя создавать волокнистую сетку (каркас) из волокон разного диаметра от 30 нм до 50 мкм. Архитектура нановолокнистых материалов подобна структуре внеклеточного матрикса. Многочисленные исследования показывают, что топография нановолокнистой поверхности и ее химический состав влияют на поведение, адгезию и пролиферацию клеток. Для выращивания функциональных органов и тканей используются как природные белки и полисахариды (коллаген, кератин, фиброин, спидроин, альгинат натрия, хондроитинсульфат, диацетат целлюлозы и др.) так и синтетические полимеры (полиэфиры, полиамид, полиуретан). В докладе представлен обзор последних достижений в области разработки нановолокнистых материалов для инжиниринга костной, нервной, эпителиальной, соединительной ткани, сосудов и др.

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Keywords: электроформование, нановолокна , биомедицина.

AEROSOL FILTRATION IN HIGH-TECH APPLICATIONS

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The theory of fine filtration of aerosols by fibrous filters is discussed. These filters are used for provision of ultrapure air for high-tech applications, for the final air purification at hazardous enterprises, and for the protection of the respiratory system. The deposition of particles in nanofiber filters at Knudsen numbers Kn ~ 0.1 - 1 has been calculated. In regard to this, particular attention is paid to the effect of gas sliding on the fiber surface. The calculated sizes of the most penetrating particles are in agreement with experiments. It also considers the limits of applicability of analytical formulas for calculating the efficiency of a layer of a large number of fibers depending on the diffusion Peclet number. Furthermore, the inertial deposition of aerosol particles in filters of ultrathin fibers is discussed.

The modification of fiber surfaces provides a foundation for the development of filters with high efficiency and low initial resistance, as well as pre-filters with high dust capacity. The deposition of submicron particles by diffusion and interception from the Stokes flow onto micron fibers with radial nanowhiskers is considered with due consideration of the gas slip effect. It is demonstrated that the quality criterion of the filter comprising modified fibers is superior to that of the filter comprising smooth fibers.

Keywords: aerosols, nanofiber, HEPA-filter, quality criterion, nanowhiskers

«ЯДЕРНАЯ ЗИМА» И ДРУГИЕ АЭРОЗОЛЬНЫЕ КЛИМАТИЧЕСКИЕ КАТАСТРОФЫ

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В докладе представлена авторская версия истории исследований гипотезы «ядерной зимы» - катастрофического изменения климата Земли в случае крупномасштабного использования ядерного оружия. Особое внимание уделено предыстории возникновения гипотезы «ядерной зимы» и научному прорыву 80-х годов XX века, когда ученые СССР, США и других стран старались осмыслить теоретическую возможность резкого похолодания на большей части земной суши в результате массовых пожаров ядерной войны и найти природные аналоги такой «рукотворной» аэрозольной климатической катастрофы. Обсуждаются также результаты совместных исследования сотрудников Института физики атмосферы и НИФХИ им. Л.Я. Карпова в области оптических и микрофизических свойств дымового аэрозоля.

CURRENT STATE OF SMALL SYSTEMS THERMODYNAMICS

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Recently it was realized that all existing thermodynamic definitions of the characteristics of surface and small systems (such as the surface tensions, contact angles, disjoining pressure, inner properties of small systems) are ambiguous. In order to choose the correct thermodynamic definitions, the second law of thermodynamics according to Clausius was used. Clausius's concept gives additional experimental information about the relaxation times for processes of transfer of a momentum, energy and mass. Such analysis of relaxation times showed that mass transfer is always a limiting stage, and local pressure always adjusts to the current mass distribution. Using the Clausius's concept distortion of the fundamentals of thermodynamics is excluded, all existing thermodynamic ambiguities are eliminated, and correct calculation of size thermodynamic functions using micromodels is ensured.

Keywords: small system, the second law of thermodynamics, relaxation times.

HYDRODYNAMIC THEORY OF A MIXED TYPE FIBROUS FILTER

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Aerosol filters of mixed type, consisting of micro- and nanofibers, have the advantages of nanofiber filters and overcome their disadvantages. The paper proposes a hydrodynamic theory of a mixed-type fibrous filter. Microscopic and macroscopic models of flow in a periodic cell containing one microfiber and many nanofibers are developed, on the surface of which non-slip and slip conditions are respectively set. In the microscopic approach, fluid flow in a rectangular cell containing micro- and nanofibers is considered in the Stokes approximation. Based on the numerical solution of the boundary value problem using the boundary element method, the velocity and vorticity fields were constructed. Parametric calculations were carried out, based on the results of which approximate formulas were obtained for calculating the total drag force and the contributions of micro- and nanofibers to it.

In the macroscopic approach, a microfiber in a periodic cell is set explicitly, and the flow in the region occupied by nanofibers is modeled by filtration flow in a porous medium within the Brinkman model. For a circular periodic cell with Kuwabara conditions on the outer boundary, analytical formulas for hydrodynamic drag are obtained. The limits of applicability of the formulas were studied based on comparison with calculations for a rectangular cell. The calculation results for both models are compared.

Acknowledgments: The work was carried out with support of a grant from the Academy of Sciences of the Republic of Tatarstan, provided to young candidates of science (postdoctoral students) for the purpose of defending a doctoral dissertation, performing research work, as well as performing labor functions in scientific and educational organizations of the Republic of Tatarstan within the framework of the State program of the Republic of Tatarstan «Scientific and technological development of the Republic of Tatarstan».

Keywords: mixed type fiber filter, drag force, Stokes model, Brinkman model

COMPREHENSIVE ASSESSMENT OF THE EFFECTIVENESS OF THE NEVA® FILTER MATERIAL FOR ITS USE IN THE MANUFACTURE OF RESPIRATORS INTENDED FOR THE USE OF ATOMIC ENERGY

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Many technological processes at nuclear industry enterprises are accompanied by the presence of aerosol particles in the air of the working area. An additional hazard factor may be the presence of radioactive substances on an aerosol particle, therefore, respiratory protection issues in the field of atomic energy use are always relevant.

According to radiation safety standards, to protect workers from exposure to the radiation factor, a respirators with maximum protective properties should be used.

In the first decades, the main filter material was Petryanova filters (FP), in subsequent years, the use and research of the protective properties of other materials, such as meltblown, in particular the new innovative NEVA® filter material, began.

The purpose of this work is to determine the effectiveness of a new domestic innovative NEVA® filter material for respiratory protection from radiation factor.

During the study, the permeability of the NEVA® filter material for non-radioactive and radioactive aerosols was determined and analyzed. An atmosphere of distribution of aerosol particles with different sizes in the air stream before and after the filter material has been formed. A conclusion has been made on the protective effectiveness of the respirators made of NEVA® filter material for use in the field of atomic energy use.

Keywords: respirators, the field of atomic energy use, radioactive aerosols, aerosol permeability, dimensional distribution.

MODELS OF FLOW PAST NANOFIBERS AND NANOPARTICLES AT LOW KNUDSEN NUMBERS

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Hydrodynamic models of flows around nanofibers and nanoparticles are used to predict the performance of aerosol fibrous filters. For small Knudsen numbers, it is permissible to use models of a continuous medium with the condition of slip on the surface of nanofibers and nanoparticles. As a rule, the slip condition is taken in the form of the Basse-Maxwell condition [1,2], when the slip velocity is considered proportional to the shear stress. Such models describe experimental data well only at very small Knudsen numbers. The report reports on the formulation and solution of problems on slow Stokes flow around a sphere and a nanofiber in the approximation of small Knudsen numbers with a new boundary condition of slip on the surface of a streamlined body. It is proposed to use a linear relationship between the tangential velocity component and flow vorticity as a slip condition. Based on analytical and numerical solutions, the aerodynamic drag forces of the cylinder and sphere are calculated as a function of the Knudsen number. The dependence of the aerodynamic drag force on the Knudsen number is shown to be in better agreement with experimental data in comparison with the Basset-Maxwell condition.

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Keywords: Stokes problem, nanoparticles, fiber filters, Knudsen number

DRY AEROSOL PRINTER FOR FORMING MICRO-SIZED OBJECTS ON VARIOUS SUBSTRATES

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The dry aerosol printer is a new approach to print without using ink, based on the use of a gas-discharge aerosol generator as a source of nanoparticles. Nanoparticles are synthesized immediately before use in a pulse-periodic gas discharge in a flowing gas between electrodes from the required consumable material. The aerosol flow of nanoparticles is focused and delivered to the surface being processed in dry form without using a solvent. The strong point of this approach is the combination of four simultaneously occurring processes in a single device: gas-discharge production, laser modification, printing and laser sintering of nanoparticles on a substrate.

The printer is designed to form objects with micron design standards from metal materials on various substrates, in particular, in electronics: interconnections, electrode structures, inductive and resistive elements. The composition of the object material is determined by the materials from which the aerosol generator electrodes are made. The printer also allows applying plasmonic nanostructures from metal nanoparticles with predetermined dimensions on the surfaces of various objects, providing multiple amplification of the optical response in optoelectronic devices (photodetector matrices, displays, semiconductor light sources), and when measuring the chemical composition of objects using enhanced Raman and fluorescence spectroscopy.

Acknowledgements: The research is supported by the Ministry of Science and Higher Education of the Russian Federation (Goszadaniye) 075-03-2024-117, project No. FSMG-2024-0009.
Keywords: dry aerosol printer; nanoparticles; sintering.

NUMERICAL METHODS AND PHASE TRANSITIONS IN THE EQUATIONS OF AGGREGATION-FRAGMENTATION OF SUBSTANCES

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In this work we discuss a famous effect of gelation (also known as zol-gel transition) using a theoretical framework of Smoluchowski kinetic equations with a source of monomers and product coagulation kernel.

The source-less case is rather well-studied and predicts the zol-gel transition moment t_g=1. However, the post-transition kinetics may vary depending on a further approach formulating the kinetic equations. The first approach is known as Flory framework and predicts exponential decay of the total density at post-gel stage. The second view of this phenomena is Stockmayer's framework giving a prediction for much slowr decay of the total density as just 1/t. In fact, both of these frameworks might be useful in applied problems and correspond to a different interaction of the gel-particle with the rest of the finite zol particles.

We generalize this difference for a case of the model with a constant source of monomers. The gelation time increases up to t_g= π/2 and the divergence between two theories becomes even more dractic. Flory's framework leads to the decay of the total mass as 1/t whereas the Stockmayers's theory gives a relaxation of the solution to a steady-state with algebraic decay of the stationary particles' concentrations as k^{-5/2}. These observations could be generalized for a more complicated case of multi-particle aggregation within a same sequence of observations.

The utilized equations also possess other interesting types of the phase transitions such as Hopf bifurcations, finite-size effects and large deviations of equilibrium solutions from scaling exponents. In all cases, we support our theories through the numerical simulations and obtain an excellent agreement of our experiments with analytical results.

Keywords: aggregation, gelation, phase transitions, kinetics, Smoluchowski equations

AEROSOL SYNTHESIS OF SINGLE-WALLED CARBON NANOTUBES

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The unique properties of single-walled carbon nanotubes (SWNTs), such as high porosity and specific surface area, low density, high ratio of optical transmittance to sheet resistance, high thermal conductivity and chemical sensitivity, and tunable metallic and semiconducting properties, open up avenues for a wide range of applications.

The presentation is devoted to a survey of SWNT synthesis by the aerosol chemical vapor deposition method. Direct integration of the SWNTs produced by this method into high-performance flexible and stretchable electronics, is discussed. Produced SWCNT/polymer composite films have exhibited excellent optical and electrical properties as well as high mechanical flexibility. The presentation also discusses a SWNT as an excellent material for aerosol filters, including pellicles.

Acknowledgements: The project was supported by the RSF grant (number 22-13-00436).

ХОЛОДНАЯ СОНОЛЮМИНЕСЦЕНЦИЯ КАВИТАЦИОННЫХ ПУЗЫРЬКОВ В ВОДЕ

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Сонолюминесценцией (СЛ) называют свечение воды и ряда других жидкостей в результате схлопывания кавитационных пузырьков, образующихся в них в результате периодического воздействия ультразвука. Однозначной теоретической интерпретации явления не существует до сих пор. Температуру внутри пузырька определяют, накладывая спектры СЛ на стандартные планковские кривые. Определенные таким образом температуры порядка нескольких тысяч градусов, хотя окружающая среда остается холодной. Существует еще одна трудность стандартных тепловых и плазменных моделей СЛ. Немногочисленные эксперименты по изучению угловой зависимости световыхода отчетливо указывают на дипольный характер излучения отдельного пузырька.

Предложена альтернативная модель сонолюминесценции в воде. В ее основе высвечивание двумерного плазмона, образующегося на поверхности кавитационной полости в результате конденсации паров воды. За счет водородных связей дипольные молекулы конденсирующегося пара прикрепляются к внутренней поверхности полостей. Их внешние взаимодействующие через кулоновский потенциал "хвосты" образуют двумерный заряженный слой. Рассчитаны свойства плазмона, связанного с собственными колебаниями этого слоя, его частота, ширина плазмонного резонанса и сечение высвечивания. В рамках модели основные закономерности сонолюминесценции объясняются не высокими температурами внутри кавитационных пузырьков, а сильными электромагнитными полями плазмонов. Модель воспроизводит общую форму частотной зависимости спектра СЛ. Тонкая структура спектра объясняется гигантским комбинационным рассеянием излучения, испускаемого плазмоном, на атомах газов, добавленных в раствор. Модель объясняет дипольный характер однопузырьковой сонолюминесценции.

ХИМИЧЕСКИЕ ПРОЦЕССЫ В АТМОСФЕРНОЙ ДЫМКЕ

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Исследование физико-химических механизмов природных и природно-техногенных явлений в атмосфере не теряет актуальности. В их числе формирование аэрозольной дымки и вызванное этим опасным явлением негативное влияние на радиационный режим атмосферы, содержание газовых примесей и здоровье населения. Имеющиеся данные о динамике превращений SO_2 в атмосфере не объясняют ни наблюдаемых темпов образования, ни уровней содержания сульфатов в частицах дымки (сотни мкг/м^3). В докладе на примере данных лабораторного моделирования процессов образования сульфатов в мало обводненных частицах (*deliquesced particles*), а также результатов мониторинга сульфатов в атмосферной дымке показано, что источником сульфатов в частицах служит каталитическая конверсия $SO_{2(газ)} \xrightarrow{Mn/Fe,\ O2} SO_{4(aq)}^{2-}$ протекающая в врожденно-разветвленном (ВР) режиме. Обсуждаются концентрационные условия этого нового механизма каталитического образования сульфатов и особенности его динамики в атмосфере. Сравнение результатов расчетов содержания SO_4^{2-} в частицах и данных мониторинга демонстрирует их удовлетворительное согласие. Эти результаты, показывают, что ВР режим каталитической реакции обеспечивает наблюдаемые темпы генерации (десятки мкг м$^{-3}$ ч$^{-1}$) и уровни содержания SO_4^{2-} в аэрозольных частицах в периоды возникновения катастрофически опасных дымок в атмосфере.

Ключевые слова*:* атмосферная дымка, диоксид серы, ионы Fe и Mn

ОЦЕНКА ЭФФЕКТИВНОСТИ СРЕДСТВ ИНДИВИДУАЛЬНОЙ ЗАЩИТЫ ОРГАНОВ ДЫХАНИЯ (СИЗОД) С УЧЕТОМ ПОВЕДЕНИЯ БИОАЭРОЗОЛЕЙ, СОДЕРЖАЩИХ ПАТОГЕНСОДЕРЖАЩИЕ ВИРУСЫ

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Аэрозольные частицы, образующиеся при чихании или кашле, состоят в основном из мокроты - смеси воды и биологических примесей. Начальное распределение по размерам патогенсодержащих частиц бимодально с максимумами в диапазонах 50…100 мкм и 100…500 мкм, но в воздухе их дисперсный состав довольно быстро меняется. Эволюция дисперсности биоаэрозолей представляет интерес как с точки зрения опасности распространения в воздушной среде вирусов, в том числе SARS-CoV-2, так и для оценки эффективности СИЗОД.

Представлен подход к оценке влияния изменчивости дисперсного состава патогенсодержащих аэрозолей в неподвижной атмосфере на эффективность средств индивидуальной защиты органов дыхания на примере защитных масок класса FFP1, FFP2 и FFP3. Рассмотрено влияние на физико-химические параметры аэрозолей сил тяжести, сопротивления, а также температуры и относительной влажности окружающего воздуха. Получены оценки времени выпадения аэрозольных частиц (с диаметром 1-1000 мкм) с учетом их частичного испарения и динамики изменения массовой доли аэрозольных частиц для относительной влажности воздуха 10 % и 100 %.

Показано, что при повышенной влажности изменение дисперсного состава патогенсодержащих аэрозолей происходит в основном за счет механизма гравитационного осаждения, что приводит к быстрому (в течение нескольких секунд), уменьшению размеров аэрозольных частиц, оставшихся в воздухе, с последующей стабилизацией концентрации. С уменьшением влажности воздуха количество первоначальных аэрозольных частиц сокращается еще значительнее, что связано с испарением жидкости в их составе. Это приводит к общему снижению концентрации и размеров первоначальных частиц. При этом СИЗОД за счет уменьшения количества вирусов будут даже эффективнее, чем в условиях без испарения.

Предложенный подход может быть использован для количественных оценок эффективности средств индивидуальной защиты органов дыхания в различных условиях генерации патогеносожержащих аэрозолей.

IMPLEMENTATION EXPERIENCE OF SCIENTIFIC AND PRACTICAL APPROACHES FOR STUDYING RADIOACTIVE AEROSOLS IN THE NANOMETER RANGE

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The report presents the main results of the research group from the Institute of Industrial Ecology of the Ural Branch of the Russian Academy of Sciences in terms of developing methods and studying the distribution of radionuclides by the size of aerosol particles in the range from 1 nm to 5 μm. The authors of the report demonstrated methods for sampling the studied atmosphere using a diffusion battery and an impactor. After this, the radionuclide composition of each collecting element was analyzed. The objects of study were the atmospheres of a glove box with a high Rn-222 concentration with progeny, warehouses of monazite concentrate with a high Rn-220 concentration with progeny, as well as the reactor hall atmosphere of a research nuclear facility with a high uranium fission products concentration - radioactive isotopes of krypton and xenon with their progeny. The study results demonstrated the presence of radionuclides in the form of aerosol particles with AMTD in the range from 1 to 300 nm in the studied objects.

Keywords: radionuclide, aerosol particles, radioactive progeny, concentration

ABSTRACTS

POSTERS

SEPARATION OF MIXTURES BY GAS CENTRIFUGES

1

UNIVERSAL FORMULA FOR THE SEPARATIVE POWER OF AN OPTIMIZED CONCURRENT GAS CENTRIFUGE

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Concurrent gas centrifuge (GC) are interesting from an academic point of view. Comparing them with countercurrent GC helps to better understand the physics of the processes in them. At the same time, concurrent GC are also interesting from a practical point of view, as devices that are capable of enriching large gas flows. In [1], we obtained an analytical formula for the separative power of an optimized concurrent GC . It gives a good agreement with the empirical data obtained for Soviet countercurrent GC [2].

However, at low rotor speeds, this formula obviously overestimates the separative power, because it surpasses the maximum of Dirac the separative power. And this is impossible. The reason is an underestimation of the axial diffusion of gas compared to axial convection at low rotational speed GC. The paradox lies in the fact that it is at low rotational speeds that the axial convection velocity becomes small and diffusion begins to dominate. We have obtained a universal formula for the separation of optimal concurrent GC for a wide range of rotation speeds, working gas parameters and GC. At high rotor speeds, the separation power is proportional to V^2, and at low rotational speeds, the separation power is proportional to V^4, as in Dirac [3], but by a factor of 0.71 less..

Keywords: super-strong centrifugal fields, isotope separation, concurrent gas centrifuge, separation power

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2 ОПТИМАЛЬНЫЙ РАДИУС РОТОРА РАЗДЕЛИТЕЛЬНОЙ ГАЗОВОЙ ЦЕНТРИФУГИ

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Центрифуга – основная технология разделения изотопов. Это обусловлено эффективностью центрифуги: высоким коэффициентом разделения и относительно малыми затратами энергии. Энергетическая эффективность центрифуги следствие реализации процесса разделения в состоянии смеси близком к равновесному. Такое преимущество делает разделительную центрифугу перспективной на многие годы вперед.

Оптимизация центрифуги необходима для повышения эффективности разделительного производства. Одним из направлений оптимизации является выбор геометрических размеров центрифуги. Центрифуга с более высокой работой разделения на единицу объема экономически выгоднее.

В литературе представлены теоретические и эмпирические зависимости разделительной мощности центрифуги от геометрических размеров: длины и радиуса ротора. Но анализ оптимальных размеров практически отсутствует. В особой степени, это касается вопроса об оптимальном радиусе ротора центрифуги. Проблема никак не освещена.

В работе получено выражение для определения оптимального радиуса ротора разделительной газовой центрифуги:

$$R = const\frac{F}{2\pi\rho D},$$

где F – поток питания; ρ – плотность; D – коэффициент диффузии

Выражение позволяет оценить оптимальный радиус ротора, для которого достигается максимум работы разделения при конечном коэффициенте обогащения центрифуги. Оптимальное значение радиуса обусловлено требованием конечности коэффициента обогащения. Критерий оптимальности радиуса ротора разделительной центрифуги получен впервые, на настоящий момент в открытой литературе нет аналогичных оценок.

Ключевые слова: разделение, центрифуга, оптимальный радиус ротора

3

ON THE POSSIBILITY OF ISOTOPICALLY SELECTIVE ATOMIC-MOLECULAR EXCHANGE IN NITROGEN INSIDE A CENTRIFUGE ROTOR

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From the balance of the vibrational energy flows of N_2 molecules entering the centrifuge rotor through the electric discharge tube as a feed flow and the entrained sum of the product and waste flows with reduced vibrational energy in the rotor volume due to dissipation on the rotor walls, the average vibrational energy per molecule ε_v is estimated. For given rotor parameters (radius, height, wall material, rotation frequency), the value of the feed flow is found at which the value $\varepsilon_v = (3\text{-}4)\cdot 10^{-2}$ eV is established in the rotor volume, for which a 30-fold enrichment of nitrogen atoms with the ^{15}N isotope was previously observed in [1, 2] at a translational temperature of T = 300 K and a concentration of N_2 molecules of 10^{17} cm^{-3} due to threshold atomic-molecular exchange. For these conditions, from the balance of the flows of N atoms entering the rotor, leaving it and recombining on the rotor walls, the ratio of the average concentration of nitrogen atoms over the rotor cross-section to the maximum concentration of atoms at the discharge outlet is estimated.

Keywords: centrifuge, atmic-molecular exchange, isotopic enrichment.

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4

РАСЧЕТ И ОПТИМИЗАЦИЯ ПРЯМОУГОЛЬНОГО КАСКАДА С ЗАДАННЫМИ КОНЦЕНТРАЦИЯМИ ^{92}МО В ВЫХОДЯЩИХ ПОТОКАХ

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Концентрирование стабильных изотопов в каскадах газовых центрифуг является актуальным в связи с их широким прменением в промышленности, науке и медицине. На практике возникает потребность решения различных задач расчета и оптимизации каскадов для разделения стабильных изотопов.
Одной из них является обеспечение заданных концентраций целевого изотопа в выходящих потоках прямоугольного каскада. Предложен метод решения данной задачи на основе использования алгоритмов «Золотого сечения» и «Роя пчел» для минимизации отклонений рассчитываемых концентраций от заданных. Проведен вычислительный эксперимент по разделению гексафторида молибдена. Показаны возможности метода по определению параметров каскада с минимальным суммарным потоком питания ступеней. Приведены примеры расчета каскадов для концентрирования ^{92}Mo до 99,9%.

Ключевые слова: стабильные изотопы, прямоугольный каскад, газовые центрифуги, расчет, оптимизация, молибден

5

DISCUSSION OF TWO-COMPONENT ISOTOPES SEPARATION IN MULTI-COMPONENT SEPARATION SYSTEM WITH CENTRIFUGE CASCADES

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Separation of two-component isotopes in multi-component separation system is one of special multicomponent separation systems in centrifugal cascade. Multiple elements in the separation medium have isotopes, while the target element have two isotope components, which decouples the components from the isotope abundance. Therefore, this multicomponent system has several characteristics of double-component separation and single cascade can be used to separate light and heavy components of target isotope at one time. Also, the efficiency of cascade can be described by value function and separative power. For this separation system, select an appropriate model cascade for calculation according to design requirements, pre-optimize the calculated flow curve, and then round off and re-optimize the obtained cascade scheme to obtain the optimized engineering cascade scheme. With this method, referring to rectangular cascade, MARC cascade and ideal cascade model, and taking the single machine separation power as the optimization goal, the design and optimization of the lithium isotope separation cascade by hexyl lithium medium is carried out, and the engineering cascade schemes are obtained. Through contrastive analysis, it is concluded that MARC cascade has the highest efficiency, while rectangular cascade has relatively low efficiency but simple rounding and less design constraints, so rectangular form is suitable for cascades of various scales.

Keywords：isotopic separation; centrifugal cascade; multicomponent separation; lithium isotope

6 ON THE PRESSURE CONTROL OF THE WASTE WITHDRAWAL OF CENTRIFUGE CASCADES

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In order to improve the anti-disturbance ability of waste end unit of stepped centrifugal cascade, the influence of electric regulating valve on the fluid state of the cascade was studied. Static and dynamic hydraulic studies of cascade are carried out. The results show that for cascade pressure disturbance, the pressure fluctuation will be transmitted to both sides of the cascade. After the steady state condition is re-established, it mainly affects the status of separation stage on concentrate side of disturbance stage; For cascade flow disturbance, the pressure fluctuation will be transmitted to both sides of the cascade. After the steady-state working condition is re-established, it mainly affects the state of separation stage on the waste side of disturbance stage.

Keywords: Centrifugal cascade, Regulating valve, Hydraulic, Pressure disturbance, Pressure fluctuation

7

NUMERICAL INVESTIGATION ON THE INFLUENCE OF PARAMETERS OF GAS CENTRIFUGE HEAT TRANSFER COMPONENTS ON THE SEPARATION PERFORMANCE

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Temperature distribution of centrifuge rotor is an important factor affecting the separation performance of gas centrifuge. A numerical iterative calculation method of the whole temperature field of centrifuge can be established by deducing the numerical theory of radiation heat transfer between the centrifuge rotor and the sleeve, and by using the continuous condition at the fluid-solid boundary. The numerical method can obtain more accurate results of the temperature field and flow field, as well as calculate separation power of the gas centrifuge. The effects of key heat transfer parameters on separation performance and temperature field of subcritical gas centrifuge, such as blackening at the inner surface of the sleeve, length of the reflector, temperature of the cooling water and the position of the water jacket, were studied using this numerical method, based on the Iguassu centrifuge model. The calculation results can provide several references for the design and optimization of the heat transfer of gas centrifuge.

Keywords: Gas Centrifuge; Radiation heat transfer; Temperature field; Separative power

8 MODELING OF MASS SOURCE-SINK ASSOCIATED WITH ADAPTIVE EXTERNAL PARAMETERS IN ROTATING CYLINDERS

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The hydrodynamic properties of rotating cylinders are of significant importance for the optimization of cylinder structures, as they can impact the operational parameters of engineering cascade systems. In this paper, a small orifice outflow model is employed to derive an expression for the extraction flux as a function of external parameters, and a corresponding mass sink model of the extraction flow is subsequently established. To enhance the precision of the model, empirical coefficients are incorporated to calibrate the calculated extraction flux with experimental data. The Iguassu rotating cylinder model, in conjunction with the homotopy continuation method, is employed to directly solve steady-state N-S equations, thereby facilitating an investigation into the influence of external parameters on the hydraulic characteristics of the rotating cylinder. The findings demonstrate that the mass source-sink model developed in this study effectively captures the primary hydraulic characteristics of the rotating cylinder influenced by external parameters during the simulation. The results obtained through simulation are in good agreement with experimental observations, with a straightforward correction of the empirical coefficients.

Keywords: hydraulic characteristics; rotating cylinder; adaptive; external parameters; numerical simulation

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SOLVING OF THE FLUID−SOLID COUPLED HEAT TRANSFER PROBLEM WITH RADIATION BOUNDARY CONDITION IN A ROTATING CYLINDER

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A numerical model of the fluid-solid coupled heat transfer problem with thermal conductive boundary condition involving radiation (the so-called radiation boundary condition) in a rotating cylinder is established. The resulting 2D N-S equations with non-linear Robin boundary condition are solved numerically by using a Newton iterative method based on homotopy algorithm. The temperature distribution on the sidewall of the rotating cylinder is obtained, and the impact on the flow field and the temperature distribution is analyzed. The results show that the temperature distribution is not linear, especially in the case of low thermal conductivity of the cylinder materials. Furthermore, it is found that the relationship is linear between the drag coefficient of the scoop and the average temperature, and so is the relationship between the drag coefficient and the maximum temperature difference on the sidewall, which both are governed by the ambient temperature and effective emissivity of the cylinder surface. The proposed model allows the temperature distribution on the sidewall of the rotating cylinder to be estimated numerically and adjusted by the radiation boundary condition.

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Keywords: Fluid-solid coupled, heat transfer, radiation boundary, rotating cylinder

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THREE-DIMENSIONAL NUMERICAL SIMULATION OF THE INFLUENCE MECHANISM OF THE EXTRACTION PRESSURE ON WASTE FLUX

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The gas extractor links the internal flow field within the rotating cylinder to the external operating parameters.

While in operation, adjusting the extraction pressure p_E can impact the waste flux W and consequently influence the equipment's operating state. In the high-speed rotating cylinder, the gas extractor interacts violently with the high-speed rotating gas flow, and the fine flow field structure around the gas extractor is of great significance for the extraction process. At present, it is unclear how the extraction pressure p_E affects the gas flow around the gas extractor and thus affects the equipment's operating state. In this paper, a three-dimensional numerical simulation study is carried out on this problem the influence mechanism of extraction pressure p_E on the waste flux W is revealed through 3D numerical simulation.

Under different extraction pressure p_E, the flow field structure around the gas extractor are different, leading to the different waste flux W. When p_E is low, the shock wave structure shields the perturbation propagation, keeping waste flux W unchanged. When p_E is high, the subsonic overflow at the mouth of gas extractor head makes W decrease with the increase of p_E.

11 HYDRAULIC ANALYSIS IN UNSTEADY STATE PROCESS WITH A MATHEMATICAL MODEL OF DUAL CASCADE

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An important factor that the adjustment and control of hydraulic parameters in centrifuge cascade system are important issues to produce stable isotope products, especially when producing two products in dual cascade. This paper establishes an unsteady cascade mathematical model of dual cascade to analyze these issues. Taking the isotope production of ^{72}Ge and ^{76}Ge as an example, the numerical calculation of double cascade is carried out, and compared with experimental data in the actual production process. The dual cascade model is used to calculate the equilibrium time of the cascade transition. Based on these calculations, this essay provides a control method in dual cascade for stable production and a reference for the adjustment of hydraulic parameters for factory during the production of stab
le isotopes.

Keywords: Multicomponent isotope separation; Unsteady state; Numerical simulation; Gas centrifuge cascade

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THE CASCADE OF INDIVIDUAL RECYCLED URANIUM FEED AND THE CASCADE OF COMBINED RECYCLED URANIUM FEED WITH DEPLETED URANIUM FEED

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China has been insisting on the development of closed nuclear fuel cycle. With the rapid development of nuclear industry, the need for recycled uranium enrichment becomes increasingly urgent. In this paper, the technical scheme of recycled uranium enrichment cascade is studied, the composition and characteristics of each nuclides in recycled uranium are analyzed, and the optimization method of multi-component cascade is selected. Based on the model of multi-component cascade, the cascade technology is studied from two different perspectives, namely, the cascade of individual recycled uranium feed and the cascade of combined recycled uranium feed with depleted uranium feed. Through the optimization calculation, uranium isotope abundances in the product all meet the restricted limits, and the extraction rate of ^{235}U is over 70%. The conversion of cascade structure can be adapted to the production under different conditions efficiently, which provides a reasonable scheme for recycled uranium enrichment and depleted uranium reuse.

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FURTHER IMPROVEMENT OF THE Q-ITERATION METHOD FOR THE CALCULATION OF CONCENTRATION DISTRIBUTION IN ISOTOPE SEPARATION CASCADES

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The so-called AQ-iteration method is proposed to resolve the non-convergence problems in the calculation of concentration distribution in cascades by alternatively performing the Q-iteration and the Q*-iteration. The Q*-iteration is a Newton Raphson method based on the gradient of the basic quantity **Q** in the Q-iteration. Numerical experiments are performed for two example cascades, for which the Q-iteration does not give convergent results. The AQ-iteration demonstrates a better performance than the Q-iteration. The results show that usually a larger under-relaxation factor gives a faster convergence. The fastest convergence is obtained when the under-relaxation factor is one, but this may occasionally yield non-convergence. Convergence can always be obtained by choosing appropriate values of the under-relaxation factors and combination of the numbers of the Q- and Q*-iterations in an AQ-iteration.

Keywords: isotope separation, cascade, Q-iteration, AQ-iteration, concentration distribution

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INFLUENCE OF WORKING SUBSTANCE LOSSES ON INTEGRAL PARAMETERS OF THE CASCADE FOR SEPARATION OF MULTICOMPONENT MIXTURES UNDER GIVEN EXTERNAL CONDITIONS

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The losses of the working substances at the cascade stages affect the efficiency of the separation process. This study aims to complement and generalize previously known results on the topic. Special attention is given to analyzing the influence of working substance losses at the stages of the cascade on its integral parameters while achieving specified concentrations of the target component in the outlet streams.

A generalized model of a quasi-ideal cascade with working substance losses at different stages was developed, which considered the presence of local losses of the working substance at those stages. A series of computational experiments were conducted to evaluate the impact of the magnitude of the loss coefficient and its assignment on the key internal and integral parameters of the cascade. In particular, the magnitude of the relative total flow of the cascade can either increase or decrease depending on the loss coefficient under the specified external conditions. In addition, in some cases, the total flow can reach a minimum depending on the loss coefficient. This feature results from the heterogeneous distribution of component masses across the stages of the cascade; for example, the losses of intermediate components at the internal stages promote a more active concentration of light components toward the end of the cascade.

Keywords: isotope separation, gas centrifuge cascade, multicomponent isotopes

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COMPARISON OF THE EFFICIENCY OF SINGLE CASCADE AND MULTI-CASCADE SCHEMES FOR CONCENTRATING COMPONENTS OF UTMOST AND INTERMEDIATE MASS NUMBERS

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Cascade systems with and without return of outgoing flows to the inputs of previous cascades are considered when concentrating isotopes of extreme and intermediate mass numbers during separation of multicomponent mixtures. Using the quasi-ideal cascade model, the efficiency of a single cascade and various cascade systems is compared when obtaining specified concentrations of the target component in the outgoing flows of the circuit. The value of the relative total flow of the cascade circuit is chosen as an efficiency criterion.
Based on the results of comparing multistage schemes with a single cascade when concentrating components of extreme and intermediate mass numbers, it is shown that each of the schemes can have its own field of application and the difference in efficiency depends on specific external conditions and parameters of the mixture.

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Keywords: isotope separation, quasi-ideal cascade, multicomponent mixture

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MASS TRANSFER REGULARITIES IN A DOUBLE CASCADE WITH A CARRIER GAS DURING PURIFICATION OF REGENERATED URANIUM

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The objective of the study was to conduct a double cascade with a carrier gas supplied to the second cascade to increase the purification effect of reprocessed uranium from the isotope ^{232}U. A series of computational experiments was conducted to study the patterns of mass transfer of components in such a cascade scheme at different concentrations of the isotope ^{235}U in the side streams of the cascade scheme and its fixed concentration in the main product flow (the flow of the heavy fraction of the second cascade). Reprocessed uranium that has undergone two cycles in the fuel of a light-water power reactor was selected as the mixture to be separated.

The influence of the ratio of the enriched fraction flows of the first cascade and the carrier gas (ratio R) on the mass transfer of components in the second cascade and the degree of purification of the product from isotopes ^{232,234}U, as well as the concentration of isotopes ^{235,236}U in the final product was revealed. For various given combinations of ^{235}U concentrations in the light-fraction flows of the first and second cascades, the characteristic value of the ratio R is estimated, at which it is no longer possible to obtain the required concentration of the ^{235}U isotope in the final product.

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Keywords: reprocessed uranium, double cascade, carrier gas

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OPTIMIZATION OF THE GENERALIZED QUASI-IDEAL CASCADE MODEL

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A generalized model of a quasi-ideal cascade with different values for the mass numbers of the key components in different sections of the cascade is proposed. A technique has been developed for finding such a set of cascade parameters at which it is possible to obtain the specified concentrations of the target component in its outgoing flows at specified integers of stages in each of its sections.
The possibility of optimizing such a cascade for given concentrations of the target component in the outgoing flows by iterating through various combinations of cascade section lengths at given concentrations of the target component in its outgoing flows and the values of the mass numbers of the reference components is shown. The efficiencies of quasi-ideal cascades with different numbers of sections and different mass numbers of key components were compared.

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Keywords: isotope separation, quasi-ideal cascade, multicomponent mixture

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DEPENDENCE OF THE HYDRAULIC RESISTANCE ON THE MACH NUMBER IN PIPES AT THE FLOW OF A GAS WITH VELOCITY CLOSE TO THE VELOCITY OF SOUND

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Hydraulic resistance coefficient λ is defined according to equation

$$\frac{d}{dx}(p + \rho v^2) = -\frac{\lambda}{d}\frac{\rho v^2}{2}$$

Conventionally it is assumed that this coefficient depends only on the Reynolds number. Understanding of the dependence of this coefficient on the Mach number is important when we deal with a compressible gas flow with high velocities. Our objective is to determine the dependence of hydraulic resistance on the Mach number. To determine this dependence, numerical modeling of the flow of air through a straight circular pipe has been performed in the ANSYS CFX CAE system for Reynolds numbers $1 \cdot 10^4, 2 \cdot 10^4, 3 \cdot 10^4$. For every Reynolds number, λ has been determined for a series of different Mach number. We found that the resistance coefficient λ does not depend on the Mach number in the limits of 0.4%.

Keywords: hydraulic resistance, compressible flow, numerical calculations

ABSTRACTS

POSTERS

PHYSICAL AND CHEMICAL SEPARATION TECHNOLOGIES

19 BIMETALLIC CATALYTIC SYSTEMS BASED ON NANOPARTICLES OF METALS OF THE 1B GROUP IN THE DEUTERO-HYDROGEN EXCHANGE REACTION

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The catalytic properties of mono- and bimetallic nanoparticles of copper, silver and gold fixed on the carrier, as well as bimetallic systems Cu_mAg_n and Au_mAg_n with different ratios of components (1:3, 1:1, 3:1) have been investigated. The samples were synthesised via the impregnation method. The experiments were conducted at 77 K and 0.5 Torr pressure.

The bimetallic samples exhibited higher activity relative to the monometallic samples. The activity of the bimetallic samples was up to six times higher in the Cu_mAg_n system and up to 13 times higher in the Au_mAg_n system. This phenomenon cannot be attributed to the inherent properties of the metals that form the nanoparticles, indicating the presence of a synergistic effect among the studied metal pairs.

The nature of the dependence of the catalytic activity of biparticles on the ratio of metals requires further investigation. In the system comprising copper and silver, the relationship between the catalytic activity of bipartite particles and the ratio of metals can be described by a parabola, with a maximum point at the composition Cu_1Ag_1. The biparticles 'gold-silver' exhibits a maximum level of activity at the Au_3Ag_1 sample, after which it declines in a linear fashion with the increase in the proportion of silver. From the above, the following assumptions about the nature of synergism can be made:

1). In the Au_mAg_n system, gold draws away the electron density of silver, which 'activates' this structure.

2). The Cu_mAg_n system becomes more active due to the non-uniformity of the surface structure, which arises from the relatively large difference in the radii of copper and silver atoms.

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Keywords: nanoparticles, copper, silver, gold, hydrogen isotope exchange

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РАЗРАБОТКА МЕТОДИКИ И ПРОГРАММЫ РАСЧЕТА НАЧАЛЬНЫХ ДАННЫХ ДЛЯ ОЦЕНКИ ИЗМЕНЕНИЯ ПОТОКОВ ФАЗ В ОБМЕННОЙ КОЛОННЕ

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Одной из важнейших характеристик массообменного процесса, отражающей его эффективность, является производительность установки, которая напрямую зависит от величины скорости потоков взаимодействующих фаз. Скорость, в свою очередь, определяется условиями процесса, такими как природа фаз, температура, давление, которые влияют на параметры, отвечающие за режим течения. Кроме того, характер течения зависит от геометрии каналов предназначенных для движения фаз.

Известно, что для организации обменного процесса широкое применение получили колонные аппараты, заполненные недорогой нерегулярной насадкой, которая создает каналы неправильной формы, что усложняет анализ структуры и характеристик потоков фаз. Поэтому оправдано использование для такого рода анализа различных программных комплексов. Однако, для создания в них достоверной расчетной модели необходимы исходных данных о физико-химических свойствах фаз, коэффициентах сопротивления среды при различных условиях и потоках в колонне. Данная работа является частью этих изысканий и состояла в разработке методики и программы расчета начальных параметров разделения изотопов бора ректификацией его трифторида в насадочной колонне.

На основе анализа литературных данных отработана методика определения коэффициентов в уравнении сопротивления, в предположении k-ω модели турбулентности течения, для нескольких вариантов насадки и выведены формулы для расчета плотности и вязкости трифторида бора в жидком и газообразном состоянии в зависимости от условий проведения массообмена. С использованием полученных результатов разработана программа расчета вышеуказанных параметров для различных начальных условий и вида используемой насадки.

Ключевые слова: насадочная колонна, ректификация, моделирование.

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COMPARISON OF THE CATALYTIC PROPERTIES OF SILVER, COPPER, GOLD NANOPARTICLES AND THEIR BINARY SYSTEMS IN THE ORTHO-PARA CONVERSION OF PROTIUM

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The catalytic and adsorption properties of Cu, Ag, and Au monometallic nanoparticles as well as bimetallic nanoparticles in Cu_mAg_n and Au_mAg_n systems with variable metal ratios (1:3, 1:1, 3:1) supported on γ-Al_2O_3 were investigated. The particles were synthesized using an impregnation method with simultaneous mixing of two salts in the impregnating solution. Reactions were studied over a wide temperature range (77–430 K) at a pressure of 0.5 Torr.

Despite the catalytic inertness of massive Cu, Ag, and Au in the isomeric conversion reaction of protium, both mono- and bimetallic nanoparticles based on these metals demonstrated activity as centers for this process. Cu and Ag monometallic particles exhibited similar, relatively low catalytic activity levels, with $\log_{10}(K_{ud})_{Cu,\ Ag} \sim 14.2$, whereas Au demonstrated a threefold increase in activity, with $\log_{10}(K_{ud})_{Au} \sim 14.7$. Notably, bimetallic CumAgn and AumAgn nanoparticles displayed comparable activity in the ortho-para conversion of protium, with $\log_{10}(K_{ud}) \sim 14.8$.

From these observations, it follows that:

1. Effects arising from the interaction between Cu and Ag within a nanoparticle lead to the synergism of the catalytic properties of the system.
2. The catalytic activity of bimetallic particles based on Au and Ag is independent of the metal ratio. The properties of the resulting system are characteristic of gold, suggesting that it forms a shell on the surface of the nanoparticle.

Acknowledgements: The work is performed in the framework of the development program "Priority-2030" of the Mendeleev University of Chemical Technology of Russia.
Keywords: nanoparticles, copper, silver, gold, hydrogen isotope exchange

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STUDYING THE INFLUENCE OF TEMPERATURE ON THE CHROMATOGRAPHIC SEPARATION OF LUTETIUM-177 AND YTTERBIUM

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Radiopharmaceuticals based on the ^{177}Lu isotope are widely used in modern nuclear medicine, for example, as part of drugs for targeted therapy of neuroendocrine tumors, prostate tumors and bone metastases. One of the ways to obtain ^{177}Lu without a carrier is to irradiate an ytterbium target enriched in ^{176}Yb with a thermal neutron flux, followed by the separation of ^{177}Lu from the ytterbium target by chromatography on ion exchange resins. The purpose of the work was to determine the main parameters of the process of chromatographic separation of ^{177}Lu and Yb at different column temperatures.

Chromatographic separation of ^{177}Lu and Yb was carried out on a thermostated column filled with Dowex 50WX8 cation exchange resin (200-400 mesh) in NH^{4+} form, in the temperature range from 20°C to 90°C. Alpha-hydroxyisobutyric acid (α-HIBA) with a concentration of 0.125 M was used as an eluent. The eluate was fractionated into 5 ml fractions and each fraction was measured on a Canberra spectrometer with a GC2018 detector.

To carry out the experiments, radioactive tracers ^{177}Lu and ^{169}Yb were used, mixed with stable lutetium and ytterbium in a ratio similar to that obtained at the end of irradiation of an enriched target with ^{176}Yb. Distribution coefficients were determined by calculation from elution curves.

Experiments and calculations have shown that with increasing temperature, the ratio of the distribution coefficients of lutetium and ytterbium with the resin increases, the distance between the peak maxima increases, but the yield decreases due to the broadening of the peaks

Keywords: chromatography, lutetium, ytterbium, separation, nuclear reactor.

23 INVESTIGATION OF THE GAS DYNAMICS OF A PACKED DISTILLATION COLUMN USING THE LOGOS CAE SYSTEM

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Film mass transfer devices have found wide application in various branches of the chemical industry. One of the most common variants of such devices is packed columns, in which various packed types are used to create a developed contact surface of interacting phases. At the same time, dumped packing is considered the most economically advantageous. However, such packing creates channels of complex and irregular shape, which complicates the analysis of the structure and characteristics of phase flows. In this work, based on the literature data, a 3D model of the packed column was created to study the influence of medium parameters on the parameters of the gas flow movement.

The numerical calculation of the fluid and gas dynamic parameters of the apparatus was carried out using the Logos CAE system. During the calculation, a turbulent flow with adhesion on the walls was considered. The solution of the system was obtained using Darcy's law for the hydrodynamics of liquid and gas flows in a porous medium.

The approbation of the obtained model was carried out with the help of the process of separation of boron isotopes by rectification of boron trifluoride. It is shown that the model adequately describes the movement of the gas phase in the packed bed of the exchange column under the assumption of a film countercurrent mode of liquid flow. This model allows numerical simulation in a wide range of pressures and velocities, changing the geometric and physical parameters of the system and can be used to analyze the dynamic parameters of the motion of interacting phases in the packed column for operating systems similar to the one studied.

Keywords: dumped packing, numerical simulation, boron rectification.

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STUDY OF CATALYSTS OF HOMOMOLECULAR HYDROGEN ISOTOPE EXCHANGE BY METHODS OF THERMOPROGRAMMED OXIDATION AND REDUCTION REACTIONS.

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Homomolecular isotope exchange catalysts play a key role in isotope separation in molecular hydrogen. In this work, nanocatalysts based on group 1-B metals are investigated by temperature-programmed oxidation (TPO) and reduction (TPV) reactions.

The samples are synthesized by impregnation of the carrier with precursor solutions followed by their thermal decomposition. Precursors: $AgNO_3$, $Cu(NO_3)_2$ and $HAuCl_4$. Carrier: γ-Al_2O_3.

It is shown that the presence of a second metal substrate under the gold shell leads to a decrease in the oxidation and reduction temperatures of gold, and this effect being different for silver and copper substrates. This suggests the formation of bimetallic structures in each case, where the second metal enhances the reactivity of the gold.

The sample with a silver shell on the gold core shows a shift in the position of the first oxidation peak towards higher temperatures, and the appearance of a low-temperature reduction peak, indicating the formation of bimetallic structures with strong interaction of metals that complicate the silver oxidation process.

The sample with a copper shell on the gold core also has a decreased oxidation temperature, but an increased reduction temperature, indicating the possible formation of structures in which the reactivity of copper to oxidation increases, and to reduction on the contrary decreases.

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Keywords: nanoparticles, isotopic exchange, copper, silver, gold.

25 THE INFLUENCE OF REACTION CONDITIONS ON THE RATE OF ISOTOPIC EXCHANGE BETWEEN WATER AND CHLOROFORM

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The object of this study is deuterated solvents, one of the most common groups of deuterated compounds. Solvents in which protium atoms are replaced by deuterium atoms are used in nuclear magnetic resonance spectroscopy.

One of the methods for obtaining deuterated chloroform is isotopic exchange between heavy water and chloroform of natural isotopic composition. In this case, the reaction catalyst is alkali.

The paper presents data on the thermodynamic and kinetic characteristics of the isotope exchange reaction between water and chloroform. It is shown that the separation coefficient of the reaction under study has values 1,048 ÷ 1,061 in the temperature range of 298 - 323 K. The reaction kinetics data indicate an increase in the reaction rate by an order of magnitude with an increase in temperature from 298 K to 323 K. The work also determined the influence of the alkali concentration in heavy water on the value of the observed rate constant (k, s^{-1}). Thus, an increase in the concentration of alkali in water from 0.01 to 0.1 M led to an increase in k from 4.79±0.25 s^{-1} to 1.82±0.10 s^{-1}.

Acknowledgement: The work is performed in the framework of the development program "Priority-2030" of the Mendeleev University of Chemical Technology of Russia.
Keywords: deuterated solvents, isotopic exchange, deuterated chloroform, homogeneous catalysis

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ISOTOPE EXCHANGE BETWEEN CARBON DIOXIDE AND WATER IN A COUNTERCURRENT COLUMN WITH A HYDROPHOBIC CATALYST

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Chemical isotope exchange (ChIE) between carbon dioxide and water is a promising alternative method to the traditional separation of oxygen isotopes – vacuum distillation of water. The most effective method for implementing ChIE is countercurrent separation in packed columns with a hydrophobic catalyst. However, such catalysts are currently not available. Previously, the authors of the work demonstrated the possibility of activating isotopic exchange between water vapor and carbon dioxide in the presence of hydrophilic granules of gamma-aluminum oxide (the observed reaction rate constant at 348 K was 1.77 ± 0.17 s^{-1}).

The paper presents data on the study of the possibility of carrying out the process of isotopic exchange between carbon dioxide and liquid water in a column filled with a mixture of hydrophilic packing and a catalyst - hydrophobized aluminum oxide in a ratio of 4:1. The experiments were carried out in independent flow mode using oxygen-18 enriched water. A blank experiment was carried out in the same column filled only with spiral-prismatic packing, as a result of which, at a temperature of 338 K, a value of the height equivalent to the theoretical plate (HETP) equal to 270 cm was obtained. The addition of catalyst to the packed bed resulted in a significant improvement in the mass transfer characteristics of the process, and the HETP value at the same temperature was 44 cm. Increasing the temperature to 348 K and 358 K resulted in a decrease in the HETP to 29 cm and 18 cm, respectively.

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Keywords: isotope separation, chemical isotope exchange, catalysis, masstransfer characteristics.

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НЕСТАЦИОНАРНЫЕ ПРОЦЕССЫ С НАКОПЛЕНИЕМ В КОМПЛЕКСНОЙ ТЕХНОЛОГИИ РАЗДЕЛЕНИЯ РЕДКОЗЕМЕЛЬНЫХ ЭЛЕМЕНТОВ

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Нестационарный режим с накоплением, предупреждающий выход каскада на опасный режим и сохранение качества получаемой продукции внедрен на предприятии Иртышская редкоземельная компания (РК) в 2006- 2015 гг. На двух экстракционных каскадах перерабатывали 300т/г концентрата РЗЭ Соликамского магниевого завода. В экстракционной части каскада искусственно создавали нестационарный режим с поддержанием фронта накопления празеодима. На двух экстракционных каскадах получали чистый дидим (99,95%), концентрат лантана-церия и концентрат иттриевой группы элементов.

Предложен «Мобильный экстракционный модуль» для разделения двух трудно-разделяемых РЗЭ с коэффициентом разделения 1,6 -1,7 и меньше с одновременным получением двух чистых компонентов с содержанием основного вещества минимум 99,9%, до 99,95% и выше и возможностью быстрой перенастройки на разделение другой пары элементов.

Предложен процесс разделения двух элементов с одновременной очисткой от примесей более легких и более тяжелых РЗЭ и выводом четырех продуктов. Подробно рассмотрено разделение празеодима - неодима, тербия-диспрозия, гольмия-эрбия с очисткой от более легких и более тяжелых элементов.

Ключевые слова: нестационарные экстракционные процессы, накопление, редкоземельные элементы

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OBTAINING OF 34-FOLD ENRICHMENT OF THE ATOMIC COMPONENT OF NITROGEN WITH ^{15}N ISOTOPES IN THE POST-DISCHARGE ZONE

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The EPR method was used to obtain an experimental dependence of the ratio of the concentrations of ^{15}N to ^{14}N isotope atoms on the time of nitrogen flow to the EPR resonator through a quartz tube emerging from the electric discharge zone. With increasing flow time, this ratio, normalized to the natural ratio, increased and reached a value of ~ 34. A kinetic model is proposed in which the observed atomic isotopic enrichment is due to the activation nature of the exchange reaction of atoms with nitrogen molecules vibrationally excited in the discharge, the upper vibrational levels of which are enriched with molecules containing a heavier isotope during nonequilibrium vibrational-vibrational exchange. In addition to the exchange, the model takes into account the dissociation of molecules, the recombination of atoms, and the loss of vibrational energy of molecules on the tube surface. Within the framework of the model, the vibrational temperature $T_1 = 1556$ K and the average vibrational energy of the molecule $\varepsilon = 0.038$ eV were estimated, which correspond to the maximum atomic enrichment at a translational temperature T = 300 K and a molecule concentration of 10^{17} cm^{-3}. Approximation of the experimental data graph using the proposed model also made it possible to independently estimate the probability of vibrational deactivation of nitrogen molecules on the wall of the quartz tube $\gamma = 1.1 \cdot 10^{-4}$ and the fraction of the discharge power spent on excitation of molecule vibrations.

Keywords: gas excitation mode, isotopic enrichment

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THE ANALYTICAL SOLUTIONS OF EQUATIONS OF A COUNTER-CURRENT CASCADE WITH ARBITRARY CUT NUMBERS OR SEPARATION FACTORS

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For the first time the analytical solutions of hydraulic equations of a counter-current cascade, the stages of which can have arbitrary cut numbers and output flows partly returned to the entrances of their self, have been found. If the stages of a cascade are characterized by arbitrary separation factors α-separation factor in product and β-separation factor in waste, the analytical expressions for flows and concentrations can be achieved.

Based on the analytical solutions of the equations of a counter-current cascade, a software was developed, which can be used to calculate the data of a counter-current cascade, such as flows and concentrations of product and waste, flow distribution and concentration distribution inside a cascade. In addition, there is no any approximation used in the software so the results provided by the software are always accurate.

Keywords: analytical solution, counter-current cascade, arbitrary cut number.

30 ИЗОТОПНО-СЕЛЕКТИВНАЯ ЛАЗЕРНАЯ ИК МНОГОФОТОННАЯ ДИССОЦИАЦИЯ МОЛЕКУЛ $^{10}BCl_3$: ПОИСК ОПТИМАЛЬНЫХ АКЦЕПТОРОВ РАДИКАЛОВ

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Исследована изотопно-селективная ИК многофотонная диссоциация (МФД) молекул BCl_3 излучением импульсного CO_2-лазера в среде 5-ти акцепторов радикалов $BCl_2^{\bullet}$ (H_2, CH_4, CH_3F, C_3H_4, CH_2F_2), которые позволяют получить газообразные борсодержащие продукты. Эксперименты проводились с естественной изотопной смесью молекул $^{10}BCl_3$ (≈20%) и $^{11}BCl_3$ (≈80%). Частота лазерного излучения настраивалась в резонанс с колебанием ν_3 = 993.7 $см^{-1}$ молекул $^{10}BCl_3$.

С акцептором пропином (C_3H_4) получены зависимости выходов и селективности МФД молекул $^{10}BCl_3$ и $^{11}BCl_3$ от собственного давления BCl_3 в диапазоне 0.5-2 Торр, а также зависимость выхода газообразного продукта от количества распавшегося BCl_3. Эти зависимости позволяют сделать вывод, что, по крайней мере, до давления BCl_3 2 Торр колебательно-колебательный обмен между возбуждаемой компонентой $^{10}BCl_3$ и невозбужденными молекулами $^{11}BCl_3$ практически не влияют на выход и состав продуктов. Для ряда акцепторов радикалов частично идентифицированы основные продукты, формирующиеся при диссоциации молекул BCl_3 и последующих химических реакций. Сделан выбор акцепторов радикалов, оптимальных с точки зрения получения единственного газообразного продукта диссоциации и достижения высоких выходов и селективности МФД молекул $^{10}BCl_3$.

Ключевые слова: изотопно-селективная ИК многофотонная диссоциация молекул, акцепторы радикалов, газообразные борсодержащие продукты

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EFFECTIVE ISOTOPE-SELECTIVE LASER IR DISSOCIATION OF $^{10}BCL_3$ AND $^{11}BCL_3$ MOLECULES UNDER MULTIPHOTON EXCITATION IN A TWO-COMPONENT MEDIUM

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In nature, boron exists in the form of two stable isotopic modifications - 10B (about 19.8%) and 11B (about 80.2%). For the successful development of nuclear energy, a fairly large amount of 10B isotopes is needed (annual consumption in Russia is up to 1000 kg). The isotope 11BCl3 is used in the electronics industry and in medicine. Therefore, the development of new technologically effective methods for separating boron isotopes is currently an important and urgent task. Among the laser methods of separating boron isotopes, the most promising is considered to be the method of isotope-selective multiphoton dissociation of BCl3 molecules by a pulsed CO2 laser radiation. However, since the BCl3 molecule is very strong (dissociation energy 110 kcal/mol), effective dissociation occurs only at very high excitation energy densities 20 J/cm2. This is a major problem in terms of developing a technological process for laser separation of boron isotopes. The main goal of this work is to find experimental conditions under which multiphoton dissociation of BCl3 molecules would be carried out at low excitation energy densities $\Phi \leq 4$ J/cm2. We have found that a significant decrease in the threshold dissociation energy density (up to 3-5 J/cm2) of 11BCl3 molecules occurs in the case of excitation of BCl3 in a mixture with SF6 molecules, which are both sensitizers and acceptors of radicals (chlorine atoms) formed during the dissociation of BCl3 molecules. It has also been established that when BCl3 is excited in a mixture with SF6 molecules, the yield and selectivity of 11BCl3 dissociation increase (by 1-2 orders of magnitude) and selectivity (by 2-5 times). The results of experiments performed under conditions of excitation of BCl3 molecules of natural isotopic composition by pulsed CO2 laser radiation in a mixture with an optically active sensitizer and radical acceptor - CH3F molecules - are presented. It was found that in this case, resonance radiative-collisional vibrational energy transfer from CH3F to 10BCl3 is observed, which leads to a significant increase in the dissociation yield (several times) of 10BCl3 and 11BCl3 molecules compared to the dissociation yield with neutral radical acceptors.

Keywords: laser isotope separation of boron isotopes, multiphoton dissociation of molecules, sensitizer, radical acceptor.

32 МАГНИТНАЯ АКТИВАЦИЯ ИЗОТОПНОГО ЭФФЕКТА ПРИ КРИСТАЛЛИЗАЦИИ

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Магнитный изотопный эффект (МИЭ), наблюдающийся в ходе химических реакций между радикалами во внешнем постоянном магнитном поле, был открыт ещё до 1979 года. Однако, МИЭ, не требующий больших затрат энергии и имеющий высокий коэффициент однократного разделения изотопов, до сих пор не находит практического применения. При этом следует заметить, что некоторые радикальные процессы в магнитном поле позволяют организовать разделительный каскад.

Наши исследования МИЭ связаны с процессом выращивания кристаллов NaCl из пересыщенного водного раствора. Раствор выпаривали при температуре 26°-27°C. В условиях насыщения раствора возрастает количество недиссоциированных молекул, оседание которых на поверхности растущего кристалла происходит по «радикальному» пути.

Соединение NaCl удобно тем, что легко кристаллизируется. При этом Na имеет один изотоп, а Cl – два. Поэтому изменение изотопного состава или их естественного распределения по объему могут быть зафиксированы методом рентгеновской дифракции. Для уменьшения радиационной нагрузки на кристаллы соли регистрировали 5 дифракционный рефлекс (угол 74,8°-75,8°) и 6 рефлекс (угол 84,4°-83,7°). Для исключения механического воздействия при измельчении для дифрактометрии, выращивали и сушили микрокристаллы размером менее 0,2 мм.

В докладе приводится экспериментальные данные и обсуждается оригинальная модель парамагнитных явлений, предложенная авторами исследования, связанная с проявлением МИЭ. Анализируется возможность получения максимального эффекта.

Ключевые слова: кристаллизация, изотопный эффект, ядерный спин, магнитное поле

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SEPARATION OF BORON ISOTOPES BY CHEMICAL EXCHANGE IN LIQUID-LIQUID SYSTEM USING MALIC ACID AS A BORON TRANSPOT AGENT

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In continuation of the complex of works on the separation of boron isotopes by the method of chemical exchange in liquid-liquid systems using aqueous solutions of boric acid and a solution of tri-n-octylamine in o-xylene, malic acid was considered as a transport agent for boron. The influence of malic acid concentration on the phase equilibrium of boron was determined, and it was found that the nature of the boron extraction isotherm is similar to the nature when tartaric acid is used as a transport agent. It was found that the organic phase is enriched with the boron-10 isotope, and the single isotope effect of boron, with an increase in the concentration of boric acid in the initial aqueous phase from 0.05 M to 0.7 M, changes from 1.0033 ± 0.0011 to 1.0433 ± 0.0056. When considering the influence of temperature on the magnitude of the single isotope effect, a decrease in the value to 1 was obtained upon reaching a temperature of 80 °C, which was accompanied by a decrease in the distribution coefficient of boron between the organic and aqueous phases.

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Keywords: separation of isotopes, boron isotopes, liquid-liquid system, single stage separation factor

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FEATURES OF HYDRODYNAMICS IN THE CO_2 – SOLUTION OF MONOETHANOLAMINE CARBAMATE IN DMSO SYSTEM IN A COLUMN WITH A SPIRAL PRISMATIC PACKING

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The article discusses the results of determining the hydrodynamic characteristics of the system CO_2 – a solution of carbamate of monoethanolamine in dimethyl sulfoxide in the concentration range of carbamate between 1 – 3 mol/l in a chemical isotope exchange column with an inner diameter of 11 mm filled with a spiral prismatic packing made of stainless steel with an element size of 1.2×1.2×0.2 mm. On average, the static retention capacity of the packing in the concentration range of carbamate of monoethanolamine in a solution of 1 – 3 mol/l varies from 0.092 to 0.125 m^3/m^3. The total retention capacity was studied at a specific fluid flow of 3.2 ml/(min · cm^2) in the same concentration range. As a result, the total retention capacity of the packing layer varies from 0.449 to 0.513 m^3/m^3. Exponential equations were obtained describing the dependence of the hydraulic resistance of the packing layer on the value of the specific fluid flow in the concentration range of carbamate of monoethanolamine 1 – 3 mol/l. Additionally, the values of maximum throughput were obtained for this system. With enlarging of the concentration the average value of maximum throughput decreasing from 6.9 up to 3.5 ml/(min · cm^2). Moreover, were studied the gas velocity at the phase inversion point for this system and were calculated the values of theoretical once. The difference between practical and theoretical values was no more than 5%, which is an acceptable result.

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Keywords: hydrodynamics, carbamate method, isotope separation, carbon isotopes, carbon dioxide

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PHASE AND ISOTOPIC EQUILIBRIUM BETWEEN BCl_3 AND ITS SOLUTION IN PERFLUORDECALIN

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The phase and isotopic equilibrium between boron trichloride and its solution in perfluorodecalin is considered.
Data obtained during experiments on the saturation of perfluorodecalin with boron trichloride in the temperature range from 12 ºC to 30 ºC indicate the high solubility of BCl_3 in perfluorodecalin, which, when expressed as a molar ratio, varies from 3.024 ± 0.004 to 0.099 ± 0.007 mol BCl_3/mol perfluorodecalin. The thermal effect of dissolution ΔH_s of BCl_3 in perfluorodecalin is estimated at 4-6 kJ/mol BCl_3, which is within the range of van der Waals interaction. Based on the results of isotope analysis of the gas and liquid phases for this gas-liquid system, a single isotope effect of boron at a temperature of 12 °C was determined to be $\alpha = 1.0085 \pm 0.0036$.

Acknowledgements: the authors express their gratitude to the Mendeleev Shared Resource Center
Keywords: perfluorodecalin, boron trichloride, boron isotopes, single stage separation factor

ABSTRACTS

POSTERS

MEMBRANE MATERIALS AND COMPOSITES

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INVESTIGATION OF TRANSPORT PROPERTIES OF MIXED MATRIX MEMBRANES BASED ON POLYSULFONE WITH ADDED GRAPHENE OXIDE NANOPARTICLES

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The process of separating gas and liquid mixtures is an energy-intensive stage in industry. In this case, the primary method used is distillation, which involves the evaporation and condensation of vapor from the mixture, a process that is also not environmentally friendly due to the emissions. An ecologically cleaner and less energy-intensive alternative is the use of baro-membrane processes.

In our work, we investigated the influence of graphene oxide (GO) on the permeability of pure water under high pressures through membranes made of polysulfone (PSF) with added GO. Samples were prepared using the phase inversion method; the casting solutions were composed of dimethylformamide (DMF), PSF, and GO, with a mass concentration of PSF in DMF of 15% and GO relative to PSF ranging from 0% to 1%.

The permeability of liquids was measured by method and experimental setup which was described in work [1]. The measurements were taken with constant temperature of 30 °C and pressure of 1.0, 1.5, 2.0 MPa

It was found that the addition of GO leads to a nonlinear change in the permeability of made membranes. The addition of 0.1% GO showed a 3.1-factor increase in permeability, while further adding GO led to a 2.8-factor decrease of permeability. There are no models that describe such behavior of permeability. The obtained results may be related to the influence of GO on the membrane formation process.

Keywords: mixed matrix membrane, graphene oxide, ultrafiltration, polysulfone

References:

[1] Grekhov A., Belogorlov A., Yushkin A., Volkov A. New express dynamic technique for liquid permeation measurements in a wide range of trans-membrane pressures // Journal of Membrane Science. – 2012. – Vol. 390-391. P. 160–163.

37 EFFECT OF GRAPHENE OXIDE EMBEDDING ON OPTICAL, THERMAL AND MECHANICAL PROPERTIES OF POLY(VINYL ALCOHOL) FILMS

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Nowadays polymer composites filled with graphene-based particles are being actively studied. Graphene is a two-dimensional material in the form of single-layer carbon sheets with outstanding mechanical, thermal and electrical properties. This allows achieving significant changes in the properties of the composite even at low filler concentrations.
The aim of this work was to study the optical, thermal and mechanical properties of polyvinyl alcohol films with embedded graphene oxide (GO) particles. The samples were prepared by solvent evaporation method, the filler fraction in the films varied from 0 to 1 wt%. In order to characterize properties of the composites tensile testing, spectrophotometric and thermomechanical analysis were carried out.
Optical density measurements of the obtained samples in the ultraviolet and visible range indicate successful dispersion of GO nanoparticles in the polymer matrix. The change in elastic modulus of the films for all filler concentrations was negligible (within 10% of the average value). Incorporation of GO improved the thermal stability of the samples, and an increase in the GO concentration enhances the effect.

Keywords: composite films, poly(vinyl alcohol), graphene oxide

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EFFECT OF SURFACE MODIFICATION OF CARBON NANOTUBES AND GRAPHENE ON DISPERSION EFFICIENCY

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The introduction of nanoparticles into polymers allows to improve their properties. Carbon nanotubes (CNT) and graphene are of particular interest; these particles have a number of unique physical properties, and their geometric shape allows to change the properties of polymers at low concentrations (<1%). Their shape and properties only begin to work, if their agglomerates can be dispersed into individual particles, which is not an easy task.

This work presents the results of a study of the influence of the method of functionalization of the surface of CNT and graphene on the optical density of suspensions and films in the visible and ultraviolet regions (190-1100 nm). For this purpose, suspensions of CNT "TAUNIT" and graphene (RG-S1) were prepared in a polar solvent (distilled water), in a non-polar solvent (chloroform) and polysulfone films with these particles (C_m=0-2%). An ultrasonic bath (35 kHz 100 W) was used to disperse the particle agglomerates. A spectrophotometer (Hach dr 5000) was used to measure the optical density. The particle surface was modified with nitric acid and a mixture of nitric and sulfuric acid.

It was found that in aqueous suspensions for graphene the difference in dispersion efficiency between nitric acid and a mixture of nitric and sulfuric acid is insignificant, while for carbon nanotubes the maximum dispersion efficiency is observed when using a mixture of nitric and sulfuric acid. In films made of polysulfone and embedded particles of different modifications, it was found that for CNT there is no fundamental difference between the use of nitric acid or a mixture of nitric and sulfuric acid. Functionalization of the surface of the particles leads to an increase in the optical density of all those studied films, i.e. to an increase in the degree of dispersion of CNTs and graphene in polysulfone

Keywords: graphene, carbon nanotube, polymer, agglomerates, dispersion

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ASSESSMENT OF CHANGES IN THE STRUCTURAL CHARACTERISTICS OF CARBON-CARBON COMPOSITE MATERIALS AND CARBON-FIBRE COMPOSITE AFTER HIGH-TEMPERATURE TESTS

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Carbon-carbon composite materials (C/C composite materials) and carbon-fibre composite having a heterogeneous structure including reinforcing fibers, a carbon matrix and pores are of considerable interest for modern scientific research due to their unique mechanical and thermal properties at a relatively low density. These materials are in great demand in space technology, modern aircraft and rocket engineering, wind energy, as well as in the automotive industry.

The aim of the work was to study the structural properties of C/C composite materials and carbon-fibre composite after conducting high-temperature tests on them at 2000 °C and 2500 °C.

The research was carried out using Raman spectroscopy and X-ray phase analysis.

The conducted studies made it possible to assess the degree of structural changes in C/C composite materials and carbon-fibre composite under the influence of high temperatures. It has been established that composite materials are resistant to high-temperature exposure, but are subject to structural changes at temperatures above 2000 °C.

The results obtained are important for the development and use of these materials in high-tech industries.

Keywords: carbon-carbon composite material, carbon-fibre composite, Raman spectroscopy, X-ray phase analysis.

40 WETTABILITY AND CHARGING OF POLYMER MATERIALS TREATED BY DIRECT CURRENT GLOW DISCHARGE

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Direct-current glow discharge treatment of polytetrafluoroethylene (PTFE) films was used for their significant hydropilization. Low-temperature plasma processing by direct-current discharge also leads to the appearance of surface charges on initially hydrophobic polymer surfaces. Storage of PTFE films after plasma treatment in environments with different relative humidity leads to an increase of water contact angle and at the same time to the decrease of urface potential. Hydrophobic recovery of plasma-treated PTFE films is considered as a consequence of charge relaxation in humid atmosphere. It was shown that the increase of hydrophilicity after plasma treatment of polymers may be assumed as the result of surface charging during plasma processing of polymer surfaces.

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Keywords: plasma treatment, wettability, polymer surfaces

41 NFLUENCE OF SYNTHESIS CONDITIONS ON CHEMICAL COMPOSITION AND DEFECTS IN POROUS ANODIC ALUMINUM OXIDE

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Porous anodic aluminum oxide (PAAO) is a nanostructured material with a high specific surface area, varying from units to tens of square meters per gram of substance. An interesting and practically important task is to create an optical sensor platform based on PAAO. To solve this problem, it is necessary to strictly control the chemical composition of the samples, the type of defects and their concentration.

Two series of the PAAO were synthesized by the anodic oxidation method in solutions based on selenium and sulfuric acid with different synthesis parameters (electrolyte concentration, current density, temperature, anodization time). Selenium and sulfur were found in the composition of the corresponding PAAO. It was found that all samples have an amorphous structure, but for the first time it was found that when the synthesis temperature of the samples is increased only to 40 °C and at a current density of 15 mA/cm^2, the samples begin to crystallize. We assume that this is due to the nanosized phase of aluminum oxide. In all PAAO samples, defects of the oxygen vacancy type were found, the concentration of which is approximately the same in both PAAO series and increases with the growth of the electrolyte temperature. This is confirmed by the data of X-ray phase analysis, according to which with the increase of the electrolyte temperature during synthesis, a decrease in the oxygen content in the PAAO is observed. It should be noted that only in the PAAO based on selenic acid were defects of the oxygen anion-radical type detected, and in a concentration more than an order of magnitude higher than oxygen vacancies. A mechanism for the observed effect is proposed that takes into account the higher oxidizing capacity of selenic acid. The obtained data can be used to obtain an optical sensor platform based on PAAO with specified characteristics.

Acknowledgements: The study was supported by a grant from Russian Science Foundation № 24-19-00402, https://rscf.ru/en/project/24-19-00402/.

Keywords: porous anodic aluminum oxide, selenic acid, sulfur acid, oxygen vacancy, oxygen anion-radical

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INVESTIGATION OF THE INFLUENCE OF CARBON NANOTUBES AND GRAPHENE ON THE PASSAGE OF TERAHERTZ RADIATION THROUGH POLYSULFONE POLYMER FILMS

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The terahertz radiation region (0.1–10 THz) is an intermediate range between microwave and infrared radiation and has several unique properties, which makes it interesting for scientific research and practical applications. A current applied task is the creation of composites capable of absorbing radiation in the terahertz frequency range. One way to solve this problem is to create polymer films with embedded nanoparticles that absorb terahertz radiation. Of particular interest due to their physicochemical properties are carbon nanotubes and graphene, which allow changing the physical properties of polymers at low concentrations (< 3%).

This work presents the results of research of the optical properties in the terahertz (THz) range (520–1520 GHz) of polysulfone (PSF) polymer films with embedded carbon nanotubes (CNTs) and graphene nanoparticles, prepared by mixing solutions of PSF/chloroform solutions and CNT/chloroform and graphene/chloroform suspensions. The measurements were carried out on an experimental setup for measurements in the THz frequency range.

It was found that the introduction of nanotubes into PSF films led to a decrease in intensity at a frequency of 960 GHz by 1.5 times at a CNT concentration of 3% and a film thickness of 55 μm. For a film with a thickness of 65 μm and a graphene concentration of 2%, it was possible to achieve a decrease in transmitted radiation compared to incident radiation by 50 times at a frequency of 1360 GHz and by 220 times at a frequency of 1520 GHz.

Keywords: Carbon nanotubes, graphene, polymer, polysulfone, optical density

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HYDROLYTICALLY STABLE POLYPHENYLENE SULFONE HOLLOW FIBER MEMBRANES

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Membrane filtration is becoming one of the most sought after water purification technologies today. The main application of membranes is the treatment of water media containing pathogenic organisms. For this reason, periodic sterilization of membrane elements is required. Of the polymers withstanding such effects on a multi-cycle basis, the most promising is polyphenylene sulfone (PPSU), which has high temperature resistance, long thermal stability, high mechanical strength and resistance to hydrolysis. In this work, hollow fiber membranes based on the synthesized PPSUs with different molecular weights were prepared and investigated in terms of transport and separation properties. The membrane that showed the best filtration result was exposed in autoclave for 250 h. Polysulfone (PSU) membranes were used as a comparison membrane. During the autoclaving process, samples were taken to study mechanical, transport and molecular weight characteristics. It was shown that the characteristics of PPSU membranes remained constant, while PSU membranes lost mechanical strength during sterilization.

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Keywords: polyphenylene sulfone, hollow fiber membrane, molecular weight, autoclaving

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THE EFFECT OF UNEVEN IMPREGNATION OF MONOFILAMENTS ON THE TECHNOLOGICAL PARAMETERS OF AUTOMATED WINDING

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Automated layout-winding with a thermoplastic prepreg is a promising method of forming thin-walled shells of composite structures. Improving the performance of these materials is an important task. One of the limiting factors for the development of an effective process strategy is the assessment of the influence of thermophysical properties during laser molding.

The purpose of this research is to solve the optimization problem according to the technological parameters of the process of automated laying-winding of composite material based on the distribution of monofilaments in an array of thermoplastic prepreg. The studies were carried out by the method of laser flash and the method of differential scanning calorimetry, as well as the study of the physical and mechanical properties of composite material samples. The obtained results were compared with an analytical model for the convergence of values, which served as the basis for solving a biparametric optimization problem.

Keywords: thermoplastic prepreg, automated layout, laser deposition, optimization task, monofilament.

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MEMBRANE BASED ON FLUORO-CONTAINING POLYORGANOSILOXANE WITH ANTIFOULING PROPERTIES

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The development of membrane materials that have an antifouling effect is a significant challenge for pervaporation separation processes. In order to obtain pervaporation membranes resistant to fouling a series of poly(decyl)-poly(pentafluoropropylacrylate)-methylsiloxane copolymers were synthesized for the first time. The near-quantitative addition of 2,2,3,3,3,3,3,3-pentafluoropropyl acrylate (F5) and 1-decene to polymethylhydrosiloxane was confirmed by ^{1}H NMR spectroscopy. The completeness of the hydrosilylation reaction in the crosslinked films was confirmed by IR spectroscopy. The influence of copolymer composition on gas-transport properties of films for CO_2, CH_4 and N_2 was considered. The introduction of F5 into poly(decylmethylsiloxane) (0F) results in an increase in CO_2 solubility and permeability coefficients across the entire concentration range studied. The interaction of side substituents in the polymer structure affects the sorption of individual liquids in a similar way. Increasing the F5 content in the copolymer leads to an increase in volumetric sorption on ethanol and acetone. The dependence of n-butanol sorption has an extreme character, with the maximum occurring for the sample with 50% mol F5 containment (50F5). Based on 50F5 copolymer characterized by the maximum value of gas permeability and sorption of n-butanol, composite membranes on MFFK-1 microfiltration substrate were prepared. A comparative study of the stability of transport properties of 50F5/MFFK and 0F/MFFK membranes after 2 months of contact with solutions of fouling agents (ABE broth, lecithin, protein) demonstrated that the presence of fluoroacrylate groups in the polymer of the selective layer allows at least halving, and in the case of ABE broth, almost completely preventing the relative permeability decrease of the composite membrane.

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Keywords: Polymethylpentafluoropropylacrylatesiloxane, polydecylmethylsiloxane, membrane, fluoroalkylacrylate-substituent polysiloxane, antifouling membrane materials

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COMPOSITE MEMBRANES FOR WATER DESALINATION BY MEMBRANE DISTILLATION

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The paper presents the methods for formation of one- and two-layer superhydrophobic coatings on the surface of hydrophilic poly(ethylene terephthalate) track-etched membrane by electron-beam deposition of polymers in vacuum. It is shown that the usage of ultra-high molecular weight polyethylene as a target makes it possible to obtain hydrophobic and highly hydrophobic coatings with morphologically developed structure. The water contact angle of this layer, depending on its thickness, varies from 92 to 125°. This change in the wettability is due to the development of roughness of the deposited layer having hydrophobic properties at the increase its thickness. The electron-beam deposition of a thin layer of polytetrafluoroethylene on their surface leads to the formation of the two-layer superhydrophobic coatings. The values of water contact angle for this type of membranes, depending on the total thickness of the two-layer coating, vary from 150 to 160°. A significant increase in the value of contact angle is due to the lower free surface energy and more considerable development of the roughness of the fluoropolymer comparison to the ultra-high molecular weight polyethylene coating. To obtain a one-layer superhydrophobic coating on the membrane surface, polytetrafluoroethylene was used as a target. It is shown that the elaborated composite membranes can be used for desalination an aqueous sodium chloride solution by membrane distillation. It is revealed that the use of the thin hydrophobic layer in combination with the thick hydrophilic substrate increases the productivity of the membrane distillation process.

Keywords: track-etched membrane, electron-beam deposition of polymers in vacuum, superhydrophobic coatings, composite membranes

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ANOMALOUS ALKANES SORPTION AND DIFFUSION IN COMB-LIKE SEMICRYSTALLINE POLYSILOXANE

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In this work, alkanes (C_2H_6, C_4H_{10}) sorption and diffusion in comb-like poly(*n*-tetradecyl methyl siloxane) (PTDMS) were investigated for the first time. The studies were carried out using the gravimetric sorption analyzer at temperatures below (5°C) and above (25°C) the side-chain melting point.

For amorphous PTDMS, it was found that the solubility *S* and diffusion *D* coefficients increase linearly with sorbed alkane concentration. The sorption and desorption isotherms coincide, and the sorption kinetics were well approximated by the solution of Fickian diffusion equation. The same sorption and transport behavior was previously observed for polydimethylsiloxane.

For semicrystalline PTDMS, the anomalous sorption and diffusion behavior was found. In a wide range of sorbed alkanes concentrations (5 – 30 cm^3(STP)/cm^3), a discrepancy between sorption and desorption was observed, as well as anomalous sorption kinetics with additional long-term relaxation stage. The alkanes diffusion coefficients in this concentration region increase by almost an order of magnitude (~10^7 → 10^{-6} cm^2/s). Moreover, the concentration dependences $S(c)$ and $D(c)$ at 5°C are strongly nonlinear. These anomalous sorption and transport properties were explained by the side-chain melting and crystallization during alkanes sorption and desorption, respectively. Such type of first order phase transition (sorption/desorption induced melting/crystallization) was detected for the first time for polysiloxane.

Acknowledgements: This research was carried out within the framework of the state program of TIPS RAS.
Keywords: polysiloxane, comb-like polymer, anomalous sorption, anomalous diffusion

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ТЕЧЕНИЕ НЕСМАЧИВАЮЩЕЙ ЖИДКОСТИ В КВАЗИЦИЛИНДРИЧЕСКИХ НАНОПОРАХ ПРИ ИМПУЛЬСНОМ ИЗМЕНЕНИИ ДАВЛЕНИЯ

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Вопрос о транспорте несмачивающей жидкости в нанопорах привлекает значительное внимание в последние годы в силу широкого спектра возможных приложений. Одним из перспективных направлений является разработка новых смарт-материалов для демпфирования импульсного воздействия, состоящих из нанопористого материала, погружённого в несмачивающую жидкость, которые могут эффективно преобразовывать и диссипировать механическую энергию. Установлено, что поглощение энергии в таких системах в первую очередь определяется откликом системы, на который влияет скорость течения несмачивающей жидкости в каналах нанопор [1].

В настоящей работе исследовано течение несмачивающей жидкости в каналах нанопор цилиндрической формы в системе «нанопористый материал-несмачивающая жидкость» в условиях импульсного (ударного) изменения давления. Для этого были проведены серии экспериментов с гидрофобизированным нанопористым материалом МСМ-41 С1. В качестве несмачивающей жидкости использовались дистиллированная вода и водный раствор этилового спирта.

[1] Belogorlov A. A. et al. Suspensions of lyophobic nanoporous particles as smart materials for energy absorption //Journal of Colloid and Interface Science. – 2021. – Т. 600. – С. 229-242.

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Ключевые слова: несмачивающая жидкость, нанопористый материал, течение несмачивающей жидкости, импульсное изменение давления, цилиндрические нанопоры.

49 ENERGETICS OF SHORT- OR LONG-TERM STATES OF NON- WETTING LIQUID DISPERSED IN NANOPOROUS MATERIAL

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Systems consisting of nanoporous material and non-wetting liquid now have a wide range of possible applications from absorption and storage of mechanical energy to drug delivery systems. The non-outflow of the non-wetting liquid was previously found to be key to determining the feasibility of such systems. This phenomenon can be considered as a transition of a part of the liquid into a metastable state, and the decay of such states is determined not only by the pore size distribution function, but also by the spatial structure of the pores.
The work presents a method of determining the energy of short- (up to 10 s) and long-term (from 10 to ~ 10^3 s) metastable states of non-wetting liquid in the case of complete and partial initial filling of pores with non-wetting liquid. For the investigated system: nanoporous material Fluka 100 C18 (60756) - non-wetting liquid distilled water the results of calculations of energy of short- and long-term metastable states of non-wetting liquid in case of complete and partial initial filling of pores with non-wetting liquid were obtained.

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Keywords: non-wetting liquid, nanoporous material, relaxation of non- wetting liquid, metastable states

50 INFLUENCE OF PORE SIZE ON THE FLOW OF NON-WETTING LIQUID IN NANOPORES

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In recent years, interest in the description of fluid transport in nanochannels has increased. These studies are mainly based on results using molecular dynamics methods. Within the framework of these studies it is shown that the filling velocity of non-wetting liquid in nanochannels can reach more than 100 m/s.

In the present work, the filling of nanoporous materials with pore sizes of 9 nm (Fluka 100 C8), 5 nm (Fluka 60 C8 PF), and 2 nm (MSM-41-C1) at pressure growth rates of 1.6 16 and 160 atm/s with non- wetting liquid (distilled water) has been studied. It is shown that the decrease in pore size increases the characteristic pore filling pressures with decreasing pore size and increasing pressure growth rate. Moreover, for the Fluka 100 C8-water system, the influence of the pressure growth rate is absent within the error of the experiment.

Acknowledgments: The work was supported by RNF, project No. 23-29-00352.
Keywords: non-wetting liquid, nanoporous material, flow of non-wetting liquid, pressure growth rate.

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SWELLING PROPERTIES OF POLYDECYLMETHYSILOXANE: INFLUENCE 1-DECENE/CROSS-LINKING DIENE RATIO

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Polydecylmethylsiloxane (C10) is a promising polysiloxane material for the volatile organic compounds (VOCs) separation from air or off gases. However, there is a problem of decreasing membrane separation properties in VOC/gas mixture, which is deals with significant polysiloxane swelling in VOC media. By chemical cross-linking the polysiloxane structure can be modified and undesirable swelling reduced. In this work, C10 was cross-linked by vinyl-terminated PDMS (molecular weight of 25,000 g/mol) and dienes (1,7-octadiene, 1,9-decadiene, 1,11-dodecadiene), marked as C10-Sil25-OD, C10-Sil25-DD, C10-Sil25-DdD, and polymer films with a 1-decene:CD ratio of 9:1 to 1:9 were obtained. The synthesis of cross-linked C10 was carried out according to the methodology previously developed at TIPS RAS, which is based on the hydrosilylation reaction. Sorption (S), swelling (Q), density (ρ) and membrane samples cross-link densities (γe) were measured in the obtained films.

It is shown that all polymers are characterized by a decrease in S, Q with increasing CD content. The lowest values are observed at 1:9 ratio for C10-Sil25-OD (S = 0.722; Q = 1.057) and the highest at 9:1 ratio for C10-Sil25-DD (S = 2.788; Q = 2.990). The obtained pattern correlates well with ρ and γe of the polymers, as ρ and γe of the polymers increase with decreasing S and Q. For example, the C10-Sil25-DD polymer has ρ and γe = 0.992 and 2.617, respectively, at 1:9 ratio and ρ and γe = 0.954 and 1.426, respectively, at 9:1 ratio. Data comparing the gas permeability of cross-linked C10 with different 1-decene/CD ratios will be presented in a poster presentation.

The data obtained in this study will help to identify the most promising polymers for the separation of VOC/gas mixtures and improve the understanding of the chemical structure of cross-linked C10. The C10-Sil25-OD polymer with a 1-decene/CD ratio of 1:9 is the most interesting for further investigation in the separation of VOC/gas mixtures as it showed the lowest swelling value (Q = 1.057).

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Keywords: polydecylmethylsiloxane; cross-linking; sorption; swelling degree

52 USE OF ULTRAFILTRATION THIN-PORE PAN MEMBRANES FOR REFINING USED OIL

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Membrane filtration of used engine oil (UEO) is a promising method for its regeneration, enabling continuous removal of contaminants such as heavy metals and polycyclic aromatic hydrocarbons under relatively mild conditions. This regeneration approach allows for the extraction of valuable oil components, conserving natural resources and reducing the environmental impact associated with improper disposal or emissions from traditional processing methods. Previously, we conducted a study on the purification of UEO using ultrafiltration membranes made from PAN (polyacrylonitrile) solution in DMSO without co-solvent additives. To enhance membrane permeability, UEO was diluted with an organic solvent such as toluene. Filtration successfully removed over 95% of key contaminants, including polymerization products and metals, which are especially harmful to the environment.

This study aims to select ultrafiltration thin-pore PAN membranes to separate the low-molecular-weight organic solvent from the permeate obtained in the prior purification stage. For this purpose, a newly developed approach of directed regulation of PAN ultrafiltration membrane porosity, achieved by adding acetone as a co-solvent to the casting solution, will be used. Varying the casting solution composition results in membranes with different pore sizes from 3.7 to 36 nm. Additionally, an analysis of the composition and physicochemical properties of waste motor oils was conducted to identify the main types of contaminants formed during oil use.

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Keywords: polyacrylonitrile, separation, asymmetric membrane, ultrafiltration, used engine oil.

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EFFECT OF TETRAHYDROFURAN AS CO-SOLVENT ON FABRICATION OF POLYACRYLONITRILE ULTRAFILTRATION MEMBRANES BY NON-SOLVENT INDUCED PHASE SEPARATION

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Membrane separation processes have become widely used across various industries due to their simplicity, environmental friendliness, energy efficiency, and nearly limitless scalability. In petrochemical applications, several tasks involve the separation of dissolved substances and impurities with molecular weights up to 5 kDa, including the recovery of petrochemical synthesis catalysts from reaction products and the separation of asphaltenes from crude oil and petroleum products. Such tasks require membranes with a molecular weight cut-off (MWCO) in the range of 1–3 kDa. Polyacrylonitrile (PAN) is a widely used material for ultrafiltration membranes due to its high chemical resistance to organic solvents, mechanical strength, and resistance to fouling by organic compounds. However, PAN membranes generally exhibit MWCO values above 10 kDa. One approach to reducing pore size involves the use of volatile co-solvents. This study investigated the effect of adding tetrahydrofuran (THF) as a co-solvent on the characteristics and structure of PAN membranes prepared via non-solvent induced phase separation (NIPS). Dimethyl sulfoxide (DMSO) and N-methyl-2-pyrrolidone (NMP) were used as solvents. Results showed that the addition of THF significantly reduced the viscosity of the casting solution. Morphological analysis revealed that with increasing THF content in NMP, the membrane structure remained unchanged. In the case of DMSO, however, an asymmetric structure with cellular micropores began to dominate. The separation performance of the resulting membranes was evaluated through the filtration of 1, 10, and 50 g/L crude oil solutions in toluene.

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Keywords: polyacrylonitrile, co-solvent, asymmetric membrane, ultrafiltration, phase inversion.

ABSTRACTS

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STABLE ISOTOPES AND RADIONUCLIDES IN NUCLEAR TECHNOLOGY AND MEDICINE

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ПРЕДПОСЫЛКИ К РАЗРАБОТКЕ АЛЬТЕРНАТИВНОГО ПРОЦЕССА ПОДГОТОВКИ ПРОБ ОБЪЕКТОВ, СОДЕРЖАЩИХ В СОСТАВЕ УРАН И ПЛУТОНИЙ, ДЛЯ АНАЛИТИЧЕСКОГО ОПРЕДЕЛЕНИЯ НЕКОТОРЫХ ПРИМЕСЕЙ

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Определение примесей в ураново-плутониевых объектах является важной частью контроля технологического процесса и аттестации продукции. Классический метод – эмиссионный спектральный анализ, не может определить такие примеси как фтор и хлор из-за их высокой энергии ионизации и образования летучих соединений в процессе анализа.

В промышленности с этой целью используют ионную хроматографию с предварительным пирогидролизным сжиганием пробы, однако этот метод требует и специального оборудования, что увеличивает время анализа. Поэтому предложенный подход к пробоподготовке — разделение на колонке с ТОМАН-сорбентом анионов от матрицы в первую очередь направлен на упрощение процедуры подготовки пробы и сокращение времени, затрачиваемого на пробу.

В докладе представлены преимущества и недостатки данного метода, показано сравнение метрологических характеристик с стандартной методикой и перспективы развития для контроля иных примесей. Измерения проводились на ионном хроматографе Metrohm 930 Compact IC Flex. Значения двухвыборочного t-критерия сравниваемых методик находятся в диапазоне 1,02 — 1,98 ($t_т = 2.78$). Правильность полученных результатов относительно контрольного раствора составляет 93,5-105,1 % и 94,1-101,8 % для иона фтора и хлора, соответственно. Данный факт указывает на то, что предложенный подход может быть использован в дальнейшем для подготовки проб при определении примесей фтора и хлора.

Ключевые слова: примеси, ионная хроматография, эмиссионный спектральный анализ, пирогидролиз, сорбция

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ИССЛЕДОВАНИЕ БАРЬЕРНЫХ СВОЙСТВ ОБЛУЧЕННОЙ ГЛИНЫ

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Глина является природным материалом, наиболее приемлемым для использования в качестве барьерного материала в захоронениях радионуклидов (РАО), образующихся в результате эксплуатации ядерной энергетики. При разрушении контейнеров с РАО происходит непосредственный контакт радионуклидов с глиной. В результате глина подвергается радиационному разрушению. В настоящее время нет систематизированных сведений об изменении барьерных свойств облученных глинистых минералов.

Цель исследования – определение коэффициента диффузии катионов щелочных и щелочноземельных элементов через слой уплотненной глины, облученной до разных поглощенных доз.

Исследование барьерных свойств минералов глины проводятся нами путем молекулярного моделирования и проведения экспериментальных исследований. В докладе приводятся и обобщаются данные экспериментальных исследований.

Для исследований собрана экспериментальная установка, содержащая диффузионную ячейку, расположенную между замкнутыми контурами с дистиллятом и 1 М водным раствором NaCl. Катионы диффундируют от контура с раствором к контуру с дистиллятом через слой толщиной 3-4 мм уплотненной до величины 1,6-2,2 г/см^3 глины. Использовали природный бентонит и бентонит, облученный до поглощенной дозы 0,3; 0,6; 1,7 МГр излучением ^{60}Co. Концентрацию катионов в дистилляте определяли с помощью кондуктометра. Расчетную формулу выводили из I закона Фика.

Экспериментальные данные показывают, что коэффициент диффузии Na^+ через бентонит, в пределах ошибки измерения, не изменяется до поглощенной дозы 0,6 МГр. При поглощенной дозе 1,7 МГр регистрируется увеличение коэффициента диффузии.

В докладе обсуждаются модели разрушения глинистого минерала, приводящие деградации её барьерных свойств.

Ключевые слова: радионуклид, барьер безопасности, глина, диффузия

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ИССЛЕДОВАНИЕ РАДИАЦИОННЫХ РАЗРУШЕНИЙ ГЛИНИСТЫХ МИНЕРАЛОВ С ПОМОЩЬЮ GEANT

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Глинистые минералы являются хорошим природным сорбентом и превосходным материалом, препятствующим распространению водных растворов. Поэтому глина считается перспективным для использования в инженерных барьерах безопасности пунктов захоронения радиоактивных отходов (РАО).

Основу каркаса глинистых минералов составляют Al_2O_3 (слой октаэдров) и SiO_2 (слой тетраэдров). За время существования глины часть атомов Al и Si были изоморфно замещены на ионы железа, магния. В качестве обменных ионов могут присутствовать Na^+, Ca^{2+}, Mg^{2+}. Например, состав глины: SiO_2 - 37,47 %; Al_2O_3 - 15,40 %; Fe_2O_3 - 2,56 %; MgO - 0,33 %; $CaO_{обм}$ -2,00 %; $MgO_{обм}$ - 0,23 %; $Na_2O_{обм}$ - 0,24 %; H_2O^+ - 4,40 %; H_2O^- - 7,68 %. В составе глинистых минералов, в количестве менее 1%, могут обнаружиться и другие элементы.

Возможные радиационные разрушение глинистого минерала, при прямом контакте с радионуклидами, изучали путем моделирования с применением пакета GEANT04. Поскольку энергия ионизирующего излучения РАО гораздо больше энергии химической связи, то пространственное распределение атомов разных элементов не влияет на разрушение минерала. Поэтому мишень, размерами 10×10×10 см, представляли в виде равномерного распределения атомов разных элементов по объему. Оценивали количество выбитых атомов и расстояние их смещения.

Обнаружено, что максимальную вероятность выбивания имеет изотоп ^{16}O ($2{,}6\ 10^{-14}$), а атом алюминия ($5{,}8\ 10^{-15}$) имеет большую вероятность смещения, чем кремния изотоп ^{28}Si ($9{,}4\ 10^{-15}$). При этом пространственные смещения выбиваемых изотопов уменьшаются в ряду: ^{1}H (390 А), ^{16}O (170 А), ^{28}Si (120), Al (106 А).

В докладе приводится анализ возможных разрушений глинистого минерала с учетом расстояния между его пакетами 10-20 А. При этом игнорировали возможностью «отжига» минерала.

Ключевые слова: глина, радиационные разрушения, поглощенная доза

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LASER AND PLASMA SEPARATION TECHNOLOGIES AND ITS APPLICATION

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КОНСТРУКЦИИ КЛАПАНОВ ДЛЯ РЕАЛИЗАЦИИ ИМПУЛЬСНЫХ ПЛАЗМЕННЫХ ПРОЦЕССОВ

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Применение высокоскоростных плотных плазменных потоков для целей обработки материалов и имитации импульсных воздействий не теряет актуальности в настоящее время. Развитие этих направлений активно ведется в ГНЦ РФ ТРИНИТИ на плазменных ускорителях КСПУ-Т и 2МК-200.

Одним из ключевых узлов плазменного ускорителя является импульсный клапан, который обеспечивает напуск плазмообразующего газа в межэлектродный зазор ускорителя. В настоящее время применяются различные клапаны: термодиффузионные, пьезоэлектрические, электродинамические и электромагнитные. Каждый тип клапана обладает преимуществами и недостатками, влияющими на решение конкретной задачи. Применимость и эффективность клапанов напрямую связаны с параметрами системы газонапуска: подклапанный объем, давление газа и время полного открытия клапана.

Клапан используемый на 2МК-200 относится к эллектромагнитному типу. Открытие клапана осуществляется индукционно-динамическим исполнительным механизмом на основе плоской электромагнитной катушки. Подобная конструкция клапана хорошо отработана. Однако, необходимость повышать характеристики плазменных ускорителей привела к потребности усовершенствовать конструкцию клапана, что негативно отразилось на эксплуатационных характеристиках. Также, в настоящее время, стоит задача по повышению частоты срабатывания клапанов, вплоть до частот 10 Гц.

В работе проведен анализ конструкции быстродействующих клапанов для импульсного напуска газа, подробно разобрана конструкция электромагнитного клапана, описаны его эксплуатационные ограничения и особенности работы.

Ключевые слова: напуск газа, электродинамический клапан, импульсные процессы, электродинамические ускорителя плазмы.

58 МОДЕЛИРОВАНИЕ И РАСЧЕТ ПРОЦЕССА РАЗРЯДА ЕМКОСТНОГО НАКОПИТЕЛЯ ЭНЕРГИИ УСТАНОВКИ 2МК-200

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Емкостные накопители энергии (ЕНЭ) являются одним из наиболее распространённых типов накопителей энергии. Например, ЕНЭ используются в регенеративной энергетике, промышленной электронике, системах аварийного и резервного питания.

Основными узлами емкостного накопителя являются конденсаторные батареи, объединенные в блоки или модули, и коммутаторы, которые полностью определяют выходные характеристики данного устройства.

Установка 2МК-200 ГНЦ РФ ТРИНИТИ укомплектована блочным накопителем энергии, состоящим из нескольких модулей конденсаторов общей емкостью порядка 2 мФ при зарядном напряжении до 45 кВ. В качестве коммутаторов используются форвакуумные разрядники, обеспечивающие коммутацию ЕНЭ на плазменную нагрузку за время порядка 10 мкс с фронтом напряжения в несколько десятков наносекунд.

В работе было проведено моделирование ЕНЭ установки 2МК-200 в среде LT Spice. Модель включает в себя оценку времени зарядки модулей, фактически учтенные параметры кабельных трасс и особенности коммутации конденсаторных блоков на пассивную нагрузку. Рассмотрены различные схемы замещение для форвакуумного разрядника. Полученные в модели осциллограммы тока на пассивной нагрузке находятся в хорошем согласии со значениями, наблюдаемыми в экспериментах.

Ключевые слова: емкостные накопители энергии, разрядники, плазменные установки.

59 DISTANT DRILLING AND LASER CUTTING OF A LARGE THICKNESS STEEL PLATE

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Experiments on remote drilling, as well as on vertical and/or horizontal separation cutting of a vertically mounted 1010 steel plate of 200 mm in thickness by radiation of a continuous ytterbium fibre laser with the power up to 20 kW at the intensity of radiation on the metal surface greater than 10^5 W/cm^2 were carried out in laboratory conditions. Through-hole and cut views and results of drilling and cutting at different modes of a vertically mounted steel plate are presented. It was revealed that the mode of periodic movements of the laser beam along the intended cut provides a higher speed of through-cutting of a steel plate of large thickness in comparison with continuous movement in one direction. The possibility of remote cutting of the same plate mounted horizontally by laser radiation of the same power at radiation intensity $(2\div3.5)\cdot10^4$ W/cm^2 without using an air jet to blow the melt out of the cutting channel was demonstrated. A sectional view as well as the cutting results of a horizontally mounted plate is presented It was found out that cutting under these conditions was only possible starting from the edge of the plate. It is not possible to make a hole in horizontally mounted plates of large thickness without using an air jet.

Keywords: laser, radiation intensity, drilling, cutting.

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ИНТЕНСИВНОЕ СВЕЧЕНИЕ НАНОУГЛЕРОДНЫХ СТРУКТУР ПОД ВОЗДЕЙСТВИЕМ ИМПУЛЬСНОГО 10МКМ ИЗЛУЧЕНИЯ

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В работе приводятся результаты исследования люминесценции оксида графена, графита, многостенных углеродных нанотрубок под воздействием излучения импульсного CO_2 - лазера на воздухе в нормальных условиях. Обнаружено, что импульсное излучение CO_2 лазера при плотностях мощности более 100 kW/cm^2 вызывает широкополосную люминесценцию углеродных наноструктур в видимой области спектра, в том числе обнаружена люминесценция многостенных углеродных нанотрубок под воздействием 10 μm излучения ранее ни где не наблюдавшаяся. Люминесценция на поверхностях, образованных массивом наноуглеродных структур образуется множеством локальных участков. Люминесценция углеродных материалов под воздействием излучения CO_2 лазера, происходит за счет многофотонного поглощения и определяется наличием графеновых структур. Предсказанное расчётами поглощение графеном электромагнитного излучения в диапазоне длин волн от нескольких микрон до десятков микрон подтверждено экспериментально.

Ключевые слова: импульсно-периодический CO_2 лазер, углеродные наночастицы, фотолюминесценция.

61 THRESHOLDS FOR MAINTAINING OPTICAL DISCHARGE IN A LASER PLASMATRON WITH A CYLINDRICAL NOZZLE

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Optical discharge in the mode of a laser plasmatron in Ar and a mixture of Ar with H_2 and CH_4 at atmospheric pressure is maintained in a vertically oriented plasmatron by focused radiation from a continuous CO_2-laser. The half focusing angle $\varphi = r_0/f$ of a laser beam with a radius of $r_0 = 20$ mm for lenses used with a focal length of $f = 160$ and 175 mm does not exceed 0.125 rad. The radius r_f of the focal spot is determined taking into account the spherical aberrations of the lens.

The dependences of the threshold power P_{th} of maintaining the discharge on the gas velocity v (0.05–2 m/s) with a change in the composition of the mixture, the focal length f and the distance L of the focus from the nozzle slice were measured.

It was found that at $L = 2$ mm, the dependences of the $P_{th}(v)$ for discharge in Ar and mixtures $Ar:H_2:CH_4=1:0.07:0.0021$ and $Ar:H_2:CH_4 =1:0.07:0.0042$ have falling and growing branches typical for lenses with $\varphi \leq 0.125$ rad.

An increase in the distance L to 4 mm for the discharge in Ar is accompanied by the absence of a falling branch and an increase in $P_{th}(v)$ on the growing branch. At $L = 7$ mm, the values of the $P_{th}(v)$ are maximum, and at $L > 7$ mm and up to $L = 17$ mm, the thresholds decrease and become close to the thresholds at $L = 2$ mm.

Measurements of $P_{th}(v)$ at $L = 17$ mm, depending on f and the composition of the mixture (concentrations $[H_2]$ and $[CH_4]$ are 0%, 7 and 0.21%, 7 and 0.42%, 14 and 0.21%) showed that a decrease in f leads, in the absence of falling branches, to an increase in $P_{th}(v)$ on growing branches due to an increase in r_f due to aberrations. At the same time, for concentrations $[H_2]$ and $[CH_4] \neq 0$, the shape of the growing branches is changed compared to $L = 2$ mm.

The results obtained can be used for the synthesis of diamond coatings on substrates in the optical discharge plasma.

Keywords: optical discharge, plasmatron, threshold power

62 TWO-WAVE PYROMETER BASED ON A DIFFRACTION GRATING SPECTROMETER

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The dependence of the blackness coefficient $\varepsilon(\lambda,T)$ of the material on the wavelength λ and temperature T can lead to a noticeable error when measuring temperature using pyrometers. For example, the measured unknown temperature excludes the use of reference data for $\varepsilon(T)$ even for gray bodies with a known constant value of ε. The error is also introduced by the dependence of $\varepsilon(\lambda,T)$ on the initial quality of the surface and the composition of the gas when it is heated.

The purpose of this work is to demonstrate the possibility of measuring close to the true surface temperature by using a two-wave pyrometer based on a spectrometer with a diffraction grating and a CCD ruler as a radiation receiver without taking into account information about the coefficients $\varepsilon(\lambda,T)$.

An algorithm for processing thermal radiation spectra has been developed and a control program for on-line temperature measurement has been created. The algorithm is based on the choice of a wavelength range $\Delta\lambda$ free from molecular bands that occur, for example, in 3D printing, excluding from the calculation formula for T the value $\ln[\varepsilon(\lambda_1,T)/\varepsilon(\lambda_2,T)]$, assuming $\varepsilon(\lambda_1,T)=\varepsilon(\lambda_2,T)$ at the edges of narrow intervals $\delta\lambda=\lambda_1-\lambda_2<\Delta\lambda$, and averaging the calculation results over the entire range $\Delta\lambda$, uniformly filled with the intervals $\delta\lambda$.

Polished plates made of St.3, titanium and tungsten were heated by laser radiation. A thermocouple and a serial single-wave pyrometer were used to control the temperature. It is shown that when heated in air at atmospheric pressure and a pressure of 1 Pa, the readings of a two-wave pyrometer with an error of less than 4% correspond to the readings of a thermocouple, and to match the readings of a single-wave pyrometer and a thermocouple, it was necessary to adjust the blackness coefficient on its panel. Dependences of $\varepsilon(T)$ reflecting their change at atmospheric pressure relative to the pressure of 1 Pa due to plate oxidation are obtained.

Keywords: surface, heating, pyrometer, thermocouple

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THE RESPONSE OF OSCILLATIONS IN THE PLASMA ACCELERATOR OF THE MASS SEPARATOR TO A MAGNETIC FIELD

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Simultaneous measurements of the amplitude-frequency characteristics (AFC) of oscillations at frequencies of 20 kHz – 30 MHz of discharge and ion currents in the plasma of an independent discharge in an accelerator with an anode layer of a plasma-optical mass separator POMS-E-3 with a change in the magnetic field at the anode B_{rA} = 205 – 1010 G, at the cathode – B_{rK} = 800 – 4200 G. The results of the AFC measurement were analyzed in conjunction with plasma emission spectra obtained in the same discharge modes in the wavelength range of 200 – 1100 nm and ion energy distributions in the range of 50 – 1200 eV. The common features of the AFC of both currents are a set of many frequencies and, mainly, the cluster nature of the oscillations. When the B_{rA} changes from 660 G to 720 G, the oscillation frequency with a maximum amplitude increases rapidly up to f_{max} ~ 4.5 MHz. In the frequency range of no more than 1 MHz, there is a threshold magnetic field $B_{rA} \approx$ 720 G, at which there are sharp surges of AFC towards higher frequencies.

The fundamental differences between AFC of the discharge current and the ion current are ~ 5 times lower oscillation frequencies with a maximum amplitude of the discharge current relative to the ion current at $205 \leq B_{rA} \leq 660$ G, a sharp decrease in f_{max} for the AFC of the discharge current, but a sharp increase in f_{max} for the AFC of the ion current when B_{rA} becomes greater than 820 G.

Keywords: plasma accelerator, discharge current, ions

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THE FORMATION OF LITHIUM-ALUMINIUM SPINELS AT THE INTERACTION OF PERIPHERAL D-Li PLASMA WITH THE ELECTRICALLY INSULATING CERAMICS IN THE TOKAMAK T-11M

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In this work we consider the interaction of peripheral deuterium-lithium plasma with the elements of ceramic electrical insulation, consisting of electrotechnical porcelain (ETP, $x Al_2O_3 \times y SiO_2$), on lithium limiters under tokamak T-11M conditions.

The theoretical assessment of the maximum possible capture of lithium was carried out based on the value of specific flux of its particles, equal to $\sim 2 \times 10^{16}$ (particles/($cm^2 \times s$)), on the periphery of plasma cord in the area of the ceramic electrical insulation elements, as well as on the value of projection area of the latters on the plasma flow path. The obtained value was compared with the results of the experiment, which involved the following:

1) The acid leaching (by 38% formic acid of analytical purity grade) of the products of the interaction of ETP with elemental lithium (presumably – $Li_xAl_yO_z$, $Li_xSi_yO_z$, and $Li_xAl_ySi_z$) from the surface of the dismantled ceramic protection elements;
2) Evaporation of the yielded solution, and
3) The elemental analysis of the dry residue for the elements Li, Al, and Si.

The results of the latter prove the irreversible nature of lithium losses assumed in [**1**], which is due to its reactions with the components of ETP, accompanied by the formation of lithium-aluminium spinels ($Li_xAl_yO_z$), lithium silicates ($Li_xSi_yO_z$), and Zintl phases ($Li_xAl_ySi_z$), and also allow to estimate the absolute and relative contribution of such processes into the total expenses of Li in the tokamak T-11M.

[1] https://doi.org/10.1134/S0036024424700055
Keywords: tokamak, plasma, lithium, electrotechnical porcelain (ETP), spinels.

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МОДИФИКАЦИЯ СТРУКТУРЫ ПОВЕРХНОСТНОГО СЛОЯ СПЛАВОВ ЖЕЛЕЗА ИМПУЛЬСНЫМИ ПЛАЗМЕННЫМИ ПОТОКАМИ

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Вопросы увеличения сроков работоспособности деталей и узлов различных механизмов остаются актуальными и в настоящее время. Одной из причин этого является желание снизить затраты на технологический цикл создания продукции, а также предотвращение возможности возникновения аварийных ситуаций. Одной из технологий упрочнения поверхностных слоёв металлов является использование концентрированных потоков энергии, в частности, потоков плазмы. Промышленное плазменное поверхностное упрочнение металлов успешно развивается. Особый интерес вызывает состояние поверхностного слоя металла при взаимодействии его с потоком плазмы. Известно о физических изменениях поверхности металлов потоками горячей импульсной плазмы с удельной мощностью от 0,3 до 0,5 МВт/см^2 и длительностью от 10 до 60 мкс. Целью работы является модификация поверхностного слоя деталей из стали 40ХМФА в плазменных потоках газов. Представлены конструкция установки и результаты воздействия плазменного потока на внутреннюю поверхность резьбовых соединений вышеуказанной стали. Генератором потока плазмы является установка ПФ-МОЛ АО «ГНЦ РФ ТРИНИТИ». Основные параметры установки:
напряжение – до 13 кВ; запасенная энергия при напряжении 25 кВ – 230 кДж; рабочее тело – неон, гелий, дейтерий, азот; расстояние от анода до мишени – от 100 до 165 мм; давление рабочего тела в камере перед пуском – от 0,1 до 0,5 торр; материал мишени – сталь 40ХМФА.
Выполнен численный анализ закономерностей воздействия теплового потока на приповерхностный слой металла в рамках уравнения теплопроводности с учётом плавления.
Основным результатом проведенной серии экспериментальных работ на установке ПФ-МОЛ является увеличение твёрдости поверхностного слоя мишени в среднем от 2,5 до 2,7 раза при плотности поглощенной энергии от 15 до 20 Дж/см^2 и длительности импульса до 10 мкс.

ABSTRACTS

POSTERS

14TH PETRYANOV AND 5TH FUKS READINGS

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MOSAIC-SKELETON APPROXIMATION IS ALL YOU NEED FOR SMOLUCHOWSKI EQUATIONS

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In this work we demonstrate a surprising way of exploitation of the mosaic-skeleton approximations for efficient numerical solving of aggregation equations with many applied kinetic kernels. The complexity of the evaluation of the right-hand side with the use of mosaic-skeleton approximations is $O(M \log M^2)$ operations instead of $O(M^2)$ for the straight-forward computation. the family of matrices with good low-parametric mosaic-skeleton approximations is much broader than usual low-rank matrices even though the complexity of the novel approach is higher by $O(\log M)$ times. In this work, we show that our ideas allow to drastically accelerate computations for a family of full rank kernels arising in the aggregation kinetics for sedimentation problems and study the systems with use of 2^{20}nonlinear equations within modest computing time.

67 PHOTOPHORETIC DEPOSITION AND SEPARATION OF AEROSOL-SYNTHESIZED SINGLE-WALLED CARBON NANOTUBES

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We report a novel, dry, and clean method to directly deposit single-walled carbon nanotubes (SWCNTs) onto a desired substrate with the photophoresis phenomenon. We demonstrate the photophoresis method to be convenient and reproducible to deposit low-bundled nanotubes to form either non-percolating or continuous networks with controlled SWCNT density and surface distribution. Employing the structure-dependent optical features of the nanotubes produced by aerosol CVD method, we show the correlation between the light source spectrum and the configuration of the deposited SWCNTs due to the selective light interaction with SWCNTs of certain chiralities. Thus, photophoretic deposition is a promising method for the fabrication of various advanced devices, such as electrically driven single-photon emitters or field-effect transistors from semiconducting SWCNTs with a desired electronic structure.

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Keywords: photophoresis, aerosol CVD, carbon nanotubes

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DEPOSITION OF RADIOACTIVE ADMIXTURE ON NANOPARTICLES IN GAS PHASE

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Aerosol particles in both outdoor and indoor environments are known to be vehicles for the transfer of radioactivity. It is very relevant to solve the problems of the transfer of contaminants both in the free atmosphere and in premises during accidents and abnormal objects using radioactive substances. However, to date, insufficient attention has been paid to solving these problems. In this work, we propose a model of coagulation between atomic radioactive impurities and aerosol particles of various sizes. For simplicity, it was assumed that the concentration of aerosol particles was not very high and coagulation between them might not be taken into account. It was also assumed that the particle concentration has stabilized and reached steady state; only collisions between aerosol particles and radioactive atoms were taken into account, which led to the redistribution of radioactivity on aerosol particles of a certain size. To describe these processes the system of differential equations were proposed. To solve these equations, the formalism of the generating function was used. The obtained analytical and numerical solutions complement each other, since when comparing theoretical and experimental data it is necessary to take into account that the number of particle fractions obtained remains finite.

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Keywords: nano particles, radioactive admixture, deposition

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AEROSOL IMPACT OF THE MEGALOPOLIS ON ITS SUBURB: ASSESSMENT OF THE TYPICAL CONCENTRATION LEVELS OF NEAR-SURFACE AEROSOLS IN THE MOSCOW REGION

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The pollution from large megalopolis is one of the topical environmental problem for adjacent territories in all regions. The paper analyzes the results of continuous observations of aerosol composition in the surface layer of the atmosphere, carried out with identical sets of equipment since 2020 synchronously in Moscow centre and in its suburb near Zvenigorod, 55 km west of of the city. Together with aerosol characteristics, the variability and trends of meteorological parameters for these two points are considered, especially including the frequency of easterly winds (from the city) in Zvenigorod. The empirical values of the rates of change in concentrations of PM10, PM2.5 and individual chemical elements from the values of pressure and relative humidity have been determined in the city and the suburb in different seasons. Also, we estimated the aerosol load from Moscow on the suburban air. The data on the aerosol composition in Moscow from the State Budgetary Institution "Mosecomonitoring" measurements allowed us to clarify the impact of the city as whole on the suburbs.

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Keywords: atmospheric aerosol, RM_{10} and $PM_{2.5}$, Moscow region, advection of impurities, empirical estimates

70 КОМПЛЕКСНЫЕ МНОГОЛЕТНИЕ ИССЛЕДОВАНИЯ АТМОСФЕРЫ НАД ОЗ. БАЙКАЛ

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Озеро Байкал уникальный природный объект Мирового уровня. В 1996 г. Байкал включен в Список объектов Всемирного наследия ЮНЕСКО, в 1999г.– принят Закон РФ «Об охране озера Байкал». Уникальность Байкала определяется высоким стратегическим значением его как крупнейшего источника питьевой воды на планете и, как уникального водоема с эндемичной флорой и фауной. В последние годы в прибрежных районах озера наблюдается «экологический кризис» - гибель эндемичных видов растений и животных и замещение их широко распространенными видами, причины которых еще до конца не раскрыты. Одной из возможных причин этой проблемы может быть и загрязнение воды озера через атмосферный канал. По объему выбросов загрязняющих веществ в атмосферу (порядка 800 тыс. тонн в год, включающих более сотни наименований, Иркутская область, занимает третье место в Сибирском федеральном округе. Анализ моделей прямых и обратных траекторий переноса воздушных масс показал, что основными путями поступления атмосферных загрязнений на Байкал от промышленных комплексов Иркутской области является северо-западный перенос (со стороны источников в долине р. Ангары), на который приходится около 60% случаев. Другой, не менее мощный источник поступления загрязняющих веществ в Байкальском регионе - лесные пожары. Эти обстоятельства делают особо актуальной оценку влияния различных источников на качество атмосферы над акваторией Байкала и состава его вод. Для исследования атмосферы над Байкалом в летние месяцы с 2019 года проводятся комплексные экспедиции с использованием оборудования дистанционного зондирования и локального контроля, входящего в состав ЦКП «Атмосфера» ИОА СО РАН, а также других приборов участников проекта. Приборы устанавливаются на верхней палубе кораблей Лимнологического института СО РАН. Общая протяженность маршрута составляет ежегодно 1600 ~1700 км. Зондирование аэрозольных полей атмосферы проводится лидарами корабельного типа «Лоза-М2», «ЛОЗА-А2». Весь период наблюдений за формированием структуры аэрозольных полей в котловине Байкала условно разделен на эпизоды: фоновая атмосфера, формирование

структуры аэрозоля за счет дымовых шлейфов «ближнего» и «дальнего» переносов примесей от лесных пожаров и от промышленных источников. Вертикальная структура аэрозольных полей сильно меняется во время дымовых шлейфов. Рост содержания дымового аэрозоля во время дальних лесных пожаров наблюдается вначале на высотах 2-2,5 км, затем фиксируется плотное заполнение всей атмосферы до поверхности воды.
Проводятся комплексные исследования газовых и аэрозольных примесей, во время крупных лесных пожаров в Сибири, при сценариях влияния глобальных, региональных и локальных источников на загрязнение атмосферы над озером. При выносе воздушных масс с прибрежных территорий, где расположены крупные населенные пункты и загрязнений, попадающих на озеро по долинам крупных притоков (Ангара, Селенга, Баргузин) регистрируются высокие концентрации оксидов азота, серы, озона, увеличивается массовая концентрация аэрозольных частиц. При лесных пожарах меняется химический состав аэрозоля. Так вблизи очага локального лесного пожара на побережье озера (бухта Сосновка, Средний Байкал 29.07.2019), фиксировались высокие концентрации оксида серы (до 47 мкг/м3) при этом заметно понижалось содержание озона. Определены высокие концентрации сажи (МВС 5-6 мкг/м3), что на два порядка превышало фоновый уровень этого вещества над озером. Во время дымового смога одновременно с ростом сажи отмечался рост полиароматических углеводородов. В составе аэрозоля увеличивались концентрации индикаторных элементов пожаров - калия, сульфатов, нитратов, тяжелых металлов V, Mn, Ni, Co, Cu, Zn, As, Cd.
Оценено поступление загрязняющих веществ из атмосферы на водную поверхность озера, оказывающих прямое действие на поверхностный слой воды. Суммарные потоки кислотных компонентов (азота и серы) на поверхность озера в два -четыре раза выше во время лесных пожаров. Загрязняется поверхностный слой воды и стойкими органическим загрязнителями – ПАУ, проведена оценка их токсичности во время лесных пожаров и в фоновых условиях.

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Ключевые слова: Байкал, атмосфера, аэрозоль, газовые примеси

71 VERTICAL PROFILES OF MICRODISPERSED AEROSOL OVER MEADOW VEGETATION AND IN FORESTRY

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The study results of the features of atmospheric aerosol deposition on the underlying surface in a forest and over meadow vegetation on the southeastern coast of Lake Baikal are presents. Based on measurements of the altitude profiles of the count concentration of microdispersed aerosol (C, cm^{-3}), it is shown that the gradients of aerosol concentration over meadow vegetation are significantly higher than in the forest under the tree crown and differ significantly. In open areas, $dC/dh < 0$ is most often maintained, i.e., the concentration of aerosol particles decreases with increasing altitude. Under the tree crown, the contribution of horizontal advection of air flows does not play a significant role due to the screening of flows by trees. Under the tree crown, a decrease in the photolysis rate and a change in vertical transport due to the presence of foliage (shading by foliage and modified vertical diffusion) are noted. The concentration gradients of fine-dispersed (VDA) particles ($0.005<d<0.2$ μm) and submicron (SMA) aerosol ($0.2<d<10$ μm) in the forest under the tree canopy vary within small limits compared to open terrain (meadow) and can be both negative and positive (dC/dh). The maximum particle concentration gradient during the experiments over meadow vegetation was for VDA particles (180 particles /cm^3)/m) during the daytime, and in the morning for submicron aerosol (SMA) (4 particles /cm^3/m). In the forest, the maximum is observed during the day for VDA particles (110 particles/cm^3/m), and for SMA particles (1 particle/cm^3/m). Low gradient values under the forest canopy indicate that the tree canopy has a significant effect on the deposition of aerosol particles in forest vegetation.

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Keywords: distribution of aerosol particles, forest, meadow.

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INFLUENCE OF OZONE AND OZONE PRECURSORS GASES ON THE PROCESSES OF FORMATION, TRANSFER AND TRANSFORMATION OF AEROSOL PARTICLES IN LAKE BAIKAL

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The paper presents the results of small gas impurities monitoring (O_3, SO_2, NOx) and aerosol in the waters of Lake Baikal during experiments on the research vessel (RV) «G.Yu. Vereshchagin» in August 2023. Abnormally high ozone concentrations in Northern Baikal were detected over a long observation period. The average daily ozone concentration from August 8 to 11 was 115 μg/m^3 with a maximum of up to 180 μg/m^3. It was found that during this period, the regions of Middle and Northern Baikal were influenced by long-range transboundary air mass transport from southeastern directions, covering industrial regions of China with high ozone and anthropogenic gas content. This is also evidenced by the results of calculations using the SILAM chemical transport model, which allows simulating the spread of chemical substances (gases, aerosols) and their mixtures with various types of interaction between them. An analysis of local emissions of anthropogenic gases from nearby territories to the lake water area was conducted. It was found that ozone and ozone precursor gases directly influence the processes of formation, transformation and transfer of aerosol particles, which is confirmed by close correlation links between them. Since aerosol particles cannot be destroyed as a result of interaction with ozone or other gases, then, apparently, variations in ozone and ozone precursor gases influence the processes of formation and coagulation of aerosol particles.

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Keywords: ozone, ozone precursor gases, aerosol, Lake Baikal.

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THE INFLUENCE OF LONG-RANGE ATMOSPHERIC DUST TRANSPORT ON PHYSICAL AND CHEMICAL CHARACTERISTICS OF NEAR-SURFACE AEROSOL IN THE CENTER OF EUROPEAN PART OF RUSSIA

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The increased interest in the research of long-range atmospheric dust transport is caused by its influence on the Earth's climate, radiation balance and atmospheric properties. According to various estimates, the increase in global dust load on ecosystems has now risen by 55 ± 30% compared to the pre-industrial period. Episodes of long-range atmospheric transport of dust aerosol from the arid zones of the Caspian and the Aral seas are also observed in the Moscow region with continuous monitoring of aerosol composition in the surface layer of the atmosphere. The sources of dust emission, the frequency and extent of exposure, as well as the variability of microphysical parameters, mass concentration and elemental composition of aerosol particles of various size fractions are discussed in this report.

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Keywords: atmospheric transport, aerosol particles, microphysical parameters, elemental composition, Moscow

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SURFACE AND INTERFACIAL TENSION OF TWO-COMPONENT CUBIC AEROSOLS

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In various situations, a non-spherical shape of aerosols can be observed, which complicates calculating physicochemical properties. The interface of the cubic shape of aerosols was studied in the simplest version of the lattice gas model taking into account the interaction of nearest neighbors in the quasi-chemical approximation on a rigid lattice. A numerical analysis of the thermodynamic definition of surface tension between a vapor or fluid and solid particles of a binary mixture and interfacial tension between two solid particles with the properties of a phases as an excess value of free energy ΔF of a two-phase system was carried out. A microscopic analysis of the definition of surface tension for the case of a complex shape of the phase boundary with the introduction of local surface tensions for faces, edges and vertices is given.

Keywords: surface tension, interfacial lattice gas model, quasi-chemical approximation, small systems.

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FORMATION OF METAL MICRO-DIMENSIONAL STRUCTURES BY DRY AEROSOL PRINTING WITH LASER SINTERING

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The results of a study on the formation of conductive micro-dimensional structures, in particular, useful for the formation of inductive elements in microwave devices, by dry aerosol printing using a printer being developed at MIPT, are presented.

Microstructures are formed by deposition of metal nanoparticles synthesized in a pulsed gas discharge in an inert gas stream onto substrates fixed in a printing chamber in a dynamic vacuum atmosphere, with simultaneous sintering by pulsed laser radiation with a wavelength of 527 nm.

The flow of aerosol nanoparticles is focused in an aerodynamic nozzle using a crimping gas stream, which makes it possible to obtain a width of the applied structure several times smaller than the outlet diameter of the nozzle.

By varying a number of printing and laser sintering parameters, namely: printing speeds from 20 to 5000 μm/s, the number of layers from 1 to 12, the repetition rate of laser pulses from 10 to 2000 Hz and pulse energy from 0 to 250 μJ, optimal parameter ranges were determined.

Micro-dimensional metal structures with a thickness of 0.5 μm and a width of 40 μm were formed on various materials substrates (silicon, glass, polyethylene terephthalate).

The advantage of the technology is the combination of all stages of the technological process of forming a metal micro-dimensional pattern in one device, including the synthesis of nanoparticles, their deposition on a substrate and sintering, which significantly increases the speed of the process and improves the economy.

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Keywords: printed electronics; nanoparticles; pulsed gas discharge; dry aerosol printing; laser sintering

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INTEGRATED HARDWARE-SOFTWARE PLATFORM FOR NANOPARTICLE MEASUREMENTS IN TECHNOLOGICAL ENVIRONMENTS: SET-UP AND FIRST TESTS

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Integrated hardware-software platform for nanoparticle measurements in technological environments has been developed and tested. The platform, which includes the diffusion aerosol spectrometer DAS 2702-M capable of precisely measuring nanoparticles of 5-200 *nm* and having total range of 5 *nm*-10 μm and other instruments of nanoparticle monitoring and sampling, was developed to measure phase transitions in the laser ablation, metalworking and material synthesis related to evaporation, condensation and chemical transformation during technological processes, which may be indicators of achieving certain operational regimes and conditions, which cannot be measured using other instrumental methods due to the limited or no access to the contact zone or other related circumstances. In this paper, the platform design and functions, including the linkage and interaction of hardware and software, digital technologies used and projected performance indicator, have been discussed and measurements of emissions from industrial laser cutting have been presented and analyzed.

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Keywords: nanoparticles, aerosol spectrometry, measurement system, technological environments, laser cutting

77 PHYSICAL CHEMISTRY OF NUCLEATION: INSIDES FROM QUANTUM SIMULATIONS, LABORATORY MEASUREMENTS AND OBSERVATIONS

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Here we report a comprehensive comparative study of different mechanisms leading to the formation of nanosized nucleated particles capable of further growth and discuss most important points regarding physical chemistry of their formation, physico-chemical properties and scaling. We discuss the importance of accurate measurements and simulations of binary sulfuric acid-water and multicomponent sulfuric acid–based nucleation mechanisms, as well as mechanisms involving amines and HOMs. Different strategies for reaching the decisive conclusions about favorable nucleation mechanisms and conditions, in which observable nucleation rates are achieved, have been discussed. The importance of quantum simulations and the role of the configurational sampling in their precession and cost-efficiency have been discussed in detail. The impact of the configurational sampling on simulated nucleation rates has been pointed out and uncertainties in nucleation rates due to system and basis-set dependencies of ab initio methods has been reviewed. We also present data showing impacts of scaling on physico-chemical properties of nucleating nanoparticles and prove that the size range, in which a quantum correction to classical nucleation theory is urgently needed is in fact very narrow and depends on the chemical composition of the nucleating cluster/small nanoparticle. The most important properties affecting nucleation rates such as Gibbs free energy changes and, in the case of ion-mediated nucleation, dipole moments of nucleating clusters, have been discussed in detail.

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Keywords: nanoparticles, quantum simulations, nucleation, Gibbs free energies, chemical kinetics

78 DYNAMICS OF DUMBELL-SHAPED AEROSOL PARTICLES

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The motion of aerosol particles of various shapes and chemical compositions in different layers of the Earth's atmosphere is an important problem of the aerosol microphysics and physical chemistry. While the use of back-trajectory methods is one of the most common ways of solving such problems, the actual particle shape has to be taken into account and its impact has to be thoroughly evaluated. The paper is dedicated to the motion of dumbbell-shaped particles, which are an important fraction of volcanic emissions but little is known about them compared to spherical and cylindrical ones. In this study, dumbbell-shaped particles are modeled by two connected spherical particles. The solution for two particles in a bispherical coordinate system was originally obtained by Stimson and Jeffery using the approximation of small Reynolds numbers. Here, the solution to this problem was obtained in the "stream function - vortex" variables and is a solution to an inhomogeneous equation in a bispherical coordinate system. Since the Knudsen number for small particles at an altitude of about a kilometer may be as large as 0.01, boundary conditions with the slippage at the particle boundary were taken into consideration and kinetically consistent difference schemes developed by B.N. Chetverushkin were used. The algorithm for calculating the distance and trajectory was obtained using such a difference scheme.

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Keywords: aerosol microphysics, dumbbell-shaped aerosol particles, motion, troposphere, difference schemes

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