XVII International Scientific Conference and School of Young Scholars
"PHYSICAL AND CHEMICAL PROCESSES IN ATOMIC SYSTEMS"

TECHNICAL PROGRAM
October 28-30, 2019, Moscow, Russia

TO THE 150TH ANNIVERSARY OF D.I. MENDELEEV PERIODIC TABLE OF CHEMICAL ELEMENTS
XVII International Scientific Conference
and School of Young Scholars
“Physical and Chemical Processes in Atomic Systems”

28-30 October, 2019

Technical Program

The book of abstracts and poster presentations at the XVII International Scientific Conference and School of Young Scholars “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 2019”. It is dedicated to the 150th anniversary of the Periodic Table of Chemical Elements by D.I. Mendeleev.

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# TECHNICAL PROGRAM

**October 28, 2019, 9:45– 14:15**  
**School of Young Scholars**  
**NRNU MEPhI, Main Building, Lecture Hall G-404**

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| 14:45 –15:30 | Membrane separation of the H$_2$-CO$_2$ mixture                       | Professor S. Koter Nicolaus Copernicus University, the city of Torun, Poland |</p>
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ABSTRACTS

SCHOOL OF YOUNG SCHOLARS
PRODUCTION OF HIGH-ENRICHED CARBON-13 BY TWO-STAGE LASER METHOD

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A variant of a two-stage laser process for production highly enriched carbon-13 (13C) with a concentration of more than 99% is being investigated. The first laser stage provides effective enrichment of 13C up to 30-50% based on the isotopically selective multiphoton dissociation of Freon-22 (CF2HCl) by pulsed radiation of a CO2 laser. Then the product of the first stage enriched in 13C, tetrafluoroethylene, is converted into the working substance of the second stage, difluorodibromomethane. At the second stage of enrichment, a component with an undesirable isotope 12C undergoes to selective dissociation, until its concentration in the residual gas decreases to 1% and the concentration of the 13C isotope is increased to 99%. The undesirable isotope 12C is concentrated in the product of dissociation. In preliminary experiments, high parameters of the elementary act of separation were achieved - the dissociation yield of the undesirable isotope component (12C) up to 20% and selectivity (for 12C) up to 100, which depended weakly on the current concentration of 12C. A productivity of the second enrichment stage for a reactor of ideal displacement is estimated. It was 0.6 and 1.2 g13C/h for initial concentrations of 13C in difluorodibromomethane of 30 and 50%, respectively.

Keywords: highly enriched carbon-13, two-stage laser enrichment process, difluorodibromomethane
SYNERGY OF SELECTIVE GAS TRANSPORT IN MULTILAYERED, HIGHLY PERMEABLE MEMBRANES

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P.M. Budd
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The ultra-permeable support with the gutter layer made from cross-linked PTMSP/PEI with CO\textsubscript{2} permeance of about 50 m(STP)/m\textsuperscript{2}·h·bar and α(CO\textsubscript{2}/N\textsubscript{2}) of 3.5-4.3 developed earlier was used to cast a thin PIM-1 layer. Microfiltration membrane MFFK-1 (Vladipor, Russia) as support and cross-linked PTMSP as gutter layer were selected to minimize the mass-transfer resistance, while the desired selectivity was expected to be provided by the thin PIM-1 film. As a result of optimization of different parameters, it was possible to obtain a series of membranes with CO\textsubscript{2} permeance of 13-22 m(STP)/m\textsuperscript{2}·h·bar and ideal CO\textsubscript{2}/N\textsubscript{2} selectivity of 36-56. It is interesting to notice that dense PIM-1 films of about 30 μm showed CO\textsubscript{2}/N\textsubscript{2} selectivity in the range of 15-22, depending on the preparation protocol. Thus, for the first time a synergy effect was demonstrated in gas selectivity for thin bilayered gas separation membranes. SEM and TEM analysis revealed that the overall selective layer thickness of optimized TFC membranes was in the range of 2.0-2.5 μm, whereas the thickness of the PIM-1 layer on top of a X-linked PTMSP gutter layer was about 0.4-0.5 μm. The prepared TFC membranes meet the criteria for post-combustion CO\textsubscript{2} capture.

As expected, all samples suffered severely from physical aging, with a 10–40 times drop in CO\textsubscript{2} permeance for the aged samples. At the same time, the ideal CO\textsubscript{2}/N\textsubscript{2} selectivity was nearly the same. The aged membranes possess lower CO\textsubscript{2} performance than required for post-combustion [3] However, the mitigation of polymer physical aging with the maintenance of high selectivity would open new potential for applications of polymers of intrinsic microporosity.

Acknowledgements: This work was supported by the Russian Science Foundation, project №. 18-19-00738.
Keywords: synergy, gas separation, CO\textsubscript{2} capture, PIM-1, polymers of intrinsic microporosity
The work deals with the theoretical description of the mechanisms of molecular transport in the subnanometer channels of zeolite membranes. The molecules in the channels of such membranes are an example of a one-dimensional system, the transport properties of which differ significantly from the transport properties of higher-dimensional systems. In particular, for a single-component gas, as the filling factor of the channel increases, the diffusion coefficient of molecules increases, and the mobility of individual molecules decreases. In the case of a two-component gas, under certain conditions, the selectivity of the zeolite membrane over one of the components can sharply increase. Anomalous transport in zeolite membranes is due to the effective interaction between the molecules in the channel and the formation of clusters of molecules with different lifetimes. These phenomena are described by the density functional method for nonequilibrium systems of arbitrary density that allows us to calculate the dynamic response function and the spectrum of relaxation of density fluctuations of 1D atomic system.

**Keywords:** Zeolite membranes, anomalous transport, single-file diffusion, 1D systems
The problem of the relaxation of metastable states in disordered media such as glasses, colloids, and polymers is one of the most urgent problems for both theoretical and experimental physics. At the same time, the applied meaning of solving the relaxation problem is important for the industry, since porous media, mainly disordered media, are widely used in such processes as catalysis and filtration. In addition to the interest in the study of the relaxation of porous media, there is the problem of the spatial arrangement of pores in a porous medium, since knowledge of such structural characteristics of the medium as pore size distribution and connectivity is often insufficient for predicting processes in porous media.

The paper presents the results of experiments on anomalously slow relaxation of non-wetting water liquid in disordered nanoporous medium - Libersorb23. A physical mechanism has been proposed that allows taking into account the collective multiparticle interactions of liquid nanoclusters in neighboring pores of different sizes on the fractal percolation cluster shell of filled pores. Such an account makes it possible to abandon the traditional contradictory approach used on the basis of the Laplace equation and to reconstruct the functions of distribution of outflowed or filled pores by size and trace their evolution over time. This makes it possible to determine the local pore configurations and its environment, which are responsible for the flow at different time. Also presented are the results of numerical modeling, which are consistent with the results of restoration of pore distribution functions by size.

Acknowledgements: this work has been financially supported by the Russian Science Foundation under grant 18-13-00398.

Keywords: disordered porous media, non-wetting liquid, configuration, surface.
The accident at the Fukushima nuclear power plant showed a particular danger of a vapor-zirconium reaction and led to the development of technologies to increase the resistance of zirconium cladding of fuel elements under conditions of the loss of coolant (LOCA, Loss-of-Cool Accident). Now the global atomic community uses the term "accident-resistant tolerant fuel" - Accident Tolerant Fuel (ATF), i.e. the fuel that ensures the safety of operation of the reactor facility even with a significant increase in the temperature of the fuel element claddings. The implementation of the program to create a tolerant fuel is largely aimed at developing heat-resistant protective coatings which have a minimal impact on fuel enrichment, the geometry of fuel claddings and neutron-physical parameters of the core of a nuclear reactor and, thus, they can almost completely suppress the formation of an explosive hydrogen mixture in case of LOCA.

The paper presents the results of studies performed at the SRC RF TRINITI for increasing the corrosion resistance of fuel claddings made from zirconium alloy E110 with the use of laser hardening and laser surface oxidation, and deposition of coatings (Al, Al2O3, Cr) by pulsed laser deposition, magnetron sputtering and electroplating of metal chromium.

**Keywords:** fuel cladding, zirconium alloy, magnetron sputtering, pulsed laser deposition, accident tolerant fuel.
D.I. Mendeleev published his first scheme of the periodic table of chemical elements 150 years ago in 1869 in the article "Correlation of properties with the atomic weight of elements". The modern interpretation of the periodic table of chemical elements is the classification of chemical elements, which establishes the dependence of the properties of elements on their charge of the atomic nucleus. The authors of textbooks on atomic and nuclear physics attribute the first idea of the modern structure of atoms to E. Rutherford's work (1911) in which he says that the results of alpha particles scattering indicate that in atoms there exists a "Central positive charge" smaller than 10-12 cm in size. It is curious that the terms "nucleus of an atom" and "planetary model of an atom" first appeared in a review of E. Rutherford's article, but not in the article itself.

In fact, the earliest planetary atom model suggesting the existence of an atomic nucleus was proposed and justified in a series of articles by B.N. Chicherin in the journal of the Russian physico-chemical society for 1887-1892. His atom model based on the mathematical analysis of experimental data on the periodicity of specific volumes of atoms from the periodic table predicted the existence of a "Central positively charged massive nucleus" and a "negatively charged compressible periphery" ("circle") of the atom. This model was highly appreciated by D.I. Mendeleev and A.G. Stoletov.

In the year of the 150th anniversary of Mendeleev’s law, we should pay tribute to our outstanding compatriot B.N. Chicherin who was inspired by this law and who substantiated the earliest planetary model of the atom with a positively charged nucleus.
HOW IS AN ACADEMIC CAREER RUN? POSSIBLE WAYS TOWARD PROFESSORSHIP

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This is not a typical lecture describing the results of the scientific research, focused on the well defined investigations. This is a lecture for young researchers starting their adventure with the science and having very often a lot of fears related to the reliable assessment of their talents. This is also a lecture for advanced researchers allowing them to assess what was excellent, and suggesting changes for the subsequent years of the efficient research work. The aim of this lecture is to present the different approaches to the academic career at its different stages: starting from master thesis through doctoral studies and tenure track positions until the full professorships. The lecture will try to discuss various problems related to the academic career, e.g.:

- is the research just a tidy, essentially linear, process where someone is moving smoothly through the various stages and reports "pop outs" at the end.
- what should be the role of a (good) supervisor?
- how (and where) to disseminate results of the investigations?
- is going to the conferences needed for the academic career?
- how to find money for the research?
- what about the international cooperation?
- what is the role of scientific societies in the development of the academic career?

The lecture will suggest answers to the above (and many other) questions, though the very strong involvement of the audience in the discussion is foreseen.
MODERN DIRECTIONS OF PRACTICAL APPLICATION OF METHODS OF SEPARATION OF LIGHT ELEMENT ISOTOPES

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The current state of technology for the separation of isotopes of light elements (hydrogen, boron, carbon, nitrogen, oxygen) in the report is considered from two points of view. Firstly, the characteristics of the technologies by which their industrial production is carried out today, and secondly, promising research works being carried out abroad and in Russia are considered, the results of which can find their practical application in the future.

Hydrogen. Currently, to produce heavy water in the world the following methods are used: low-temperature distillation of hydrogen, chemical isotope exchange (ChIE) in systems of hydrogen sulfide-water and ammonia-hydrogen. Additionally to solve of tasks of water detritiation, rectification of water and ChIE in the system of water-hydrogen is used. Of the new methods for the separation of hydrogen isotopes, one should mention the method which is based on the phenomenon of quantum sieving - the transfer of hydrogen in a electrochemical solid polymeric cell using graphene deposited on an electrocatalyst. According to published data, this method is characterized unusually large single separation effects.

Boron. The main industrial methods for the separation of boron isotopes are rectification of trifluoride ore trichloride boron, as well as the ChIE in system of BF₃ - its complex with methoxybenzene. In the last 6 years, at MUCTR an extraction method for the separation of boron isotopes in a system of an aqueous solution of boric acid - the organic phase is being developed.

Carbon. For the separation of carbon isotopes in industry, the process of rectification of carbon monoxide or methane is used. As promising methods, one can mention the processes based on the use of benzene vapors for the separation of carbon isotopes in centrifuges studies conducted at the MUCTR on the isotopic exchange of carbon dioxide with amine solutions in octane, and the laser separation method using freons as working substances.
Nitrogen. The traditional method for the separation of nitrogen isotopes is based on the isotopic exchange of nitrogen oxides with solution of nitric acid. On a smaller scale, nitric oxide rectification technology is used. In MUCTR research is being carried out on the use for the large-scale production of nitrogen-15 the process of rectification of molecular nitrogen, the advantage of which lies in an unlimited source of raw materials.

Oxygen. The main industrial technologies for producing the isotope of oxygen-18 are based on rectification processes. As working substances, water and oxides of carbon and nitrogen are used. As a promising process, a pilot installation should be noted, which was tested at the MUCTR for the study of a new separation method based on the catalytic process of ChIE in the carbon dioxide-water system in the new contact devices of membrane type.

In conclusion, the report states emerging in recent positive trend in Russia associated with the construction of large facilities for isotope separation. So, in Sarov, the installation of boron isotope separation by the BCl₃ rectification method was launched; in Gatchina and Ozersk, hydrogen isotope separation installations are being built by the methods of ChIE in the system of water-hydrogen and by water rectification, respectively, the Radium Institute named de V.G. Chlopin is active in relation to the project for the construction of a large installation for production of isotope oxygen-18.

Acknowledgement: the author is grateful to the staff of the Department of Isotopes of the MUCTR, who are active followers of their teachers' research in developing new methods for the separation of isotope of light elements.
A numerical simulation of the processes of flow and diffusion in hyper-speed gas centrifuges (GC) with a rotor speed of 1000 m/s and more was carried out. Modeling was carried out both in the framework of the axisymmetric approximation and in the three-dimensional formulation. The main attention is paid to obtaining the dependence of the optimal separative power of the GC on the rotational speed, length and diameter of the rotor. It is shown that the problem of finding the optimal separative power of GCs can be successfully solved in the framework of the axisymmetric approximation and the source-sink model. The dependencies of the optimal separative power and optimal parameters on the length, rotation speed and diameter of the rotor of hyper-speed GCs with rotor speeds of 1000 m/s to 1500 m/s, a rotor length of 1 m to 5 m and a rotor diameter of 12 cm to 20 cm are obtained.

Acknowledgements: The present work was supported by Russian science foundation, project N18-19-00447

Keywords: gas centrifuge, isotope separation, numerical modelling
Molybdenum is considered as one of the substitutes for zirconium in making fuel cladding for safe reactor designs. Optimized double-cascade separation schemes consisting of the Q-cascade model are employed for studying massive production of IMM and evaluating the economic feasibility of production. By making use of the data (price for separative power unit) for uranium enrichment, a simple formula is derived to be able to assess the cost per kilogram of IMM. Various factors can be taken into account by the formula, such as the feed material cost, the separation cost, the separation properties of separation units, and the material recovery, provided that the the same separation technology is used for IMM production and uranium enrichment. The results demonstrate that it is feasible to produce massively the IMM with a total thermal neutron absorption cross section equivalent to that of zirconium.

Acknowledgements: This research is supported by Natural Science Foundation of China (Grant No. 11575097), and the Sino-Russian joint project from National Natural Science Foundation of China (Grant No. 11911530087) and Russian Fund for Basic Research (Grant No. 19-58-53002 GFEN_a).

Keywords: isotope separation; matched abundance ratio cascade; quasi-ideal cascade; relationship
The operation of nuclear power plants inevitably leads to the accumulation of spent nuclear fuel (SNF). At the same time, reprocessed uranium (RepU) recovered from SNF usually has a higher content of the valuable $^{235}$U isotope compared to natural uranium. This allows its use for the production of fresh low enriched uranium (LEU) for nuclear reactors. In addition, spent fuel contains plutonium, which can also be used as fuel material. The storage of spent nuclear fuel is expensive, and there are difficulties with the choice of a place for its disposal.

In this regard, the reprocessing of spent nuclear fuel and the subsequent use of fissile materials separated from it is an important step towards the closure of the nuclear fuel cycle. However, there are serious obstacles to the achievement of this goal. First, the reprocessing of SNF is a complicated procedure that is expensive and potentially environmentally hazardous. Second, RepU contains artificial isotopes $^{232}$U, $^{236}$U, and also have a higher concentration of $^{234}$U than in natural uranium. These factors complicate the process of enrichment of the RepU because of the need to comply with the requirements for the isotopic composition of commercial LEU.

In the work, we carried out a critical analysis of the options for using RepU in the fuel of thermal neutron reactors. The possibilities of its use both in the composition of uranium fuel and in the composition of various types of mixed (uranium-plutonium) fuel are considered. For every option, we showed the role of uranium enrichment technologies in RepU reusing.

**Acknowledgements:** The study was carried out with the support of the grant from the Russian Science Foundation (project No. 18-79-00249).

**Keywords:** reprocessed uranium, multiple uranium recycling, closed nuclear fuel cycle, separation cascade, spent nuclear fuel.
RESPONSIVE MEMBRANES

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Modifying the membrane surface has the potential to retain the properties of the bulk membrane material but tailor the interactions between components of the feed and the membrane surface. Surface modification may be used to produce responsive membranes. Responsive membranes contain monomer units that can change their conformation in response to an external stimulus such as pH, ionic strength, temperature, light, electric field, magnetic field etc. The change in conformation of the monomer units may be used to change the separation properties of the membrane in response to changed environmental conditions. Porous membranes are generally made responsive by grafting responsive polymer layers from the membrane external surface and, often, the pore walls. Surface modification must ensure that the properties of the base membrane are preserved while grafting responsive groups to the membrane surface. This presentation will describe membranes that respond to various stimuli: pH, ionic strength, temperature and magnetic field. The focus will be on the novel magnetically responsive membranes that we have developed. In this case, magnetically responsive nanobrushes that have been grafted from the barrier surface of commercially available nanofiltration, ultrafiltration and microfiltration membranes. The ability to modify membrane performance in an oscillating magnetic field will be discussed.

Acknowledgements: Funding for this work was provided by the Arkansas Research Alliance
Keywords: atom transfer radical polymerization, flux, fouling, rejection, surface modification.
MEMBRANE SEPARATION OF H₂/CO₂ MIXTURES

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One of the renewable sources of energy is hydrogen produced by fermentation. In such process the H₂-CO₂ mixture is created which should be further separated. H₂ is used in the fuel cells whereas CO₂ can be used as a substrate in photo-bioreactors to grow microalgae, being recycled as a raw material for biocatalyzed H₂-evolution [1].

In this presentation we focus on the membranes which can be used for H₂-CO₂ separation. These include: polymeric, inorganic, mixed-matrix, metal-organic-framework (MOF) membranes, and other types of membranes (containing ionic liquids, carriers, enzymes, based on carbon materials like graphene). Among them the polymeric membranes, which are easily formed, have the limited H₂/CO₂ separation ability as indicated by the Robeson upper bound plot. According to that plot the higher membrane selectivity the lower its permeability and vice versa. Other types of membranes go beyond this limit; for graphene with defects the theoretical calculations show that the H₂/CO₂ selectivity reach one hundred, for 2D polyphenylene layer it is even much higher. However, the basic problem is how to form such membranes.

Apart of that, various approaches to the modeling of gas membrane separation with a special emphasis on the H₂/CO₂ mixture is given. The transports through the membrane and in the membrane module are discussed. Diverse approaches to the membrane transport are presented, including phenomenological equations, Maxwell-Stefan equations, and the molecular simulations. Regarding the membrane module, the influence of various flow patterns on the gas separation efficiency is presented.

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PERCOLATION EFFECTS IN POLYMERIC MEMBRANES WITH EMBEDDED CARBON NANOTUBES

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In recent years, the properties of mixed matrix membranes (MMM), inorganic polymer with embedded nanoparticles, are intensively studied in the context of both membrane materials science and separation technology. MMM generated by adding the polymers to carbon nanotubes (CNT) are of particular interest. At present, there is no any unified approach to describe the mechanisms of membranes permeability increase when embedding the CNT. Supposedly, the permeability of membranes may increase when diffusing through open channels in the CNT or in case of diffusion in a modified polymer layer at the CNT surface. However, many polymers demonstrate a nonlinear change in the permeability of the MMM membranes as the CNT concentration increases. To explain these phenomena, one should take into account non-linear changes in the membrane structure during the formation of a percolation cluster from embedded particles.

In this work, conditions of formation and parameters of a percolation cluster of cylindrical particles in 3D films are calculated by the Monte Carlo method. It was found that at the same concentrations of nanoparticles in the MMM samples, the changing membrane geometry affects the percolation cluster structure and causes a change in the transport properties of these membranes. The results obtained explain a instability in the parameters of MMM membranes with percolation structure. The unstable change in the MMM transport characteristics, when particles with a large aspect number are embedded, can be associated with a poorly developed percolation cluster and, as a result, a small fraction of the membrane area, in which the transport channels are formed.

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Keywords: mixed matrix membranes, CNT, percolation, agglomeration, Monte Carlo method.
PLASMA CENTRIFUGE WITH AXIAL CIRCULATION
FOR ISOTOPE SEPARATION OF ALKALINE AND
ALKALINE EARTH ELEMENTS

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We propose a new type of a plasma centrifuge (PC) with a phased high frequency electromagnetic field and axial circulation excited by a traveling magnetic field (TMF), to increase separation performance and to separate isotopes of certain types of chemical elements efficiently. Elements of particular interest are those possessing masses in the range of 40–200 a.m.u., but without a suitable volatile compound form required for use in a GC. The new PC concept rotates a weakly ionized isotope gas mixture with a resultant rotating HF electromagnetic field, while an axial circulation flow, necessary for multiplying the radial separation effect, is created by an axial TMF. By assuming that the plasma medium is weakly ionized, diffusion separation can be assumed to undergo processes that are similar in behavior to a neutral gas.

Applying an external HF field to the arrangement avoids the development of "spoke-like" plasma instabilities, which can be observed for plasmas rotating in stationary crossed electric and magnetic fields. A model of the PC was developed to determine its operational parameters and isotopic separation performance for a partially ionized medium. In contrast to the HF wave system described in the recently published papers, the new PC concept rotates a weakly ionized isotope gas mixture with a resultant rotating HF electromagnetic field, while an axial circulation flow, necessary for multiplying the radial separation effect, is created by an axial TMF.

Acknowledgement. This study is carried out with the support of the Program for Improving the Competitiveness of the National Research Nuclear University MEPhI under contract No. 02.a03.21.0005 of August 27, 2013 and the Russian Science Foundation, project no. 18-19-00447.

Key words: plasma centrifuge; isotope separation; axial circulation; traveling magnetic field.
CONTROLLED PROCESSES AT LASER COATING DEPOSITION

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A coating method based on irradiating gas-dust medium which is an ensemble of microparticles moving in the gas in the form of a free vertical jet by a horizontal laser beam is proposed. The threshold laser radiation intensity is estimated for evaporation of particles in dependence on their size. Under experimental conditions no optical breakdown occurs near particles. Selecting smooth regions in the radiation spectra corresponding to the thermal radiation allowed determination of the true temperature of particles without information about blackness coefficients. Coatings on various substrates were produced, measurement results of coating characteristics were presented. An experimental setup including a cw CO$_2$-laser for diamond coating deposition in optical discharge plasma was created. Spherical aberrations of the plasmatron focusing lens considerably affect thresholds of discharge maintenance. Plasma radiation spectrum and two-dimension temperature distribution across the substrate surface were measured. Diamond film on the tungsten substrate surface was received.

A system including a compact spectrometer for surface temperature measurement at surface illumination by laser radiation was developed and created. The system operates in real time, its rapidity is equal to 30 ms. The system test was performed at laser overlying of metal powder under pilot-scale production conditions.

Keywords: laser, coating, spectrum, surface, temperature.
The existing laser isotope separation techniques are discussed. The main
target is paid to the so-called “low-energy” separation methods
(activation energy $E_a < 1 \text{ eV}$), based on the selective prevention of
molecular clustering and the selective dissociation of small clusters by IR
laser radiation in molecular-cluster beams. The results of the study of
these processes by the example of molecules with a large ($^{32}\text{SF}_6 / ^{34}\text{SF}_6,$
$\Delta \nu_{is} \approx 17 \text{ cm}^{-1}$) [1] and a small ($\text{CF}_3^{79}\text{Br} / \text{CF}_3^{81}\text{Br},$ $\Delta \nu_{is} \approx 0.25 \text{ cm}^{-1}$) [2]
value of the isotopic shift $\Delta \nu_{is}$ in the frequency of the molecular vibration
under laser excitation are presented. The realized selectivity values for
suppressing the clustering of $^{32}\text{SF}_6$ molecules are $\alpha (^{32}\text{SF}_6 / ^{34}\text{SF}_6) \geq 25-30,$ and for $\text{CF}_3^{79}\text{Br}$ molecules, $\alpha (^{32}\text{SF}_6 / ^{34}\text{SF}_6) \approx 1.18.$ The
possibilities of increasing the separation parameters, as well as the
prospects for their practical implementation, are discussed.

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Keywords: laser isotope separation, molecular and cluster beams.
TRANSFER PROCESSES IN DENSE DEGENERATE PLASMA

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A method has been developed for the calculation of tensors of the electrical conductivity, Seebeck coefficient, and thermal conductivity of a nonideal plasma in a magnetic field within a unified approach where the kinetic coefficients are calculated together with the equation of state of the nonideal plasma within a quasichemical model. It has been shown for the first time that there is a density range where all components of the Seebeck tensor in xenon change their sign because of the Ramsauer minimum in the cross section for scattering of electrons on neutral atoms in the region of comparable values of cyclotron and transport frequencies of electrons.

Various methods for determining the Coulomb logarithm in the kinetic theory of transport and various variants of the choice of the plasma screening constant, taking into account and disregarding the contribution of the ion component and the boundary value of the electron wavevector are considered. The correlation of ions is taken into account using the Ornstein–Zernike integral equation in the hypernetted-chain approximation. It is found that the effect of ion correlation in a nondegenerate plasma is weak, while in a degenerate plasma, this effect must be taken into account when screening is determined by the electron component alone. The calculated values of the electrical conductivity of a hydrogen plasma are compared with the values determined experimentally in the megabar pressure range. It is shown that the values of the Coulomb logarithm can indeed be smaller than unity.

Acknowledgement. This work was supported by the Russian Science Foundation (project no. 16-12-10511).
Targeted alpha-therapy is one of the most promising methods of oncological diseases treatment. Of certain interest is $^{212}\text{Pb}$ beta-emitter with its daughter nuclides ($^{212}\text{Bi}$ and $^{212}\text{Po}$) undergoing alpha-decay, which allows one to regard $^{212}\text{Pb}$ as an \textit{in vivo} alpha-emitters generator. In this connection, a new method of $^{212}\text{Pb}$ production has been developed and implemented. A method of $^{212}\text{Pb}$-labeled complex based on synthetic peptide Tyr$_3$-octreotate conjugated with bifunctional DOTA chelating agent (DOTATATE) synthesis has been implemented. It is specific to SSTR2-type somatostatin receptors whose overexpression is observable in cells of a number of tumors, especially in case of neuroendocrine neoplasms. Radionuclide $^{212}\text{Pb}$ was produced with the designed $^{228}\text{Th}/^{212}\text{Pb}$ generator. The operation principle of the generator is based on the transfer of gaseous $^{220}\text{Rn}$ from a vessel with the $^{228}\text{Th}$-containing ion exchange resin into a separate collector. Such phase separation ensures high radionuclide purity of the therapeutic $^{212}\text{Pb}$. Dependences of the yield of the DOTATATE labeling reaction with $^{212}\text{Pb}$ have been studied in cases of different molar activities, synthesis durations and temperatures. Dissociative stability of the synthesized complex in biologically relevant media has also been studied. Investigations on the $[^{212}\text{Pb}]$DOTATATE cytotoxic effect have also been carried out on tumor cells by MTT-assay.
WAVE PROCESSES IN GAS CENTRIFUGES

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Waves in gas centrifuges are generated by scoops for withdrawal of the gas. The physics of the waves and their role in the gas dynamics are under discussion. Strong centrifugal and Coriolis forces have dramatic impact on the properties and dispersion relation of the waves. The conventional sound, vertex and entropy waves split into 3 families with different dispersion. The entropy wave has zero velocity of propagation but variation of temperature in this wave is accompanied by toroidal motion. Pressure is not perturbed. The rest two families of the waves have nonzero velocities of propagation. Upper family has frequency above doubled frequency of rotation of the rotor with exceptional case of the wave (named acoustic wave) propagating exactly in the axial direction. This wave propagates with the conventional sound velocity and is polarized only in the axial direction. Unique property of this wave is the weakest damping due to the molecular viscosity and heat conductivity. All other waves are damped on distances compared with their wavelength. Computer modeling allowed us to determine the damping decrement of the acoustic wave in dependence on the parameters. At the conventional parameters of the IGUASU centrifuge the acoustic waves are damped due to the viscous interaction and heat exchange with the wall of the rotor. This wave is able to propagate from one end of the rotor to another. Numerical experiments show that the waves can affect the axial circulation and gas content in the centrifuge.

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ABSTRACTS

POSTERS

SEPARATION OF ISOTOPE AND NON-ISOTOPE MIXTURES BY GAS CENTRIFUGES
The rapid development of technologies for the production of new materials in the future may provide the opportunity to create new gas centrifuges (further GC) with rotor speeds of 1000 m/s and more. However, the question of the effectiveness of such GCs remains open. At present, there are no data of an experimental and theoretical-numerical nature regarding the separation performance of such GCs. In this work we present the results of calculations of the optimized separation performance of countercurrent hyper-velocity Iguassu GCs with a length of 1 to 5 meters and rotational speeds from 1000 to 1500 m/s. The calculations were carried in axisymmetric approximation within the source-sink model. It is shown that for hyper-speed GCs the optimized separation performance, pressure on the rotor wall, feed flux and gas friction power linearly depend on the rotor length, while the temperature difference at the end caps of rotor does not depend on the rotor length. The obtained dependencies are characteristic of all the studied GC with rotor velocities from 1000 to 1500 m/s.

Acknowledgements: The present work was supported by Russian science foundation, project N 18-19-00447.

Keywords: gas centrifuge, optimization, numerical simulation, isotope separation
ENRICHMENT OF MOLYBDENUM-99 IN GAS CENTRIFUGES

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The quality of many medical radionuclides used for diagnosis and therapy is determined by their specific activity. Enrichment in gas centrifuges, radioactive isotopes are known and used in practice. [1] However, in many cases it is necessary to enrich short-lived radioactive isotopes at their ultra-low concentrations in the working substance.
The report presents the results of experimental studies on the enrichment of Molybdenum-99 (half-life of 66 hours) in gas centrifuges using molybdenum hexafluoride as a working gas.
The developed technology is supposed to be used for the production Molybdenum-99 - of Technetium-99m generators. [2]


Keywords: Molybdenum-99, gas centrifuges, enrichment, medical radionuclides, short-lived radioactive isotopes.
Currently, factories for the separation of isotopes of uranium in the world has accumulated about 2 million tonnes of depleted uranium hexafluoride (DUHF) with a concentration of 235U in the range of \( y = 0.1-0.4\% \) by weight per metallic uranium. DUHF is a dangerous chemical compound, safe storage costs or on its translation into a more secure form of uranium dioxide UO2 counted in costs of enriched uranium product and, as a result, the cost of electricity the plant. In the work are the methods and results of calculations of energy and economic value of resources DUHF as a secondary source of nuclear fuel. Due to DUHF enrichment to the concentration of natural uranium equivalent (NUE), you can not only increase the resource base of nuclear power, but also strengthen the profitability of the processing plants through the sale of NUE and reduce the cost of safe storage DUHF or transfer it to the DUHF dioxide as a result of the DUHF weight reduction. The concept of “DUHF economic value” is formulated, and assessments of the economic feasibility of natural uranium equivalent outputs of OGFU are calculated at different market conditions.

**Keywords:** depleted uranium hexafluoride (DUHF), natural uranium equivalent, re-enrichment DUHF, DUHF economic value
During the operation of gas centrifuge (GC) cascade for the multicomponent isotope mixture separation there are nonstationary hydraulic processes when the values of pressures and process gas flows change in the cascade stages and in outgoing flows. One of the most frequent origins of nonstationary processes is change of cascade flow rate (feed, light or heavy fraction). Research of these processes is of interest for determination laws of isotope concentration change. This article contains the research results for nonstationary transfer of isotopic mixture in GC cascade caused by the change in values of cascade feed flow. The research considers the case of germanium isotopes that are applied in production of semi-conducting materials and research of neutrinoless double $\beta$-decay. Germanium isotopes are also used as a starting material for arsenic radioactive isotopes. It was determined that during a nonstationary process, the concentrations of isotopes with intermediary mass number in light and heavy fraction flows may cross the range limits restricted by the initial and final stationary values and exceed the maximum reachable values for a threeflow cascade. Time for stationary isotope concentrations to settle is different for isotopes and depends on the final values of cascade flow.

**Keywords:** isotope, gas centrifuge, nonstationary process, germanium
The stationary separation mode is preceded by non-stationary, which can conditionally be divided into two phases: filling the cascade with a working substance and a transition process. During second phase stationary concentration of the components of the isotopic mixture in the steps and flows of the cascade is established. The study of the transition process in view of its considerable duration and, as a consequence, the negative impact on the efficiency of the cascade is of particular interest. The transition process is a non-stationary hydraulic and separation when flows, pressure of the working substance and concentration of components change are changed. The transient process is studied by the example of obtaining in a cascade of gas centrifuges germanium enriched with 72Ge up to 50%. The character of the influence of cascade flows on the dynamics of isotope concentrations and the duration of the transition process is determined. The conditions for accelerating the accumulation of the target isotope in the cascade and reducing the duration of the transition process are given.

**Keywords**: cascade, isotope, separation, germanium, transition process
NUMERICAL STUDY ON COUPLING MODE OF MECHANICAL AND THERMAL DRIVE CIRCULATIONS IN GAS CENTRIFUGE

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In modern gas centrifuge (GC), circulations driven by stationary scoops and temperature difference between end caps, also called as mechanical and thermal drive circulations, have very important effects on its separation performance. The flow patterns of mechanical and thermal drive circulations in a GC are different and whether the coupling mode of them is linear or nonlinear is not clear. In this research, an axial circulation in the model Iguassu GC is simulated for single mechanical, thermal, and both kind together drives. In addition, the product and waste baffles are also considered in the model GC, making the flow patterns much more complicated. Besides, the rotors with different aspect ratios are also investigated. We take the absolute value of the stream function along an axial cross section to define the intensity of various types of axial circulations. The simulation results demonstrate that the coupling mode of mechanical and thermal drive circulations in a GC is close to linear even though the circulations are reshaped by product and waste baffles. The result obtained may simplify the procedure of optimization for the separative power of a single GC for isotope separation.

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Keywords: gas centrifuge, mechanical and thermal drives, decay of axial circulation
The boron isotope \(^{10}\text{B}\) with a relative concentration of 80 – 95% is the most in demand in the nuclear power industry at present. \(^{10}\text{B}\) is used mainly as an integral part of control rods in a reactor construction. The heavy isotope \(^{11}\text{B}\) is used to create heat-resistant and “transparent” for neutrons structural materials. A method of numerical-analytical optimization of cascades of uniflow gas centrifuges for the separation of boron isotopes in the form of BF\(_3\) has been developed. As a criterion, the minimum of the total number of gas centrifuges for given external parameters of the cascade scheme was adopted. The method is based on analytical relationships for stage flows obtained in the approximation of minimizing the total feed flow. The calculations used estimates of the efficiency of the separation of boron isotopes in a uniflow centrifuge with a central body, which determine its optimal mode of operation. Various cascade schemes of BF\(_3\) enrichment for each of the isotopes \(^{10}\text{B}\) and \(^{11}\text{B}\) are considered.

**Keywords:** boron isotopes, separation cascade, uniflow centrifuge, optimization.
The problem of highly concentrated molybdenum isotopes production in multiflow cascades is considered. A method of the cascade with two additional product flows optimization has been developed. Two components intermediate in weight are concentrated simultaneously in those flows. The optimization problem is solved using a variation of the partial flow cuts of the cascade stages with large separation coefficients. The optimization criterion is the minimum of the stage total feed flow while ensuring a given concentration of isotopes. A computational experiment was carried out to separate a mixture of molybdenum hexafluoride. The experiment demonstrated the features of intermediate components concentrating in additional product flows of the cascade.

**Keywords**: isotope separation, optimization, multi-flow cascade, intermediate components.
RESEARCH ON THE PERFORMANCE OF PRESSURE REGULATOR IN DIFFERENT CASCADES

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The pressure regulator is an important component of centrifuge cascades, whose performance has a significant influence on the hydraulic behavior of centrifuge cascades and has played a decisive role in the change of cascade’s fluid parameters. In this paper, a mathematical model of cascade is established for research on the performance of pressure regulator. This paper has simulated a square-off cascade in different situations by establishing mathematical models of pressure regulator and the recovery process after the stable state of cascade is destroyed has been studied based on the cascades dynamic numerical calculation theory. Certain disturbance, including a bypass of separation stage is considered to analyze the influence of regulators on the cascade. Analysis of changes on the pressure of waste pipe and tails flow in cascade are given with a dynamic process. Thus, the proper ranges of the parameters are obtained for the pressure regulators by comparing the dynamic influence on the cascade with different regulators.

Keywords: cascade hydraulics; pressure regulator; mathematical model; square-off cascade
RESEARCH ON MULTI-SCALE COUPLING METHOD BASED ON SIMUWORKS AND FLUENT FOR CASCADE SYSTEM

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Based on 1D second-development system code SimuWorks and 3D computational fluid dynamic code FLUENT, a multi-scale coupling code was proposed by means of using application programming interface and user-defined functions of FLUENT. Steady and transient flow simulation in cascade system were selected to perform Code-to-Code verification between coupling code and SimuWorks code. The results show that the simulation results of coupling code are in good agreement with the SimuWorks calculation results and the multi-scale coupling code for cascade system has achieved initial success. Through further improvement and fully validation, the multi-scale coupling code can be used to carry out complex 3D hydraulic phenomena analysis in cascade system. The simulation results of multi-scale coupling code for cascade system also show that the movement law of solid particles of different types and sizes in cascade system.

Keywords: multi-scale coupling, cascade, simulation, hydraulic, solid particles
EFFECT OF UNEVEN VARIATION OF ZONES WITHIN SEPARATION STAGE ON CASCADE

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Centrifuge cascade calculation is the basis of centrifuge engineering design. The usual calculation method treats the separation stage as a smallest separative element. In order to consider the differences between zones within the separation stage, this paper establishes a mathematical model by using zones as separative elements. Based on this, improve the traditional cascade calculation method. And write a program to calculate a cascade. The results show that when the feeding of a single zone decreases, the cascade separative performance is reduced, and the difference between zones is obvious. When the cut and separation factor in partial zones are reduced, cascade efficiency drops. Compare single-stage mixing losses under two calculation methods. When the zone is calculated as a separative element, the mixing loss mainly occurs in the junctions of product and waste between zones.

Key words: Centrifuge cascade, Cascade calculation, Zone, Mixing loss
Understanding the relationship between the quasi-ideal cascade (QIC) and the matched abundance ratio cascade (MARC) is very helpful to analyzing and understanding the separation mechanism of a cascade and practical applications of the cascade theory. For different cases of separation factors and separation condition, the relationship between QIC and MARC is investigated. It is found that they are different types of cascades. Only when the separation factor is constant and the separation is symmetrical, they are equivalent. Therefore, in practice, the two types of cascades should be considered separately to select the optimal cascade and achieve the best separation performance.

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**Keywords:** isotope separation; matched abundance ratio cascade; quasi-ideal cascade; relationship
FEATURES OF TRANSIENT PROCESSES IN SEPARATION CASCADES WITH ADDITIONAL PRODUCT FLOW

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One of the important stages of the separation campaign for enrichment of specified isotope from the multicomponent isotopic mixtures is attainment of the stationary mode of its operation, including the achievement of the specified concentrations of the separating components in the withdrawal flows. This process can be characterized, depending on the chosen separation method, by a relatively long time which is associated with consumption of a working substance and operating costs. It follows that the search for the values of the cascade control parameters at which they would reduce the time of the transition process is an important problem either for the theory or practice of separation of isotopes by separation cascades.

In parallel with the above, one of the developing areas of the modern theory of separation cascades is the study of the physical laws of the stationary mass transfer in the cascades with additional outgoing flows. Such cascades are finding more and more applications for solving a number of urgent problems, in particular, obtaining relatively high concentrations of intermediate mass isotopes. At the same time, the laws of unsteady mass transfer in such cascades remain poorly understood.

The paper analyzes the key patterns of the transient processes in a square cascade with an additional product flow. Also, the interconnections between the time to achieve the stationary mode of cascade operation and the external conditions that determine the process of isotope mixture separation are revealed as well.

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Keywords: isotope separation, transient process, multicomponent mixtures, separation cascade, additional product flow
MULTI-CASCADE ENRICHMENT SCHEMES FOR REPROCESSED URANIUM RECYCLING

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The paper deals with the problem of reprocessed uranium (RepU) enrichment in cascades of gas centrifuges with simultaneous fulfillment of requirements on concentrations of isotopes $^{232,234,236}$U. These harmful isotopes bred by nuclear chain reaction are responsible for an increase in radioactivity level and neutron poisoning of fresh nuclear fuel. The study examines the cascade schemes that aim at closing the nuclear fuel cycle by satisfying the formal condition of the complete uranium reclaim. The prospective VVER fuel cycle strategy of multiple U recycling is considered. Schemes under consideration are multi-cascade ones. Such configurations are stipulated by the necessity to fulfill both a series of requirements on concentrations of even-numbered isotopes in commercial low-enriched uranium and condition of “full return” of uranium extracted from spent nuclear fuel from particular reactor to produce fresh fuel load for the same reactor.

The research provides a basis for comparison between three various multi-cascade schemes designed to re-enrich RepU under mentioned above conditions. We used the unified metrics (related to ordinary cascade and normalized to LEU product) of natural uranium savings, separative work, and depleted uranium consumption and their derivative. The calculations take into account the necessity of RepU dilution to compensate for the adverse effects of $^{232,234,236}$U isotopes. As the reference cascade scheme, a simple modification of a single triple-flow cascade for RepU enrichment was considered. It is demonstrated that some modern cascade schemes could provide sustainable recycling of uranium.

Acknowledgements: The study was carried out with the support of the grant from the Russian Science Foundation (project No. 18-79-00249).
Keywords: reprocessed uranium, multiple uranium recycling, closed nuclear fuel cycle, separation cascade, spent nuclear fuel.
The separative power $\delta U$ of a gas centrifuge for isotope separation (GC) is characterized by the extremum depending on a working substance pressure $P$ near a rotor wall. During the normal operation, the dependence $\delta U(P)$ is displaced in the coordinate space $\{\delta U; P\}$ with the shape which changes up to the formation of a" plateau" in the vicinity of the extremum. This eliminates the possibility of applying the negative feedback principle on the $\delta U$. For automatic control of the separation process, the optimal mode sign is the value of the derivative $d\delta U/dP = g > 0$ found from the derivative of the function $\delta U(P)$ which is close to zero. In this case, even the occurrence of a plateau in the region of the extreme insignificantly changes the indication of the separative power of a GC. Automatic stabilization of the derivative above $d\delta U/dP = g$ is carried out by the adaptive search algorithms in terms of the finite differences. The Simulink MATLAB simulation demonstrates that the step-by-step automatic search algorithm stabilizes the optimal mode of the separation process with an accuracy of hundredths of a percent for deviation from the maximum value of $\delta U(P)$ under the conditions of displacement and change in the shape of $\delta U(P)$.

**Keywords:** gas centrifuge; isotope separation; automatic optimization.

**Acknowledgement.** This study is carried out with the support of the Program for Improving the Competitiveness of the National Research Nuclear University MEPhI under contract No. 02.a03.21.0005 of August 27, 2013 and the Russian Science Foundation, project no. 18-19-00447.
The problem of obtaining relatively high concentrations of stable isotopes of intermediate mass numbers is considered. The object of research is a connection of three ordinary square cascades. The possibility of simultaneous concentration of isotopes of intermediate masses in different output flows of cascades is shown. The dependencies of the parameters of the cascade schemes under consideration are investigated. The method of optimization of such system of square cascades according to the criterion of minimum relative total flow at given concentrations of target components is proposed. Calculations were made on the example of isotope mixtures with the number of components from 3 to 6.

Acknowledgements: The study was carried out with the support of the grant from the Russian Science Foundation (project No. 18-79-00249).

Keywords: isotope separation, multicomponent mixture, intermediate isotope, square cascade.
GAS DYNAMICS IN THE IGUASSU GAS CENTRIFUGE WITH NESTED ROTORS

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Iguassu centrifuge contains a significant vacuum area that doesn’t provide isotope separation. Centrifuge with nested rotors is one of the methods to utilize vacuum area. This type of centrifuge consists of two working cameras separated by a partition wall. In this work we conduct numerical modelling of the gas flow in the Iguassu gas centrifuge with nested rotors.

Acknowledgements: The present work was supported by Russian science foundation, project N18-19-00447

Keywords: gas centrifuge, isotope separation, numerical modelling
CENTRIFUGAL SEPARATION OF CARBON ISOTOPIES USING CARBON TETRAFLUORIDE AS PROCESSING GAS

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At present, the application of carbon isotope is becoming more and more extensive, especially in the field of medical testing, and the demand for \(^{13}\)C in high abundance is fast increasing. Using carbon tetrafluoride (CF\(_4\)) as separation medium, study on centrifugal separation of carbon isotopes was carried out. Single-centrifuge experiments were done based on modified domestic gas centrifuges. As a result, the separation factor and single-centrifuge separative power under different working conditions were obtained. Based on the results of single-centrifuge separation experiments, cascade calculation of the enrichment of \(^{13}\)C isotope was conducted by ideal cascade. According to calculation results, through two cascade separations, \(^{13}\)C isotope could be enriched from 30% to above 99% in abundance. The study laid a good basement for production of \(^{13}\)C isotope in high abundance.

**Keywords:** \(^{13}\)C; gas centrifugation; carbon tetrafluoride; separation factor; separative power; ideal cascade
Natural occurring boron has two stable isotopes: boron-10 and boron-11. Boron-10 has high thermal neutron cross section in a wide range of energy and the product of boron-10’s neutron reaction contains alpha particles. So, it is a good material for neutron absorbing and neutron tracing. Enriched boron-10 material is used in many areas, such as nuclear reactor, radioprotection, neutron therapy and neutron detector. In order to enrich boron-10 from natural boron, several methods had been proven to be feasible: chemical exchange distillation, cryogenic distillation and ion exchange resin method. However, only chemical exchange distillation was applied to industrial production. The market now places higher demands on the economics of the separation method, so study on production of boron-10 by gas diffusion method is carried out. Using BF$_3$ as processing gas, it is feasible to enrich high abundance of boron-10 by gas diffusion. The single stage separation effect and the hydraulic status of single stage was estimated. Binary gas diffusion cascades were designed and compared. Under given production requirements, the scale of the cascade was estimated and optimized. Finally, step cascade was picked for the production of 90% boron-10. Based on the cascade design, economic estimation of this separation method was conducted, and the target product cost was calculated. This study laid a good foundation for the expansion of boron isotope separation methods.

**Keywords:** Boron Isotopes, Gaseous Diffusion, Economic Estimation, Boron Trifluoride
ABSTRACTS

POSTERS

PHYSICAL, CHEMICAL AND PLASMA SEPARATION TECHNOLOGIES
The work analyzes the existing technologies and schemes of treatment of highly concentrated wastewater of complex composition, based on various combinations of Physico-chemical, membrane and biological methods of water treatment. The system of wastewater treatment with removal of the main part of pollutants from them at the stage of preliminary preparation and extraction of solid-phase sludge is proposed. This system allows the most optimal treatment of wastewater and its preparation for the membrane treatment stage, which significantly increases the efficiency of the reverse osmosis treatment stage.

In the process of work, an experimental plant for water purification and transfer of pollutants into the solid phase was created. The plant includes the following blocks: clarification, reagent flotation, ultrafiltration, as well as a sediment collection block for pollutants. Studies have been conducted on the purification of various types of real water, characterized by high concentrations of organic and inorganic pollutants. As objects of research filtration water of solid waste landfills, wastewater of pulp and paper mill, as well as effluents of pig complexes were used. Studies have shown that when using the proposed system, it is possible to significantly reduce the initial color and turbidity of the wastewater, and also reduce the concentration of the main pollutants by tens of times, which greatly facilitates the subsequent post-treatment with reverse osmosis.

Keywords: water treatment, wastewater, Physico-chemical methods, coagulation, sediment
In the work, the sorption properties of the synthetic zeolites HF 512O and NaX were studied. In the course of the study, the sorption capacities of zeolites for nitrogen, oxygen and air were obtained by the volumetric method. The experimental setup for determining the sorption capacity by the volumetric method consisted of two tanks. The first tank has a known volume, and the second tank is filled with the studied sorbent. Helium was used to determine the free volume of the second tank. The gas whose sorption capacity is to be determined is supplied to the first tank, the second tank is pumped out using a vacuum pump, after which the tanks are connected and the pressure in the tanks is equalized. Thus, the sorption capacity of the sorbent can be calculated by the pressure drop in the system. In addition, sorption isotherms for pure gases and for air were obtained. The selectivity of sorbents for nitrogen – oxygen pair for pure gases and the selectivity for sorption of a binary air mixture were calculated. Based on the isotherms of nitrogen, oxygen and air, the ratio of sorption of nitrogen and oxygen for a binary mixture of air is determined. Based on the results obtained, a cyclogram of the operation of the sorption block of the hybrid membrane-adsorption oxygen concentrator is proposed.

Acknowledgements: The work was financially supported by FASIE 13707GU/2018.

Keywords: gas separation, adsorption, synthetic zeolites, PSA, oxygen concentrator.
The chemical isotope exchange (ChIE) process in the water-hydrogen system is used to heavy water recycling and to detritiation of water waste. Industrial progress of this system became possible due to development of heterogeneous hydrophobic catalysts. However, the low heat resistance of these catalysts limits their operational temperatures.

In this work, the ChIE mechanism in the water–hydrogen system was studied in the temperature range from 285 to 368 K on the new hydrophobic catalyst RCTU-4 (Pt/CDVB). It was shown that at 323 K the maximum value of the mass transfer coefficient is observed, which decreases with a further increase in temperature. This dependence is explained from the point of view of hydrogen and water vapor competitive adsorption at the catalyst active sites. This is confirmed by direct measurement of temperature dependence of the catalytic reaction between water vapors and hydrogen. At a relative humidity of RH = 100%, the reaction rate decreases at temperatures above 343 K. If the ratio \( P_{H_2O}/P_{H_2} \) in the mixture is kept constant, the catalyst activity increases in the all studied temperature range (\( E_a = 15 \text{ kJ/mol} \)).

**Acknowledgements:** The reported study was funded by RFBR, project number 19-38-90014.

**Keywords:** hydrophobic catalysts, activation energy, isotope exchange, water-hydrogen.
From a historical point of view, the first separation of isotopes by the chemical exchange method (CHEX) for industrial purposes was carried out more than 80 years ago at a concentrating of $^{15}\text{N}$. Since then, this method has gone through various stages of development, demonstrating its capabilities in the separation of numerous isotopes from hydrogen to uranium and its particular viability for large-scale production of isotopes of the lightest chemical elements. At present, the CHEX method is the basis of the technology for the production of isotopes such as deuterium, lithium-6, boron-10 and others.

The report discusses both industrial technologies for the concentration of isotopes by the CHEX method (from deuterium to $^{235}\text{U}$), as well as the results of many studies devoted to new directions of isotope separation processes by this method. This is a change in industrial technology, and the development of new isotope separation methods. In particular, the results of determining both the thermodynamic and mass transfer characteristics of many processes for the separation of stable isotopes, in particular, isotopes of nitrogen, carbon, silicon, germanium, and others, are presented.

**Keywords:** isotope separation, chemical exchange, isotope production, research and development.
INVERSION OF BORON ISOTOPE EFFECT DURING CHEMICAL EXCHANGE IN EXTRACTION SYSTEMS

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In the processes of boron isotopic exchange in liquid-liquid systems using boric acid as the main working substance, the lighter boron isotope is concentrating in the organic phase, which takes place both in the case of phase exchange (tributyl phosphate, TBP) and at the chemical (trioctylamine, TOA) isotope exchange [1]. That is, boron-10, as a rule, predominantly passes into the organic phase.

In contrast to the previously observed effects, our studies for several extraction systems using secondary amines (diethyl, dipropyl, and dibutylamine as the organic phase) demonstrated the inversion of the boron isotope effect when a more light isotope $^{10}$B is concentrated in the aqueous phase. At the same time, the level of the values of the single stage separation factor of boron isotopes turned out to be quite high and amounted to 1.020 - 1.028.

The paper discusses the possible causes of the discovered phenomenon, and also considers the potential for practical application of such an effect.


Keywords: boron isotopes, single stage separation factor, isotope effect inversion.
GLOBAL DYNAMICS OF PHASE TRANSITION
EVAPORATION INTERFACES IN THE FORM OF
TRAVELING FRONTS IN HORIZONTALLY EXTENDED
DOMAINS OF POROUS LAYERS

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The present paper is devoted to validity of the model Kolmogorov–Petrovskii–
Piskounov–Fisher equation (KPP) in description of phase transition evaporation
interfaces in the form of traveling fronts in horizontally extended domains of
porous layers where the water is located over the vapor. It was indicated that for
the case of close planar phase transition fronts the dynamics of the system is
described by the (KPP) equation. We have shown, that even in case when the
plane stationary interfaces are not close and formally we cannot use the KPP
equation for description of fronts, the maximum deviation of the dimensionless
traveling front amplitude from the corresponding (traveling with the same speed)
KPP front is small enough. Moreover, the asymptotics of the front at infinity is
always described by the KPP equation. For stable asymptotes the most dangerous
perturbations are evidently travel with the front. All other do not have time to
develop and the front runs away from them. But when one of these asymptotes
is unstable in order the front can run away from stationary perturbations it is
necessary that this instability be the convective one in the reference frame firmly
connected with a traveling front. There are two scenarios for the development of
instability. In the first case, the solution is transformed into a traveling wave. In
the second scenario of instability, a finger is formed, which rapidly increases in
amplitude. The problem is solved numerically using the boundary element
method. For this solution, the boundary of the water- saturated region is
represented by a polygonal line consisting of sections-panels. Each panel is
associated with the source of the potential of the double layer the density of
intensity of which is determined by solving a system of linear equations for each
panel. These linear equations are obtained under the assumption that the potential
created by all panels in the middle of each of the panels is equal to the pressure
at this point.

Acknowledgements: The work was carried out with support from the Russian
Science Foundation under the grant No. 16-11-10195.

Keywords: phase transition surface, fingering, travelling wave, instability.
This work examines the mechanisms of destruction and synthesis for macromolecules, which may be propelled by external acoustic fields in the flows of polymeric liquids containing a large number of gas bubbles. In the present case, the emergence of a huge number of cavitation nuclei is brought about by the developed internal structure and the presence of various degrees of freedom for polymer macromolecules. The dynamics of these bubbles is assumed to govern by changing the flow geometry and exciting sound oscillations in the flow. Special attention is drawn to the process of changing liquid density owing to the effect of internal airlift in the polymer medium. Mechanically-induced kinetic changes in macromolecules (destruction and synthesis of polymer chains) will occur when the bubbles collapse. These features may be used for the oil treatment.

**Acknowledgement.** This work is supported by the RFBR (No. 19-32-90105), Russian Science Foundation (No. 15-19-00151)

**Keywords:** polymeric liquid, density collapse, chemical kinetics, airlift
The multi-functional Tritium Removal Facility (TRF) has been designed for the heavy water research reactor PIK in Gatchina, Russia. Along with the extraction of tritium and protium from a heavy water reflector of the reactor, TRF provides the processing of heavy water waste and the production of tritium-free heavy water. Combined Electrolysis & Catalytic Exchange (CECE) process and hydrogen cryogenic distillation are used at TRF. A number of investigations have been made to obtain data for the TRF design in the NRC «Kurchatov Institute» - PNPI. At present, the facility is under construction and detailed design is being completed. Possibility of processing of heavy water waste to produce heavy water simultaneously with the extraction of tritium and protium from heavy water reactor will improve the functionality and economic efficiency of the Tritium Removal Facility. The key design parameters, basic technological scheme of the facility and the main modes of its operation are presented along with a progress of the construction of the facility building and engineering systems.

**Keywords:** heavy water, hydrogen isotope separation, tritium removal facility.
The motivation for researchers to address the elaboration of processes of mass separation from a mixture of elements in a plasma state was the problem of the disposal of spent nuclear fuel. The theory of plasma technology shows the possibility of separating mixtures into elements or groups of elements. However, the first experiments demonstrate the mixing of heavy and light components at the receivers. The experiments carried out on the POMS-E-3 plasma-optical mass separator allow us to say that the low resolution is a consequence of the “intervention” of plasma effects accompanying the process. These are anomalous acceleration of ions, generation of a field of charges separation, density jumps, various behavior of the density with a change in the orientation of the magnetic field, the appearance of isomagnetic potential jumps, and the generation of plasma electrostatic oscillations in the zone of the $E \times B$ discharge. The report presents the characteristics of the listed effects and the regularity of their manifestation. The necessity of finding the effects to which the ions are most sensitive is emphasized. Some ways of compensating for their influence on the efficiency and productivity of plasma-optical mass separation are described.

Acknowledgment: this work was partly supported by Russian Science Foundation (grant №18-79-00037).

Keywords: plasma-optical mass separation, plasma accelerator
According to the Szilard-Chalmers effect, recoil atoms of the 99Mo radionuclide can be produced in nuclear reactions and retained in surrounding buffer substance. Nanolayers of molybdenum with thickness of 30 to 220 nm were produced by magnetron sputtering on sapphire plates. Measurements of the yield of recoil 99Mo atoms in the 100Mo(p,x)99Mo nuclear reaction under irradiation of nanolayers in the U-150 cyclotron with 28 MeV protons as a function of metallic Mo nanolayer thickness were carried out after eluation of parent Mo nanolayers [1]. The optimal yield of 99Mo recoil atoms in relation to the starting isotope was found to be the highest with the molybdenum layer thickness of 80 ± 5 nm. The mass of parent Mo in collector was determined by activation analysis. The enrichment factor (EF) has been defined as EF = 1200 ± 150. The specific activity (SA) of 99Mo produced in the collector was estimated to be equal to 25 Ci·g−1. An intermediate 5nm Cr nanolayer was used as a thin diffusion barrier that detains the penetration of parent Mo and passes the 99Mo recoil atoms. The use of Cr interlayer increased the resulting of 99Mo SA more than 10 times.

**Keywords:** isotope separation, Mo-99, Mo nanolayers, Szilard-Chalmers effect, yield of recoil atoms.

**Reference**
DIELECTRIC CONSTANT OF PLASMA ROTATING IN CROSSED ELECTRIC AND MAGNETIC FIELDS

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Rotating plasma is applied for isotope separation of chemical elements which do not have convenient gaseous compounds under normal conditions. The paper considers unsteady plasma rotation in crossed radial electric and axial magnetic fields. The situation is studied when the medium is sufficiently rarefied and highly ionized as well as its viscosity and other dissipative processes can be neglected. The estimated time of speed rotation and the effective dielectric constant for lithium plasma are calculated.

Acknowledgment. This research is supported by the Russian Science Foundation (grant No 18-19-447) and the Program for Improving the Competitiveness of the National Research Nuclear University MEPhI (grant No. 02.a03.21.0005 of August 27, 2013).

Keywords: isotope separation, rotating plasma, dielectric constant of plasma.
The project of a fusion neutron source (DEMO-FNS) involves the combination of fusion and fission technologies (in a hybrid energy system) based on a tokamak. On one hand, stated DEMO-FNS parameters, as well as the stationary mode operation, lead to a fuel load in the tokamak (via injection of 3 types) compared to JET (and significantly lower than ITER). On the other hand, the total content of tritium in all systems depends on the selected processing technologies, and now is estimated about 2 kg (that is half of ITER tritium inventory). The fuel tritium-deuterium cycle is one of the main fusion facility systems. Within the framework of the fuel cycle, there is carried out: providing fuel to injection systems into the plasma, removal of gases from the plasma chamber (divertor), separation of hydrogen from gas mixtures, hydrogen isotopes separation, gas detritiation.

Closed fuel cycles were implemented on TFTR and JET fusion facilities, within which various methods of handling tritium and tritium-containing gases, separation of hydrogen isotopes, etc. were tested. ITER, CFETR and DEMO fuel cycle systems design and testing are on the way. The requirements for these facilities are much higher, in view of significantly larger amounts of tritium.

In this report the general approaches to the fuel cycle DEMO-FNS design described. It also contains comparison with various technologies used or to be used in fusion facilities (TFTR, JET, ITER, CFETR, DEMO).

The work was supported by the NRC “Kurchatov Institute (14.09.2019 № 1805)

Keywords: fusion fuel cycle, tritium inventory, DEMO-FNS, fusion neutron source, hydrogen isotopes separation.
Metals in a nanostructured state exhibit new physico-chemical properties concerned with to bulk metals. This phenomenon is used in many branches of science and technology, including catalysis. In this work, to evaluate and compare the catalytic properties of different studied objects, we used the reactions of homomolecular isotopic exchange of hydrogen and ortho-para conversion of protium.

The objects of study are copper, silver, and gold nanoparticles deposited on $\gamma$-Al$_2$O$_3$. Nanoparticles of copper and gold were obtained by impregnating the support with a solution of a metal salt and its further decomposition. Silver nanoparticles are synthesized in reverse micelles.

The catalytic activity of the samples was studied in the reaction of ortho-para conversion of protium at the boiling point of liquid nitrogen (77 K).

The main results and comparison of the specific catalytic activities of the nanoparticles of the studied metals are given in the table.

<table>
<thead>
<tr>
<th>Metal</th>
<th>$K_{77}^{\text{spec}}$, molecules $\cdot s^{-1} \cdot \text{sm}^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>(1,484±0,028)$\cdot 10^{14}$</td>
</tr>
<tr>
<td>Ag</td>
<td>(1,84±0,24)$\cdot 10^{14}$</td>
</tr>
<tr>
<td>Au</td>
<td>(3,00±0,19)$\cdot 10^{14}$</td>
</tr>
</tbody>
</table>

The following conclusions can be drawn from the presented research results:

1. In contrast to bulk metals, copper, silver, and gold nanoparticles exhibit catalytic activity;
2. Nanoparticles of 1B-group metals in the reaction of ortho-para conversion of protium show a high specific catalytic activity comparable with the best catalytic systems;
3. According to the catalytic activity of metal, the nanoparticles are arranged in the following order Au > Ag > Cu.
Main parameters of the vacuum pump system for boron isotopes separation by the SILARC method, such as mean values of gas flow pressure, temperature and velocity, averaged over respective vacuum pump inlet area, are calculated by solving the system of material, momentum and energy balance equations for different characteristic stations along core and rim gas flow vacuum pump system tracts. As a result, pumping out speeds of respective vacuum pumps for rim and core gas evacuation, required to provide optimal pressure and temperature level in supersonic gas flow have been evaluated.

Acknowledgements: This work was supported by the Russian Science Foundation grant 17-11-01388.

Keywords: boron isotopes, laser assisted methods of isotopes separation, hydraulic approximation, turbomolecular vacuum pump, supersonic gas flow
ABSTRACTS

POSTERS

MEMBRANE SEPARATION
SEPARATION OF A GAS MIXTURE IN NANOSIZED POROUS MEMBRANES. EFFECT OF ADSORPTION AND SURFACE DIFFUSION

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Results of the theoretical analysis of the separation effect for a binary gas mixture diffusing in a porous membrane are shown. The analysis is based on the capillary model of the porous medium, which takes into account the effects of adsorption and surface diffusion of one of the components on the channel walls. We consider the Knudsen-flow regime, characteristic for nanosized porous media at normal gas pressures. Expressions for mean molar fluxes of mixture components in the membrane, derived in this model, the adsorption isotherm and data on surface diffusion coefficients are used to obtain relations for the concentration jump in the membrane for the given pressure drop on the membrane. The resulting expressions contain corrections due to the adsorption and surface diffusion of one of the mixture components. Calculations of the concentration jump and separation factor for the adsorbed component in the membrane are carried out for a series of industrial-relevant gas mixtures, such as, for example, H2/CO, H2/CO2 and H2/C3H8. It is demonstrated that taking into account of the surface effects can lead to an up to ten percent change in the separation factor, compared to its limiting Knudsen value (in the absence of adsorption).

Acknowledgements: this work has been financially supported by the Russian Fund for Basic Research under Grant No. 18-08-00211A.

Keywords: nanoporous membrane, adsorption, surface diffusion, mixture separation, Knudsen flow.
INTELLIGENT AIR CONDITIONING SYSTEM BASED ON MEMBRANE GAS SEPARATION TECHNOLOGY

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Air quality has a significant impact on both health and human performance and productivity. In the urban environment, where there are such polluting factors as road transport, industrial enterprises and dense buildings, air quality issues are most acute. To create a safe and comfortable environment, many enterprises invest heavily in climate systems. However, at present, most of these systems only support air exchange and air temperature. One of the most promising methods of air purification, at present, is the method of membrane gas separation. Installations based on membrane technology have the following advantages: compactness and low weight, relatively low operating costs, the ability to work in a wide range of gas pressure, ease of installation and maintenance, quick start and stop, as well as a long service life. In this work, we consider an air conditioning system based on membrane technology that can control the following indoor air parameters: humidity and oxygen and carbon dioxide concentrations. The system operation was modeled and the effectiveness of using the membrane method was shown when removing carbon dioxide formed in the process of human life. It is shown that the use of membrane technology as part of intelligent air conditioning systems helps to reduce the required air exchange rate to maintain a normal indoor air composition.

Keywords: gas separation, membrane, intelligent conditioning, air exchange, carbon dioxide recovery
Production of efficient rGO/PVDF membranes using graphene oxide nanocrystallites nc-GO as inclusions on the surface in standard polymeric PVDF membranes is demonstrated. Composite rGO/PVDF membranes consist of a larger number (15–20) of rGO layers, the thickness of the rGO layer reaches 1500–1700 nm, the thickness of one rGO sheet is 70–100 nm, each rGO sheet consists of rGO flakes of different orientations. rGO/PVDF membranes have shown the best filtration efficiency as compared to the standard polymeric PVDF membranes. The dependence of the rate of water transport through interlayer nanochannels of rGO/PVDF membranes on the reduce time of rGO was revealed. An increase in the reduce time of rGO leads to a decrease in the number of hydroxyl OH and carboxyl CO groups, which leads to an increase in the hydrophobicity of rGO and a decrease in the size of the interlayer channels of rGO. This, in turn, leads to an increase in the rate of water passage through rGO / PVDF membranes due to a decrease in the activation energy of shear viscosity of water in rGO nanochannels. Application of pulsed photon annealing PA allows producing the stable rGO/PVDF membranes. PA leads to an increase in the crystallinity of the rGO/PVDF membrane structure, which depends on the duration of PA. An increase in the duration of the annealing pulse leads to an improvement in the perfection of the crystal structure of rGO flakes.

Keywords: rGO/PVDF membranes, graphene oxide nanocrystallites
WATER ACTUATION THROUGH NANOMEMBRANES USING SURFACE ACOUSTIC WAVES (SAW)

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Nanofiltration technology for water desalination and other fluids purification from salts, germs, bacteria and viruses are based on the so called nanopumping (NP) effect, when a fluid flow through nanomembranes and nanochannels is actuated using Surface Acoustic Waves (SAW) is presented. The paper considers processes of water nanofiltration through a carbon nanomembrane using ultrasonic waves, which were generated by SAW devices under different RF power and frequencies. We considered a droplet of water with the volume in the 2 and 5 μl range, and used SAW devices with different frequencies of 34 and 58.2 MHz. The effect of frequency on microfluidic performance, such as moving, atomization, and passage of nanodroplets has been studied using a video camera in a range of SAW power. Our study made clear that SAW having higher resonant frequencies have an increased power for moving, atomization, and passage of droplets through nanomembranes. The SAW device consisted of a Lithium niobate (LiNbO₃) piezoelectric substrate and a graphene nanomembrane placed on the substrate. Such nanopumping devices will be of practical interest for the development of future energy sources, e.g., for fuel cells, hydrogen energy, pharmaceutical processes and nanoengines for medical robots, as well as for use in a wide variety of chemical, food and agricultural applications. It is demonstrated that the process of nanofiltration of water includes the processes of droplet moving, atomization and passage through nanopores and will be useful for future water desalination processes. The dependences of the travel time of droplet moving and atomization of water on the power, frequency and volume of the droplets were established. It is shown that with an increase of power and frequency of SAW, the filtration process proceeds rapidly and has a power-law character. The results of modeling were thoroughly compared by existing experimental data.

Keywords: Nanofiltration, water desalination, purification of fluids from salts, germs, bacteria and viruses, nanopumping effect.
ASYMMETRIC FILTRATION MEMBRANES BASED ON POLYIMIDE (R-BAPB)

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An important scientific task that is in focus of leading scientific membrane groups is the fabrication of membranes for the filtration processes under aggressive environment conditions. Insoluble polyimides are the most promising group of polymer materials to solve this problem, since they are stable at temperatures above 200 °C and when exposed to organic solvents. However, in order to obtain asymmetric membranes from polyimide, it is necessary to form membranes from a prepolymer solution (polyamide acid – PAA) by non-solvent induced phase separation method, and then imidize PAA.

The thermoplastic crystallizable polyimide R-BAPB, which is resistant to a number of known organic solvents, was chosen as a membrane material. It has been experimentally proved that water is the strongest non-solvent for the studied polymer, being the preferred precipitant for fabrication of filtration membranes by the phase-inversion technique. For the first time, polyimide-based membranes from R-BAPB having the asymmetric porous structure with the selective layer are fabricated. An increase in the glass transition temperature of the material to 220°C confirms the formation of R-BAPB polyimide, which is also accompanied by a significant increase in the elastic modulus. The results of filtration experiments indicate that the pores of the microfiltration level are present in the membranes.

Acknowledgement: This work was supported by the Russian Foundation for Basic Research (RFBR), Grant No. 18-29-17040.
Keywords: R-BAPB, insoluble polyimide, porous membrane, filtration
Commercial polymeric membranes have asymmetric structure with a fine selective layer having narrow pores and a macroporous support layer. In the case of integrally skinned asymmetric membranes, such a porous structure is formed during membrane preparation by the non-solvent induced phase separation technique (NIPS). The vapor-induced phase separation (VIPS) technique can be considered as an alternative to NIPS. The combined variant is possible when limited in time vapor exposition is used prior to casting in liquid nonsolvent to obtain the desired porous structure. Such combination of vapor exposure and immersion in nonsolvent allows varying the membrane formation conditions and, therefore, to obtain a wide range of possible porous space configurations. Most papers reported on VIPS technique consider four polymers: PVDF, PS, PES and PEI. However, a limited number of works focuses on the fabrication of polyacrylonitrile (PAN) membranes according to this method despite the fact that this polymer is the second most common membrane material for the development of filtration membranes. PAN possesses high mechanical, chemical and thermal stability, solvent resistance, low cost and good fouling resistance.

In this work, series of PAN membranes were obtained by the combined VIPS/NIPS method with a wide range of casting conditions. These membranes were investigated by using liquid-liquid displacement method for membrane pore size distribution and membrane permeance measurements. Porometer POROLIQ 1000 ML was used for the membrane investigation. Wide range of pores was obtained in the range of 5-50 nm depending on casting conditions. Membrane permeance measured at pressure 1-30 bar reached 400 kg/m²·h·bar.

Acknowledgements: This work was funded by the Russian Science Foundation (Project no. 18-79-10260)

Keywords: porous membrane, PAN, pore size, polyacrylonitrile, liquid-liquid displacement, filtration, asymmetric membrane, ultrafiltration
Processes of C$_1$-C$_4$ hydrocarbons gas separation with membranes yielding in methane and C$_{3+}$ fractions are highly attractive. The significant breakthrough on this issue can be achieved by development of novel gas separation modules based on C$_{3+}$ hydrocarbons-selective hollow fiber membranes. The efficiency of this technology significantly depends on the module design, that should take into account the mass and heat transfer processes within the module with simultaneous external constrained flow in the fiber system, the internal flow in hollow fibers, and molecular transport in selective membrane layer considering the thermal effects of hydrocarbons separation. The developed simulation model includes the theory of convective diffusion transport in hollow fiber membrane modules with an ordered and disordered arrangement of fibers. The simulated dependencies of the Sherwood number for circular and noncircular fibers in a fiber system within a model module with longitudinal, transverse and transverse-radial external flows on the Reynolds and Peclet numbers, fiber packing density, temperature, mass transfer coefficient in the membrane, will be presented. The dependences of the impurity absorption efficiency of fibers from three-dimensional external flows on the Reynolds and Peclet numbers under different packing densities, membrane properties, module parameters and separation conditions, will be considered. Transport in modules with a disordered arrangement of fibers and the effect of polydispersity of fibers on the Sherwood number will be shown. The limits of model approach applicability to the description of transport within real modules will be described.

**Acknowledgements:** This work was carried out in A.V. Topchiev Institute of Petrochemical Synthesis (Russian Academy of Sciences) and was funded by Russian Science Foundation, grant number 19-19-00647.

**Keywords:** hollow fiber membrane, hollow fiber module, gas separation, simulation, mass transfer, heat transfer.
ABSTRACTS

POSTERS

MOLECULAR TRANSPORT UNDER EXTREME CONDITIONS AND ITS APPLICATION IN INNOVATIVE TECHNOLOGIES
Quality of ingots of light alloys (aluminum, titanium, niobium) is determined by casting technology, in particular by melt temperature, cooling rate and casting speed. Stirring increases heat transfer between the hot core and the cooled edges of the ingot. This increases the speed of the casting process providing homogeneous and fine structure of the alloy in comparison with the conventional casting and improves the ingot quality and reduces the wast product. In addition, the electromagnetic forces allows us to develop a novel technology of casting without contact of the ingot with the walls of the mold (levitation of the metal) providing production of the ingots which do not need further mechanical scalping. Development of these technologies requires special numerical codes for modeling of these processes. These codes are under development in the laboratory of extremal hydrodynamics of NRNU MEPhI. In particular in this work we discuss a new method of numerical modeling of the casting process taking into account the thermal convection in the liquid phase. Convection plays a key role because the heat transfer due to convection strongly exceeds the heat transfer due to thermal conductivity in light metals especially in titanium alloys. A buoyancy term \( g(\rho - \rho_{ref}) \) in the Navier-Stokes equation is usually used to simulate thermal convection. However, inappropriate choice of \( \rho_{ref} \) can lead to an incorrect result at the modeling of the casting. To avoid the problem of selection of reference density, a new method of modeling of convection is proposed and tested in this work. 3D numerical simulation of casting of an aluminum alloy (as an example) with magnetic stirring was carried out using a software packages ANSYS CFX and ANSYS Emag.

**Keywords:** casting, light metals, numerical modeling.
Dissection of metal structures, blocking the mouth of oil or gas well in case of uncontrollable blow-out is an actual task, as it allows carrying out operations on the replacement of wellhead equipment and the elimination of spouting. The modern and safe way of conducting emergency response and restoration operations in the current circumstances is the distance severing of metal structures using laser radiation. The effectiveness of this method was successfully demonstrated by the mobile laser technological complex MLTK-20. The success of laser radiation application for the above-mentioned purposes largely depends on the effectiveness and loss-free transportation of such radiation to the place of its action. Obviously, if the beam propagates through the flame, the radiation attenuation occurs. Degree of the attenuation depends on the composition of burning hydrocarbons and the length of the combustion area. This paper is devoted to investigation the possibility of laser radiation use for conducting restoration operations on emergency oil wells. Measurement results of the averaged over the flame length the absorption coefficient of laser radiation by diffusion oil flame have been presented. Efficiency of the remote laser cutting of thick-walled metal and concrete has been determined.

Keywords: flame, radiation absorption coefficient, cutting.
APPLICATION OF MODERN LASER TECHNOLOGIES FOR MONITORING OF THE COMPOSITION OF THE AIR ENVIRONMENT ON MANNED SPACECRAFT AND VOLATILE METABOLITES IN EXHALED AIR DURING LONG SPACE FLIGHTS

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The current strategy of monitoring the composition of the air environment of manned spacecrafts (MSC) and orbital stations (OS) during long flights envisages acquiring of the maximum scope of information on a real-time basis. The cornerstone of this strategy is high-precision, continuous, dynamic control of the content of a number of volatile compounds polluting the air environment of MSC and OS. Such control is required for taking optimal medical and technical managerial decisions aimed at maintaining the crew performance and correcting the operation of life support systems of MSC and OS.

Besides, as the duration of human stay in space flight will get longer, noninvasive methods of the real-time integral assessment of the physiological condition of a person will make the basis of space medicine. One of the major steps in this direction is the development of a medical technology based on a study of volatile metabolites, i.e. biomarkers of peroxide oxidation of lipids in the human exhale air during physiological adaptation to space flight conditions.

This paper reports on a new promising model of an analytical complex based on modern diode lasers, quantum-cascade lasers, and optical multipass cells for precision continuous air quality control on board a MSC and OS and the analysis of the chemical composition of the air exhaled by a person with detecting limits at the level of 5-10 ppb. In order to ensure the overlapping of the nomenclature of the substances to be
detected in the MSC and OS air environment and human exhalation with regard to compounds of special importance, it is suggested to use simultaneously gas analyzers of several types based on Diode Laser Spectroscopy, Cavity Ring Down Spectroscopy, and Integrated Cavity Output Spectroscopy. The latter two types ensure optical paths of considerable lengths (up to 1 km and longer). The adaptation of such system would make it possible to analyze a wide range of substances and provide continuous precision quality control of the MSC and OS air environment and the composition of the air exhaled by a person during a long space flight.

This work was performed within the state order of the Ministry of Science and Higher Education of the Russian Federation (topic 0082-2019-0017, registration No.AAAAA19-119010990034-5).

**Keywords**: spacecraft, atmosphere, analysis, laser technology
Mass spectrometry of metastable ions is sufficiently well-researched and used in chemistry to determine and control fragmentation reactions. Peaks of metastable ions are substantially wider than peaks of real ions and, as a rule, non-symmetrical. They negatively affect spectral resolution and are the main cause of background ion current in a wide range of mass numbers.

Iridium hydride tetrakistrifluorophosphine Ir(PF3)4H has a well-developed spectrum of ion groups, suggesting presence of metastable transitions with generation of metastable ions. The research encompassed tests on a MI-1201 static magnetic sector mass spectrometer. Table 1 shows the relative intensities of ion groups in Ir(PF3)4H.

Table 1. Relative intensities of ion groups in Ir(PF3)4H mass spectrum.

<table>
<thead>
<tr>
<th>Ion group</th>
<th>Ir(PF3)4H+</th>
<th>Ir(PF3)3H+</th>
<th>Ir(PF3)2H+</th>
<th>Ir(PF3)H+</th>
<th>Ir+</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative intensity</td>
<td>200</td>
<td>900</td>
<td>900</td>
<td>1000</td>
<td>200</td>
</tr>
</tbody>
</table>

Decay pattern with generation of “apparent” masses was selected with detachment of one trifluorophosphine PF30 radical.

\[
\text{Ir(PF3)4H}^+ \rightarrow \text{Ir(PF3)3H}^+ + \text{PF30} \quad m^*=382.2 \\
\text{Ir(PF3)3H}^+ \rightarrow \text{Ir(PF3)2H}^+ + \text{PF30} \quad m^*=296.9 \\
\text{Ir(PF3)2H}^+ \rightarrow \text{Ir(PF3)H}^+ + \text{PF30} \quad m^*=212.9 \\
\text{Ir(PF3)H}^+ \rightarrow \text{IrH}^+ + \text{PF30} \quad m^*=131.7 
\]

No Ir(PF3)H+ → Ir(PF2)H+ + F0 transitions with detachment of one fluorine inside PF3+ radical were recorded. Thus, with electron impact ionization in Ir(PF3)4H compound, ions are fragmented by the primary pattern with detachment of PF3 radical. Ir(PF2)H+, Ir(PF)H+, IrPH+, IrF+ and IrH+ ions are an insignificant part of the constitutive share of ions. The developed spectrum of metastable ions in Ir(PF3)4H compound indicates significant lifetime of “offspring” ions. Apart from the main cause, associated with redistribution of internal energy when a molecular ion is ionized in an ion source, fragmentation is affected by the high molecular mass of Ir(PF3)4H+ ion and associated significant time of ions drifting in a mass spectrometer chamber. The resulting “apparent” masses
of metastable ions may be used to give a correct interpretation of peak background values in mass spectra of gases and have more accurate calculations of both isotopic and impurity content. Besides determining metastable ion values and probability of one or another decay (fragmentation) pattern, the lifetime of these ions was also assessed, and it constituted $2.90 \times 10^{-5}$ s.
The stable isotope tellurium Te130 is used in nuclear medicine to produce radioactive iodine I131. Tellurium hexafluoride is the operating gas for the separation of tellurium isotopes by centrifugal method. However, tellurium isotopes are used in oxide and elemental chemical forms. The literature describes the technology of conversion of tellurium hexafluoride into dioxide by aqueous hydrolysis. The authors studied the possibility of synthesis of tellurium dioxide by interaction of tellurium hexafluoride with silicon dioxide by reaction:

\[ 2\text{TeF}_6 + 3\text{SiO}_2 = 2\text{TeO}_2 + 3\text{SiF}_4 + \text{O}_2 \]

in the temperature range 25–850 °C. Kinetic dependences of reaction rate on temperature are obtained. The activation energy of the process is determined.

With noticeable speed, reaction begins at 400 °C, but rapidly slows down due to the blocking reaction surface formed TeO2. Above 750°C tellurium dioxide evaporates from the SiO2 surface and condenses in the cold zone. The process was carried out in a reactor from a quartz tube, which was both a reagent and a product collector. The output of the target product reaches 90%.

Keywords: isotope tellurium, tellurium hexafluoride, silicon dioxide, chemical conversion.
Impact on the surface and volume breakdown in a barrier discharge of both the pre-postponed charge on a barrier and its electric activation by low voltage will be presented in the report. The experiments were performed in argon and air at atmospheric pressure with a barrier corona in geometry "a metal pin - a flat barrier electrode" and with the barrier discharge between two flat electrodes covered with a dielectric. At the research of surface breakdown, the HV pin electrode was tightly pressed to a surface of a dielectric barrier. The DC voltage of the necessary polarity with an amplitude either insufficient for surface breakdown or exceeding it was applied to the pin. In the first case, at an exposition of dielectric with a high voltage about 5 minutes, there was its activation, i.e. formation of the induced polarization and giving to dielectric of electret properties. In the second case, on a barrier surface there was a deposition of a charge the amount of which depended on the excess of the applied voltage compared to the breakdown voltage. At the research of volume breakdown between two flat barriers, the pin electrode was used only for charging of one dielectric barrier and was spaced from its surface at distance 0.3 - 30 mm. The detailed results will be presented in the report showing that not only pre-postponed charge but the electric pre-activation of a dielectric barrier influences the breakdown of the barrier discharge as well.

Acknowledgements: This work was supported by the RFBR (project No. 19-52-53003).
Modern pipeline systems are operated at high pressure, up to 200 atmospheres. It is clear that the destruction of equipment under such pressure will lead to the appearance of intense shock waves. The hazard also increases due to the fact that the destruction of the pipeline does not occur over the cross section, but sectional linear rupture with a length of up to 100 m are formed. The resulting shock waves have a shape close to the cylinder (close to the route).

Modeling of such processes is of great practical importance, but it does not receive due attention. Its methods often do not give correct results. In this paper, we consider the problem of breaking a pipe with a diameter of 1.2 m under a pressure of 212 atm.

The sizes of the damaged areas are determined. Destruction of buildings is possible at distances up to 70 m. The applicability limits of the cylindrical approximation of the solution are determined: it is possible up to distances comparable to the length of the pipe opening.

Keywords: gas pipeline, rupture, shock wave
Channel surface discharge (CSD) is a type of surface (sliding), and in the incomplete stage - dielectric barrier discharge. In the work experimental studies of both incomplete (low-current) and high-current, completed stage, of the channel surface discharge are carried out. The temporal waveform of the current pulse of the incomplete stage of the discharge was studied, and the influence rate of increase voltage $dU/dt$ on the discharge electrodes on it. Experimental dependence amplitude of the current pulse incomplete stage CSD of rate of increase $dU/dt$ was obtained over a wide range of variation of the latter. For the completed stage CSD, a relation between intensity of the discharge radiation in the UV region and the amplitude of current pulse has been received. Using UV radiation from the CSD for ionization of atmospheric pressure nitrogen, the dependence of the maximum electron concentration on UV radiation intensity of the high-current stage CSD, is obtained.

**Keywords:** channel surface discharge (CSD), dielectric barrier discharge, pulse of a current, incomplete stage, complete stage, rate of increase voltage, intensity UV radiation, ionization of nitrogen.
APPLICATION OF THE PERTURBATION THEORY FOR THE CALCULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES OF HYDROGEN AND ITS ISOTOPES

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The KLRR perturbation theory is well suited for determining an equation of state and properties for gases included supercritical fluids. In this work the equation of state based on the perturbation theory is used for evaluation of the thermodynamic and transport properties of hydrogen isotopes at atmospheric and at high pressure.

The application of molecular kinetic theory for ideal gases is unrealistic for calculating the transport properties of dense gases in the high-pressure region. The analytical expressions for the calculation of transport coefficients based on the Chapman-Enskog kinetic theory using the Lennard-Jones pair interaction potential were analysed. In the proposed equations for viscosity of individual substances use the values of the radial distribution function and the hard-sphere diameter, which can be obtained on the basis of the perturbation theory previously used only to estimate the thermophysical properties. Thus, the obtained equation of state allows to calculate not only the thermal properties of hydrogen isotopes, but also transport properties such as viscosity, diffusion and thermal conductivity in a wide range of pressure. It has been shown good agreement of predicted thermophysical and transport properties with the available experimental data and molecular dynamics simulation.

Acknowledgements: The work was carried out with support from the Russian Science Foundation under the grant No. 16-19-00188.

Keywords: the perturbation theory, transport properties, hydrogen isotopes, viscosity.
Optimization of Laser Writing Process for Fabrication of Light-Guiding Structures in Chromophore-Containing Polymers

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Electro-optical (EO) polymer materials, containing chromophores of donor-acceptor structure, are prospective for the creation of high-speed active elements of integrated optical circuits: switchers and modulators [1]. For the formation of light-guiding channels in thin films of EO polymer while fabricating those circuits one can use the method of laser image writing, based on irreversible photo-destruction of EO chromophores in the material under the influence of intense radiation of visible range.

The dependence of the laser writing rate on the process parameters (the intensity and wavelength of the radiation) while creating light-guiding structures in films of EO polymer DO1/PMMA [2] has been investigated. For this purpose thin films (up to 1 μm) of the EO polymer had been fabricated on SiO₂ substrates. It has been shown, that the laser writing process is efficient only when the laser light wavelength lies within the absorption band of the EO material. In this case the minimal time required for the image writing can reach 11 minutes.

Acknowledgements: the work was supported by the Ministry of Science and Higher Education of the Russian Federation within the State assignment FSRC “Crystallography and Photonics” RAS in part of the synthesis of electro-optical polymers, Russian Foundation for Basic Research (Project № 18-32-00948) in part of optimization of the laser writing process.

Keywords: electro-optical polymers, chromophores, channel waveguides, thin films, photo-bleaching.
Laser techniques for treating joint diseases require the development of medical diagnostic methods. Structural diagnosis of joints using synchrotron radiation and X-ray contrast nanoparticles is a promising method for visualizing cartilage defects. Oxide compounds of metals Fe, Ti, W, and Mo belong to the transition group of elements of the table D.I.Mendeleev can serve as such nanoparticles [1].

It is proposed to contrast the internal structure of cartilage with nanoparticles of metal oxides and oxide bronzes for visualization using high-resolution X-ray tomography.

Targeted transport of magnetic nanoparticles of iron oxide in non-homogeneous magnetic field of magnetic trap with axially symmetric distribution of magnetic induction is used to impregnate tissue with a colloidal solution of X-ray contrast substance. This trap consists of 2 oppositely magnetized ring permanent magnets, between which a tube is co-axially installed with a colloidal solution of magnetic nanoparticles.

An analysis of the distribution of the magnetic fields in the trap showed a linear dependence of magnetic induction on the distance along the axis of the magnets. This dependence allow us to control the gradient of magnetic field and the magnitude of the force acting on the transport of magnetic nanoparticles in interstitial space of cartilaginous tissue.

The kinetics of impregnation of iron oxide nanoparticles from the solution into cartilage placed in the magnetic trap was experimentally studied. Using thin section of the tissue, with the different exposure times placed in a colloidal solution in the trap, and further photometry of cartilage staining intensity, the dependence of the depth of tissue impregnation on time was obtained.

Based on the equations of magnetic nanoparticles motion in a viscous biotissue placed in non-homogeneous magnetic field of the magnetic trap, the mathematical model of cartilage impregnation with X-contrast substance is constructed. The calculated values of the depth of tissue
impregnation coincide with experimental data, both in depth and in the rate of impregnation of cartilage with nanoparticles. This method of impregnation of cartilage with biofunctional nanoparticles can be used to detect the pathologic structure of biotissues with X-ray synchrotron radiation.


Acknowledgements: This work was partially supported by the Ministry of Science and Higher Education within the State assignment FSRC «Crystallography and Photonics» RAS.

Keywords: Synchrotron radiation, diagnostics of biological tissue, X-ray contrast nanoparticles, impregnation of cartilage, magnetic nanoparticles.
Additive manufacturing enables a substantial decrease of the production cycle of complex shape parts. A direct numerical simulation (DNS) is an efficient tool for the reduction of experimental work needed for complex technology optimization. Numerical models are needed to be verified before the application in the process parameters optimization. The developed multiscale model of selective laser melting (SLM) allows calculating macro and micro parameters of produced tracks. Macromodel is validated for Ni-based powder SLM in a wide range of technical parameters taking into account the evaporation effect. The comparison of the substrate melting depth and track width with experimental data is held. The error in the numerically determining the track width was in the range of the measurement accuracy. For Inconel 718 powder we show that the effect of the evaporation on the heat balance is needed to be accounted for the laser energy density (LED) values above 250 J/mm and could be omitted for the values below. The track average crystalline size was calculated for the wide range of scanning speeds. The verification of the microscale part shows the adequacy of the average crystalline size with published metallographic data analysis. The increase of scanning speed leads to the cooling rate increase at the solidification front which results in the reduction of the grain size.

Acknowledgements: This work was supported by the Ministry of Science and Higher Education within the State assignment FSRC «Crystallography and Photonics» RAS in part of «development of the computer algorithm for researching SLM taking in account for the evaporation», RFBR (Project No. 16-29-11743 ofi_m) in part of «validation of the hydrodynamic multiscale model of microstructure evolution for SLM taking in account for the evaporation».
Development and creation of mobile laser systems for various sectors of the economy is one of the scientific and technical areas traditionally developed in the JC "SRC RF TRINITY". A revolutionary achievement of the 21st century in laser technology was the appearance of powerful fiber lasers. This work describes the possibility of applying powerful mobile laser technological complexes for the solution of perspective tasks. The scope of the complex includes remote separation cutting of reinforced concrete structures, underwater gas-laser cutting of bulk structures, remote ignition, cleaning, including decontamination, of surfaces, pest control. Remote separation cutting is used in the elimination of accidents in oil and gas fields without any risk to human life. Underwater gas-laser cutting can be used for dismantling the underwater part of oil platforms or for cutting radiation-contaminated materials in spent fuel storage pools. Remote setting fire is used for cleaning water, soil or ice surfaces when they are contaminated with various hydrocarbons. In addition, this approach can be used for remote detonation of mines. Laser decontamination is applicable for cleaning the surface radioactive contamination of metal and concrete surfaces. The mobile laser system can also be used to destroy agricultural pests, such as locusts.

**Keywords**: laser, decontamination, underwater, distant cutting.
Holes up to 10 mm in depth and less than 1 mm in diameter are often used in design of devices and facilities. Traditional drilling methods for such holes are inefficient, for small diameter drills are frequently replaced and difficultly sharpened for reuse. Under these conditions, the laser drilling method is more productive, despite the increased overall energy cost.

We describe the production of high quality holes of up to 200 mm in diameter in stainless steel or corundum plates by drilling vertically arranged plates with a horizontal beam of a fiber Yb laser operating in pulse-periodic mode with variable pulse duration and repetition rate with the average focal spot radiation intensity $10^8$ W/cm$^2$, spherical aberrations of the used lenses being taken into account in calculation. It is found that the drilling time and the quality of holes depend on radiation parameters, focusing conditions, magnitude and sign of the displacement of the focal plane relative to the surface. Selecting these parameters allowed holes of 100 mm in diameter in 1.5 mm thickness steel and holes of 120 or 180 mm in diameter in 5 or 9 mm thickness corundum, respectively, taper and diameter irregularity along the length not exceeding 10%.

**Keywords:** laser, drilling, plate, steel, corundum.
AUTOMATIC SYSTEM OF TEMPERATURE CONTROL AT LASER CLADDING

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Complexity of the equipment used and high requirements to the laser cladding quality lead to the necessity to control the cladding process in real time. Controlled parameters are the electron temperature in a plasma flame, the deposited layer shape, the brightness or color temperature of the melt. The temperature control is technically most simple but the brightness or color temperature measurements require the emissivity data which are unknown for many materials.

The algorithm to control the melt temperature without using the emissivity data is based on step-by-step temperature calculation for two closely spaced radiation wavelengths $\lambda_1$ and $\lambda_2$ in the thermal radiation spectrum measured by a compact spectrometer. The emissivity dependence on $\lambda$ is neglected for $\lambda_2-\lambda_1=\delta\lambda\approx2$ nm and for the spectral range $\Delta\lambda\approx50\delta\lambda$ for which the measurement results are averaged. The received mean temperature is taken as a real surface temperature for each spectrum measured at the given time. System rapidity is equal to 30 ms, the deviation from thermocouple measurements doesn’t exceed 5%.

System testing was performed under the pilot-scale production conditions. The optical elements were attached to a device of combined coaxial powder and fiber laser radiation supply mounted on the arm of a robotic manipulator.

Keywords: laser, cladding, control, spectrum, temperature.
IMPROVED TUNABLE DIODE LASER ANALYZER FOR MOISTURE MEASUREMENT IN NATURAL GAS

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The measurement of moisture in natural gas is an important parameter for the processing, storage and transportation of natural gas globally. Tunable Diode Laser Absorption Spectroscopy (TDLAS) refers to one of the methods of automatic online measurement of moisture in natural gas. The presented here new patented TDLAS measuring instrument for the concentration of water vapor in natural gas is characterized by recording analytical and reference absorption spectra in the wavelength range of 920-960 nm. The said spectral band is optimal for measuring, since only the water absorption band is observed in it. For measurements, a multi-pass analytical cell with a sample of natural gas and a reference cell with pure low-pressure water vapor are used. The measurement technique includes linking the analytical spectrum to the absolute wavelength scale, determined by the reference spectrum, and determining the water vapor concentration as a linear regression coefficient of the measured analytical absorption spectrum in the absolute wavelength scale from the calculated absorption spectrum of water vapor of a reference concentration. This non-contact technology requires minimal maintenance and provides class-leading measurement performance, stability and detection sensitivity.

Keywords: natural gas, tunable diode laser absorption spectroscopy, moisture, laser hygrometer, regression analysis.
The process of low temperature synthesis of graphene-like nanocomposites films on 3d islands of porous silicon nanocrystallites (nc-PS) is considered. It was shown that the low temperature synthesis of graphene-like nanocomposites on nc-PS is due to the excess surface energy of porous-Si nanocrystallites and, in this case, nanoscale effects that occur on local parts of the atomically rough nc-PS surface play a specifically role. The self-organization of nanoscale systems with the formation of periodically ordered structures on the real nanocrystallites surface of a porous Si is determined by quantum effects, which are caused by atomic roughness in the form of atomic steps, protrusions and determine the appearance of long-range capillary-elastic forces of surface tension. Besides long-range capillary-elastic forces, defect-deformation forces play an important role strength as well the effects of self-organization of nanoscale structures on the surface of a solid under the action of these forces are clearly manifested in the processes of their epitaxial growth. Also he boundary conditions of nanocrystallites in the ысудуешт of a porous silicon are essentially the boundary conditions of the meta-surfaces of 2DM and Q2DM materials, which can dramatically change the components of the electric and magnetic fields on both sides of the nanocrystallite lattices and the crystal matrix, which leads to a reformulation of the laws of reflection and refraction in the meta-surface are discussed. The report features of these forces and their influence on the energy of low-temperature synthesis of graphene-like nanocomposites on the surface of porous silicon nanocrystallites are considered.

**Keywords:** nanosize systems energy, nanocrystallites surface, nanocomposites, synthesis.
MODELING OF DIELECTRIC SHIELDING EFFECT BY WATER AND EXPERIMENTAL VALIDATION ON HVAC SETUP

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Significant part of electric power losses in the air associated with corona discharge on super high voltage transmission lines, especially under wet weather conditions. In this work, a computer modeling and an industrial-size test of the corona discharge mitigation effect were investigated by depositing a hydrophilic thin film on HVAC transmission lines. The tests were conducted under rain conditions. We have tested a number of aluminum wire coatings to reduce corona losses from transmission lines. Aluminum wires and bundles were coated with a porous high-temperature α-Al₂O₃ aluminum oxide reinforced with graphene oxide and carbon nanotubes additives. Industrial high-voltage tests show that the significant reduction of the power loss due to corona of 30-50% has been measured for wires with a super-hydrophilic layer. The corona ignition threshold voltage increased up to 40% for the rain weather conditions.

The first stage of the computer modeling of electrostatics using a finite element method (FEM) has shown a significant dependence of a local electric field enhancement factor (β-factor) on the surface hydrophilicity (wettability). Modeling explained a new finding that the β-factor from a micro-tip on a high-voltage line can be decreased depending on a contact angle. It was shown that highly porous and hygroscopic properties of the modified surface reduce the contact angle of water droplets on the wire, and the β-factor of a rough surface due to dielectric shielding [1, 2]. The second stage was simulation of the corona discharge processes with water vapor around the wire in a coaxial cylinder at 500 kV by using a plasma package of the COMSOL Multiphysics software. The model based on solving the equation of motion for electrons and ions, as well as the Poisson equation for the electric field, also taken into account secondary electrons arising from the ion bombardment of the cathode surface. The radial ion concentration and their average energy dependences were obtained by solving the diffusion equation for the electron drift current density.

Keywords: FEM modelling, Dielectric shielding, Anti-corona coating, coaxial cylinder, Corona discharge.
ABSTRACTS

POSTERS

PHYSICS AND MECHANICS OF FLUID IN NANOPOROUS MATERIALS
The stability of vertical flows through a horizontally extended two-dimensional region of a porous medium is considered in the case of presence of a phase transition front. The porous medium contains water and an air-steam mixture between the aquifer and the structure ceiling. The water and the humid air are separated by a phase transition interface. The low-permeability region is bounded from above by a highly permeable aquifer or reservoir bottom. The lower boundary of the low permeable area is the ceiling of the underground structure (tunnel). The underground structure is well ventilated and constant humidity of air is maintained in it. There is the surface of the phase transition inside the low-permeability region. The water comes in the porous medium from the aquifer and evaporates on the surface of phase transition. The vapor that is formed during evaporation diffuses through the porous medium into the underground construction. If a porous medium is non-wettable, then two stationary solutions with a plane phase transition front can exist. The finite perturbation can cause destabilization of the basic flow, which is stable with respect to any infinitely small harmonic perturbation. This can occur when the perturbation amplitude is substantially larger than the distance between the equilibrium levels. We find an approximate analytic expression for threshold value of the amplitude of the localized perturbation, which leads to a catastrophic restructuring of the solution. For this we obtain an approximate equation. This amplitude equation may be reduced to the form of the Kolmogorov-Petrovskii-Piskunov (KPP) equation.

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The system "nanoporous medium - non-wetting liquid" is a smart system, and damping devices can be created on its basis [Borman et al, J. Phys.: Conf. Ser. 1099, 1, 012026, 2018]. A feature of such systems is an existence of a regime of filling a nanoporous medium with a non-wetting liquid at a constant (critical) pressure [Borman et al, JETP, 108(3), 389-410, 2009]. This mode will allow controlling the maximum force transmitted to the protected object [Sun et al, Mater. & Des., 66, 545-551, 2015]. Critical constant filling pressure conditions during an impact of the system "nanoporous medium - non-wetting liquid" were studied in this work. To define parameters affecting the presence of the constant filling pressure, series of experiments were performed on an impact of systems: Fluka 100 C18 (50756-50G), Fluka 90 C18 (50757-50G), Fluka 100 C8 (60755-50G), Fluka 100 C8 (60759-50G) - distilled water.

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**Keywords:** non-wetting liquid, nanoporous medium, constant filling pressure, damping devices
The modern clinical oncology key task is to increase the efficiency of cancer chemical therapy. The main direction of provided investigations are to ensure targeted delivery of drugs to cancer cells with the minimization of the harmful effect to normal cells, as well as overcoming the multiple drug resistance of cancer cells. One of the possible solution is to use nanoporous medium filled with non-wetting liquid (drug) as a carrier. Interest to such systems is caused by two effects observed for such systems: the effect of non-wetting liquid dispersion in pores and it’s anomalously slow relaxation (outflow). It has also been shown that these effects are critically dependent on temperature. The work is present results of experimental study of the kinetics of model liquid outflow from nanoporous medium at the temperature range 20-40 °C. Results obtained for systems with different granule sizes and surface modifications.

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Keywords: non-wetting liquid, nanoporous medium, drugs delivery.
RELAXATION OF NON-WETTING LIQUID DISPERSED IN NANOPOROUS MEDIUM WITH PARTIAL FILLING

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It has now been established that when the nanoporous medium is fully filled with a non-wetting liquid and the overpressure is then decreasing to zero, the non-wetting liquid may not flows out of the pores in full or in part. It has been shown that as the observation time increasing, the non-wetting liquid does not flow out and abnormally slowly relaxes (flows out). Such behavior was described as the formation of states of strongly interacting liquid clusters in pores. The process of relaxation itself is characterized by fluctuations there energy barrier is overcoming and local metastable states are decaying with the subsequent outflow of liquid in effect of surface ejection forces. The previously proposed model described relaxation in case of a fully filled porous medium with non-wetting liquid, but was not checked in case of a partially filled porous medium. In this work we present are technic and experimental studies which are necessarily to confirm the applicability of this model. Experimental data were obtained for the system Fluka 100 C₈+C₁—water at temperature range 20 – 60 °C. Observation time was from 1 to 10000 seconds after the overpressure was reduced to zero.

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Keywords: non-wetting liquid, nanoporous medium, partial filling, relaxation of metastable states.
Nowadays, porous media models are widely used for modeling various physical and chemical processes, such as transition from one phase to another, non-Newtonian flow, flow not according to Darcy law, reaction transport, thermodynamics of oil-bearing layers. The feasibility of such modeling, i.e. the reliability of their predictions, largely depends on the quality of the correspondence between the pore space of the real environment and the pore network built as its representation.

The paper suggests a mechanistic approach based on the cherry pit model. The porous space is the space inside the spheres. Calculated algorithms and methods are presented, and it is shown that it is possible to describe qualitatively not only the hysteresis depending on the volume of the system - the applied pressure, but also relaxation curves of the remaining volume of non-wetting liquid in a porous medium from time at different temperatures.

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**Keywords:** disordered porous media, non-wetting liquid, configuration, modelling.
It is known that for the most nanoporous medium - non-wetting liquid systems is observed non-outflow phenomenon. It is shown that this phenomenon may depend on many factors, one of which is a waiting time. The observed anomalously slow relaxation (non-wetting liquid outflow) caused by formation of strongly interacting states of liquid clusters in pores. Previously was shown that relaxation of such states can occur due to relaxation of metastable local configurations of filled and empty pores. In the present work the relaxation of non-wetting liquid (water) dispersed in disordered nanoporous medium (hydrophobic silica gel Libersorb 23) is considered. The pore size distribution functions of captured liquid in the model of cylindrical pores and quasispherical pores are obtained. Some local configurations are analyzed and their lifetimes are defined.

Acknowledgements: This work was supported by the Russian Science Foundation (project no. 18-13-00398).

Keywords: non-wetting liquid, nanoporous medium, local configurations, relaxation of metastable states.
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