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**IMPORT SUBSTITUTION OF SOFTWARE FOR DIGITALIZATION
OF INDUSTRY IN THE REPUBLIC OF KAZAKHSTAN**

Abstract. The state program "Digital Kazakhstan" aims to digitalize all spheres of life and economy of Kazakhstan, leading the country to the fourth industrial revolution. In order to increase digital competitiveness on the world stage, domestic developers should pay attention to international experience, study the experience of leading companies and create their own product aimed at the economy and infrastructure of the Republic of Kazakhstan. The paper reviews foreign and domestic developments in the field of mathematical modeling of chemical and technological processes. Authors describe software complexes "SPK-01-20" and "PVC" created for mathematical modeling of nanostructured sorbents, and determining the optimal configuration of catalytic converters.

Key words: software, airtel, nanomaterials, catalytic converter, mathematical modeling, digitization.

Against the background of the situation in the world, the government of our republic pays great attention to the program "Digital Kazakhstan". The main objective of the program is digitization of all the spheres of Kazakhstan life and economy in order to take the opportunity to occupy the frontline on the world scene, as well as to enhance the quality of the public life and to establish favorable conditions for entrepreneurial development [1-2]. In the coming years it is planned to widely introduce digital technologies into business and industry, attract investments in domestic IT start-ups, commercialize scientific developments, work on import substitution of software. In order to increase digital competitiveness on the world stage, domestic developers should pay attention to international experience, study the experience of leading companies and create their own product aimed at the economy and industry of Kazakhstan.

Today such companies as Unisim, Predict, Ansys, MSC occupy the leading place in digitalization of a wide range of physical and chemical processes both in the world and in Kazakhstan.

Honeywell Predict is a real-time corrosion control system used in refining, transportation, gas refineries and refineries, in exploration and oil and gas production. More than 20 years of experience in modeling and developing solutions to problems has allowed the company to build up an extensive database, allowing for the most accurate forecasts. The value of these technologies for corrosion protection lies primarily in the financial effect. Another product by Honeywell, UniSim Design Suite provides an accurate and intuitive process modeling solution that enables engineers to create steady-state and dynamic models for plant and control design, safety studies, performance monitoring, troubleshooting, operational improvement, digital twins, business planning and asset management [3]. The software enables users to create models quickly to evaluate many scenarios. The interactive environment allows for easy 'what-if' studies and sensitivity analysis. The top candidates can be used to create high fidelity models in which additional equipment and process details are included.

ANSYS and MSC are universal multidisciplinary integrated environments for virtual product development and engineering calculations, existing, solving problems in various fields of engineering (structural strength, thermodynamics, fluid and gas mechanics, electromagnetism and many others). ANSYS exists and develop over the past 30 years currently having 200,000 business and university jobs

worldwide. With the help of MSC, the most advanced samples of aviation, automobile, space technology, high-tech devices and structures in other fields of technology are being developed.

Starting in 2015, «D.V. Sokolsky Institute of Fuel, Catalysis and Electrochemistry» JSC began its way to study the process of creating digital twins and engaged in mathematical modeling of chemical and technological processes. In 2017, within the framework of the scientific project “High-precision modeling for structure prediction and properties of functional and composite nanomaterials using parallel computing”, the first software-computing complex “PVC” was developed. The complex allows to predict the process of adsorption of solid model substances in nanopores of inorganic aerogels.

“PVC” consists of two sections: "Structure Generator" and "Chromatography and Adsorption." Due to the fact that the process of chromatography and, in particular, adsorption is an extremely long process (can take up to 48 hours per sample), these processes are modeled in “PVC” so that research could be carried out without using of reagents, expensive instruments and extra time. Through the comparative analysis of modeling methods using parallelisms of different types (coarse and fine grain), 3 models of generation of chaotic structures were selected: weakly overlapping spheres model (OSM), diffusion limited aggregation with multiple crystallization centers model (MultiRLA), diffusion limited cluster aggregation model (DLCA). Monte Carlo techniques used in these cell-automatic models effectively produce important parameters such as pore size distribution, cluster structure dimensions, and local particle concentrations in the system. In order to bring the simulation results closer to the conditions of real tests and increase the accuracy of calculations, such environmental parameters as temperature, properties of adsorbed solid substance, pressure are taken into account. The software allows to perform calculations on supercomputers using OpenMP and MPI cluster computing technologies, as well as using CUDA fine grain parallelism technology. The software module is implemented in the C# programming language and has the first edition. “PVC” can be used in higher education institutions, specialized research institutes, scientific centers of Kazakhstan, which deal with the problems of creating a new generation of sorbents, as well as the development of new porous materials with a chaotic structure for the chemical, pharmaceutical, medical, space, construction fields.

Software "SPK-01-20" was developed in 2020 within the framework of the scientific project "Modeling of processes in neutralizers of toxic gases for determining their optimal composition and design using parallel computing". It is intended for users for users who do not have special knowledge in the fields of chemistry, mathematical modeling and programming, based on the initial data (composition, temperature and gas flow rate), to quickly obtain the optimal catalyst parameters necessary for the most effective purification of toxic exhaust gases of motor vehicles, diesel generators and industrial facilities by simulating processes taking place in the catalytic converter using parallel calculations. The software complex is a modular hierarchical structure, this allows a gradual deepening in the details of the process being studied by complicating the number and hierarchy of mathematical models as the program develops, thereby gradually creating a full digital twin. The basis of numerical modeling of processes in the neutralizer is the approach based on the theory of cell automata on Boltzmann lattices. This method has proven itself in the simulation of dynamic processes, it is easily to parallelize. Modeling the dynamics of the gas flow passing through the catalytic converters allows to obtain the resistance of the catalytic units and choose the correct geometry to avoid pipe rupture. Data processing module of experimental research results is a constantly replenishing virtual MySQL database storing data on results of aerodynamic as well as physical and chemical tests of catalytic converters. The reference to the experimental database accelerates the modeling process, allows to carry out comparative analysis of calculated and experimental data, thus guaranteeing adequacy of the mathematical model used in the “SPK-01-20”. The software complex is implemented in the programming language C#, the results visualization module is built in the Unity development environment. In the perspective of further development of the software complex it is planned to create a chemistry module. This module will allow to investigate the process of neutralizing gases of various compositions, as well as determine the degree of purification for a particular catalyst configuration. Rapid and automatic selection of the catalyst composition will allow to establish the production of catalytic converters for many types of toxic exhaust gas sources. Currently, "SPK-01-20" is successfully used in the catalytic converter manufacturing workshop at the institute.

Created software is oriented for a wide range of scientific problems, it is based on adequate mathematical models, has high performance, provides high accuracy and representativeness of the

estimated parameters and meets the basic requirements for such products in order to be competitive in the domestic software market.

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ҚАЗАҚСТАН РЕСПУБЛИКАСЫНДА ӨНЕРКӘСІПТІ ЦИФРЛАНДЫРУ ҮШІН БАҒДАРЛАМАЛЫҚ ҚАМТАМАСЫЗ ЕТЕТІН ИМПОРТ АЛМАСТЫРУ

Аннотация. Қазіргі әлем төртінші өнеркәсіптік революцияның – алдыңғы қатарлы технологиялар экономиканың тұтас саласын түбегейлі өзгертетін инновациялар дәуірінің табылдырығында тұр және барлығы жылдам қарқынмен жүріп жатыр. Кәсіпорынның цифрлық трансформациясы нәтижесінде болашақ бұйымның, өндірістік желінің немесе жалпы кәсіпорынның цифрлық қосындыларын – виртуалды модельдерін қолдана бастайды. «Цифрлық Қазақстан» мемлекеттік бағдарламасы елімізді төртінші өнеркәсіптік революцияға жетелей отырып, Қазақстан өмірі мен экономикасының барлық салаларын цифрландыруды мақсат етеді. Әлемдік аренадағы цифрлық бәсекеге қабілеттілікті арттыру мақсатында отандық әзірлеушілердің халықаралық тәжірибеге назар аударуы, жетекші компаниялардың тәжірибесін зерделеуі және Қазақстан Республикасының экономикасы мен инфрақұрылымына бағытталған өнімін жасауы тиіс. Жұмыста химия-технологиялық үдерістерді математикалық модельдеу саласындағы шетелдік және отандық әзірлемелерге шолу жүргізіледі. «ПВК» бағдарламалық-есептеу кешені бейорганикалық аэрогельдер нанопорында қатты модельді заттардың адсорбция үдерісін болжауға мүмкіндік береді. «СПК-01-20» мамандандырылған бағдарламалық кешені бастапқы деректердің негізінде (газ ағынының құрамы, температурасы және жылдамдығы) автокөлік құралдарының, дизель генераторлардың және өнеркәсіптік объектілердің ұйғты пайдаланылған газдарын параллель есептеуді қолдана отырып, бейтараптандырғышта өтетін үдерістерді модельдеу жолымен тиімді тазарту үшін қажетті бейтараптандырғыштың онтайлы параметрлерін жедел алуға мүмкіндік береді.

Түйін сөздер: бағдарламалық қамтамасыз ету, аэрогель, наноматериалдар, каталитикалық бейтараптандырғыш, математикалық модельдеу, цифрландыру.

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ИМПОРТОЗАМЕЩЕНИЕ ПРОГРАММНОГО ОБЕСПЕЧЕНИЯ ДЛЯ ЦИФРОВИЗАЦИИ ПРОМЫШЛЕННОСТИ В РЕСПУБЛИКЕ КАЗАХСТАН

Аннотация. Современный мир находится на пороге четвертой промышленной революции – эпохи инноваций, когда передовые технологии радикально меняют целые отрасли экономики, и все происходит довольно быстрыми темпами. В результате цифровой трансформации предприятия начинают применять цифровые двойники – виртуальные модели будущего изделия, производственной линии или предприятия в целом. Государственная программа «Цифровой Казахстан» ставит своей целью цифровизацию всех сфер жизни и экономики Казахстана, ведя страну к четвертой промышленной революции. С целью повышения цифровой конкурентоспособности на мировой арене отечественным разработчикам следует обращать внимание на международный опыт, изучать опыт лидирующих компаний и создавать собственный продукт, нацеленный на экономику и инфраструктуру Республики Казахстан. В работе проводится обзор зарубежных и отечественных разработок в области математического моделирования химико-технологических процессов. Программно-вычислительный комплекс «ПВК» позволяет предсказывать процесс адсорбции твердых модельных веществ в нанопорах неорганических аэрогелей. Специализированный программный комплекс «СПК-01-20» на основе из исходных данных (состав, температура и скорость потока газа) позволяет оперативно получать оптимальные параметры нейтрализатора, необходимые для наиболее эффективной очистки токсичных выхлопных газов автотранспортных средств, дизель генераторов и промышленных

объектов путем моделирования процессов, проходящих в нейтрализаторе с применением параллельных вычислений.

Ключевые слова: программное обеспечение, аэрогель, наноматериалы, каталитический нейтрализатор, математическое моделирование, цифровизация.

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