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State of the art and research development prospects of energy and resource-efficient environmentally safe chemical process systems engineering

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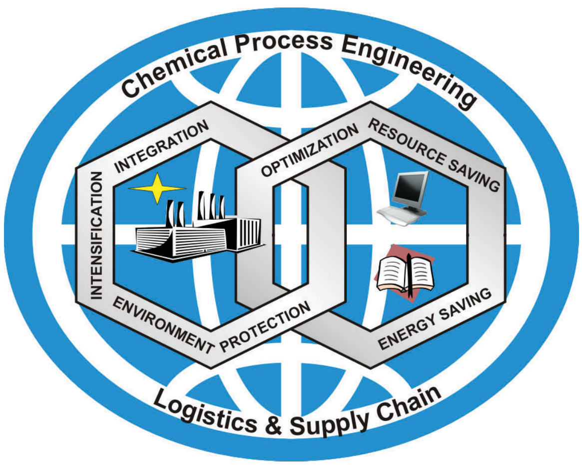
In this focus overview, the main types and directions of engineering, methods and techniques of intensification of chemical process systems (CPS) and process optimization of energy- and resource-efficient processes for the representative production of titanium compounds, mining waste processing systems, electrochemical coating technologies, combined technologies for the treatment of industrial effluents and energy-and resource-efficient technologies for cleaning soils from petroleum and chemical pollution products are reviewed. The following issues have been discussed: methods of complex assessment of production energy efficiency and software and information support for automated synthesis of optimal energy-efficient regenerative heat exchange systems using pinch analysis; methods and algorithms for fractal-statistical characteristics analysis of nonstationary gas flows in complex gas pipelines; methods of ecological and economic optimization of production, infrastructure supply chains; methods for assessing and preventing the dangerous environmental impact assessment of chemical pollution; organization and logistics management of business processes engineering for improving the energy efficiency of plants; engineering of problem-oriented computer systems, heuristic-computational models and algorithms for intelligent integrated logistics support of the equipment life cycle; engineering developments in the field of digital transformation of energy-efficient CPS and technological production systems; application of methods for optimizing reliability factors optimization, digitalized risk and safety management in the engineering of energy- and resource-efficient CPS.



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Introduction

The term ‘Chemical Engineering’ was introduced by British chemist, Professor George E. Davis (Manchester University, UK) in 1887.[1,2]

The modern general concept of engineering, including chemical technology, can be defined as follows. Engineering is a complex technical, computational, graphic, organizational, economic and consulting activities, that implements the accomplishment of the wide spectrum of intellectual operations in such areas as: research, design, calculating, analysis, management and economic, at all stages of the life cycle (pre-project research, feasibility study; business planning; design management; development of technical and operational projects; construction and commissioning; operation and maintenance management) of any industrial systems, including technical and socio-economic systems.[3–5]

The most important tasks of the petroleum and gas chemical industry (PGCI), being the complex CPS, are intensification of chemical and technological systems and reconstruction of existing plants, as well as designing and commissioning of environmentally safe energy-saving plants, in the shortest possible time. The successful solution of these tasks became possible due to widespread use of computers, methods of cybernetics, computer science and mathematical modeling of technogenic systems. It was also facilitated by the rapid development of the new scientific discipline in the field of theoretical foundations of chemical technology – ‘Process Systems Engineering’ (PSE) or ‘Process Engineering’ (PE), first formulated by Robert H. Sargent in the late 1960s and early 1970s.[3,4] The objects of research of ‘Chemical Process Engineering’ are ‘Chemical Process’, ‘Process System’, ‘Process’, ‘Chemical Processing Systems’, ‘Processing System’, ‘Chemical Plants’.

It was proclaimed by the UN General Assembly in 2000, that for the successful implementation of economic, social, and environmental goals of sustainable development (SDGs), the advanced and developing countries shall pursue scientifically based engineering methods, industrial implementation and operation management of digitalized energy- and resource-efficient environmentally safe manufacturing facilities and enterprises in the chemical industry, PGCI and in the chemical-metallurgical sector. All these fields represent the complex CPS.[3] Highly intensive unit operations (UO) and energy resources efficient and environmentally safe CPS ensure the following: the sustainable natural resources management; protection of the environment from pollution; preservation of the biological diversity of natural systems; socio-cultural harmonization of society; increasing the economic efficiency of production, industrial enterprises and supply chains (SC); improving the quality and life expectancy of people.

These achievements comply with the sustainable development goals under the conditions of the industrial revolution ‘Industry 4.0’ and the development strategy of society ‘Society 5.0’.

1. The basic types and branches of engineering in the digital economy

The entity, main types, methods and computer tools of the engineering of technological structure, technological and business processes of energy- and resource-efficient CPS, as well as facilities and supply chains of competitive PGCI products (substances and materials) are covered in the review.[5] The description of the compliance of CPS properties and quality indicators of manufactured products with the requirements of the National and International standards, as well as with the indexes

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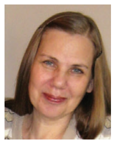

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of the Best Available Techniques Reference Documents (BAT-BREFs) are given.

The concept of engineering is closely interrelated with the concept of logistics. Logistics in a global sense represents an interdisciplinary science that studies the methods of 'detailed planning of any complex research and engineering operation'. As an applied science, logistics studies methods of managing not only the material flows of various industrial products, goods and services in the supply chains, but also the intellectual flows of various knowledge, skills and abilities, which are the most important intellectual products of the modern digital economy and the knowledge economy.[5–8]

At present, the basic types of engineering are distinguished as follows: functional and production, comprehensive technical, civil, operational, international and computerized.[5]

Types of functional and production engineering differentiated by economy branches and sectors of the economy, as well as by branches of technology:[5] system engineering, chemical engineering, process system engineering (PSE), power engineering, heat engineering, mechanical engineering, logistics engineering, knowledge engineering.

Computer-aided engineering performs multidisciplinary, multiscale (multilevel) and multi-stage developments and research of projects. Such developments and research ensure the automated execution of all types of engineering and technical works for the creation of technical systems and industrial facilities. They rely on the extensive use of computer technology tools and equipment, as well as the high-tech information and communication technologies (ICT), including instrumental complexes of technical and software tools: computer-aided design (CAD) and computer-aided logistics support (CALS) technologies. Upgrading these tools allowed one to expand significantly the range of functions covered by them.

Now the abbreviation CALS stands for continuous acquisition (information) and life-cycle support.

2. Technique and methods of intensification of chemical and technological systems in the engineering of energy- and resource-efficient industrial facilities

The National Standards of Russia and the International Organization for Standardization (ISO) in the field of resource and energy conservation, energy and environmental management, as well as the stipulations of legal acts regarding the BAT-BREFs, established the technical requirements and specifications, engineering guidelines and characteristics of high-tech production systems, technical devices, business processes, products and services. It is necessary to follow the provisions of these documents in order to ensure high energy efficiency, reliability and environmental safety in the engineering of various CPS for the production of competitive high-quality chemical products.[5]

Methods and algorithms of the theory of analysis, optimization and synthesis of CPS as well as methods of logistics, resource conservation and optimal organizational and functional design of energy- and resource-efficient SC shall be widely used to obtain scientifically sound engineering results of optimal energy-efficient and highly reliable CPS and CS PGCI.[5–7]

Technique and methods of UO and CPS intensification are considered as the important part of CPS engineering, and their promotion can make a substantial contribution to ensuring the steady development of the chemical industry.[8,9]

The main driving forces of CPS intensification for the innovative development of the chemical industry are described.[6,7,10] They include the following: improving the quality and efficiency of raw materials usage, reducing capital costs, miniaturization of unit equipment (UE) and reducing safety risks.

In industry, raw material costs may constitute up to 70–80% of total production cost. Consequently, any cost savings on raw materials, for example, because of higher efficiency of CPS of raw materials preparation, can result in the large economic effect. Resource and energy saving together with simultaneous reduction of carbon dioxide emissions is also an important factor of decreasing the cost of chemical products and reducing the dangerous environmental impact of chemical pollutants PGCI.[8] Thus, chemical industry in the European Union (EU) has reduced its power consumption per ton of product by 25%.

The study, conducted by the European Federal Union for the Chemical Industry (CEFIC) among 10 000 Europeans, revealed that the social acceptability of the chemical industry is only 48%, mainly due to its hypothetical low safety.[11] In fact, the chemical industry is very safe. The number of victims and injuries per million man-hours is very small, but it matters for public perception. The situation can be improved by the use of chemicals with a lower perceived risk, in accordance with REACH (Registration, Evaluation, Authorization and Restriction of Chemicals) Regulation (EC), as well as the use of highly reliable miniature UES to ensure safety.[12]

Techniques and methods for UO and CPS processes intensifying (PI) in chemical engineering are documented.[13,14] PI often includes an approach of combining individual operations (such as chemorectification, chemoextraction, chemosorption, *etc*., including both reaction and separation) into one UE. This combining leads to a more resource- and energy- efficient, environmentally friendly, and cost-saving manufacturing process.[8]

In the context of globalization and the transition to sustainable development, four main theoretical and experimental directions of chemical engineering can be distinguished. They are the following: increasing productivity and selectivity owing to the intensification of technological operations and a systematic multilevel approach to CPS management (for example, nanostructure or microstructure of catalysts); engineering of new miniature combined EOS, based on scientific principles and new production methods; process intensification of CPS when using multifunctional combined reactors and highly efficient catalysts; CPS engineering using the triple engineering methodology 'Product Engineering – Process Engineering – Plant Engineering' (for short, the 3P-3E) to obtain the needed final high-quality product; application of multiscale computer modeling methods in any Unit operations and phenomena, as well as live situations from the molecular, micro- or macrolevel to the production scale.

Digitalization is a modern direction of fundamental improvement of resource and energy efficiency and environmental safety of PGCI production facilities, enterprises and supply chains in the frames of 'Industry 4.0', 'Society 5.0' and the digital economy. Companies accept digitalization as a tool for transforming their business processes, for stimulating the development of innovations and for reengineering of business and technological processes.

PI promises new ways of solving the current problems related to the increasing of energy efficiency in the chemical industry, that leads to a rapid increase in interest in this field of research. There are various approaches to the synthesis of intensive CPS, most of them are based on the methods of the theory of synthesis and optimization of CPS.[3,4,8,15] The present analytical review will summarize these methods and present their applications for CPS intensification, it will also overview and compare approaches to CPS modernization by using PI methods and criteria for evaluating PI options.

The methods of designing and modeling integrated UOS in the production of biodiesel from food waste have been proposed.[14]

3. Physicochemical engineering of energy- and resource-efficient chemical-technological process for the production of titanium compounds

The problem of development of Russian titanium ore deposits is the main obstacle to the sustainable development of the titanium industry. Russia, which takes the third place in the world in terms of proven reserves of titanium, unfortunately, does not develop any previously discovered deposits. The world's largest titanium producer, PJSC VSMPO-AVISMA, fully buys ilmenite concentrates and titanium slag in the Ukraine, the Norway and other countries.

The only way to solve the problem of import substitution for titanium products is the development of the Yarega oil and titanium field, which is the largest in Russia. More than half of the national titanium reserves are located in the depths of the Yarega. The mine produces high-viscosity oil, while the titanium component of the ore, quartz–leucoxene concentrate, is a waste product of high-viscosity oil production and, regrettably, it is not used. The reason for the lack of demand for Russian titanium ore is its unique mineral composition, characterized by an increased content of quartz.

Russian scientists have conducted scientific research to find the new ways of titanium ore processing. It was shown,[16] that quartz–leucoxene concentrate has the lowest reactivity during chlorination in comparison with other types of titanium raw materials. However, even a slight decrease in the silica content in the raw material, which can be achieved by pretreatment of the concentrate with an alkali solution, significantly increases the activity of concentrate in the CPS of its further processing into $TiCl_4$.[17] An original kinetic model of UO leaching has been developed,[18] and the technological parameters of UO for obtaining a high-quality concentrate of a given composition have been determined.[19] Further study[20] established the optimal technological parameters for the synthesis of $TiCl_4$, a new energy- and resource-efficient CP chlorination of Yarega concentrates in fluidized bed reactors. The end product is suitable for getting both high-quality titanium sponge and pigmented titanium dioxide.

The obtained results[19,20] demonstrate that Yarega concentrates should become the main source of titanium raw materials in Russia. This would allow for not only full coverage of the needs for titanium raw materials, but also significantly increase the profitability of production of high-viscosity oil.

4. Scientific foundations of digitalized engineering of energy- and resource-efficient environmentally safe chemical energy process systems (CEPS) of mining waste processing

The depletion of mineral resources and environmental problems of storage of technogenic waste of ore dressing of mining plants make it necessary to create combined energy- and resource-efficient technologies for waste processing and disposal. These complex systems, CEPS, shall include the multichamber conveyor type roasting machines, sintering machines and ore-thermal furnaces. General techniques[21,22] and various methods[23] of complex processing of technogenic waste and increasing the energy and resource efficiency of complex chemical thermal power plants in chemical-metallurgical and mining and processing complex (M&PC) have been described.

The authors[24,25] have been considering the processes only in one layer of pellets and/or in separate technological zones of CEPS. Theoretically and experimentally determined parameters of the kinetics of sintering processes and the values of the parameters, characterizing the shrinkage of the sintered charge layer, were presented.[26] The coefficients of energy exchange in the zone of pellet drying were studied; the criteria equations of heat and mass transfer processes were obtained.[26] Mathematical model of sintering kinetics of an agglomeration charge was proposed.[27] This model takes into account the shrinkage of the layer and the change in pressure losses in the technological zones of melting and formation of the final agglomerate, and it correlates well with experimental data. A multifactorial relationship between chemical and metallurgical processes and the conditions of heat and mass exchange (transfer) in the sintered layer of the agglomeration charge was identified. The adequacy of the mathematical model allows us to use it for the analysis of highly efficient modes of agglomerate production.

Increasing energy and resource saving during drying of dispersed material in a dense layer is a crucial problem. A multiscale mathematical model of heat and mass transfer in a moving dense layer of pellets, with a cross flow of a heat carrier gas, has been developed, and its adequacy has been proved.[28] This solution allows for optimization of energy consumption basing on the intensification of the drying process of layers, through the formation of a damped heat wave, propagating deep into the dense layer of pellets.

Multiscale mathematical and computer models of a multistage chemical and energo-technological process of pellets firing have been developed.[29] The process includes the reaction of carbonates dissociation and the sintering process of a moving dense multilayer mass of phosphorite pellets in a complex CEPS, corresponding to a conveyor firing machine – roller kiln (Figure 1). The conformity of the proposed mathematical model was verified. Computational experiments were carried out to determine the operating parameters of firing of the primary phosphate raw material with various physicochemical characteristics and the external flow of the coolant gas.

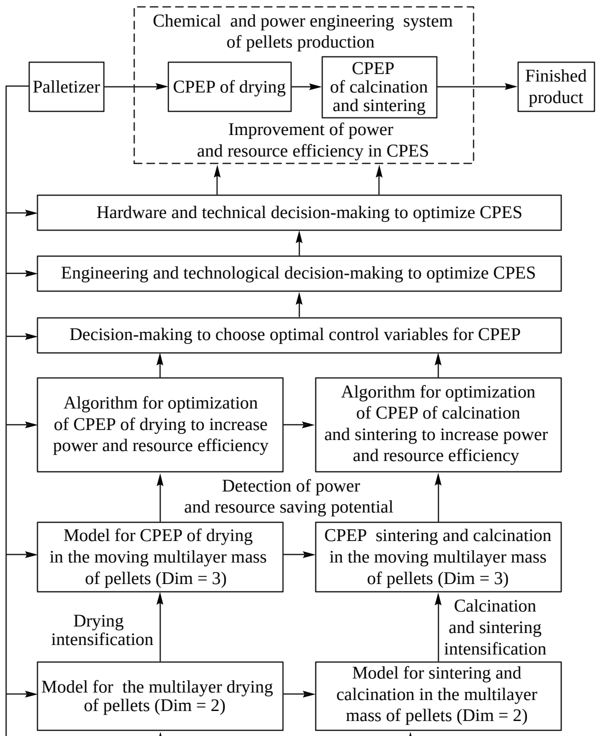

Figure 1 Flow block diagram of the algorithm for multiscale modeling and multilevel optimization of the CEPS of pellet production. CPES – chemical and power engineering system, CPEP – chemical and power engineering process.

Proposed and studied are mathematical models that encompass the following parameters: the intensity of the internal moisture transfer process inside the pellet; the processes of waterlogging of individual horizons in a heated multilayer moving mass of pellets; various physical and chemical characteristics of technogenic raw materials and the external flow of heat carrier gas.[30]

The concepts of engineering of energy- and resource-efficient, environmentally safe CEPS of extracted raw materials waste processing at M&PC are proposed.[31] This allows one to solve the problems of recycling and converting waste into competitive products with high added value and to reduce the negative impact on the environment.

A substantial engineering and technological formulation of the problem of engineering a multistage CEPS for the production of phosphorite pellets from technogenic waste of apatite-nepheline ores of M&PC is presented.[32] Generalized multiscale mathematical model of CEPS for phosphorus production, applying the notation of the international standard for function modeling IDEF0, is developed.

An original hybrid fuzzy differential-production model of the dynamic drying process of a multilayer granulated pellet as a dispersed spherical body was proposed.[33] The model represents the velocity of the localized evaporation front within the pellet being dried. It is characterized by the following features: using a system of differential equations of thermal conductivity and drying rate with fuzzy parameters representing the interval values of the thermophysical properties of dispersed pellet particles; computational operations for reducing the accumulation of the errors of the applied finite-difference methods; replacing the approximating multidimensional finite-difference system of equations with a set of special fuzzy production rules describing the complex dependence of the velocity of the localized evaporation front on the fuzzy thermophysical and heat-and-mass transfer parameters of the drying process.

The analysis of the chemical and metallurgical processes of iron ore raw material pelletizing is carried out, the CEPS of raw materials sintering in steel industry and mathematical models for their description are considered.[34]

An original high-speed computational heuristic algorithm for optimizing the energy and resource efficiency of a local multistage drying process of a moving mass of phosphorite pellets is proposed.[35]

Complex processes, which are used in practice in the heat treatment of raw materials in HTS, such as: drying, coke combustion, phosphorite decarbonization, melting of charge particles, the appearance of sinter, condensation of moisture vapors in the lower layers, have been studied.[36] All these processes are thermally activated and occur in phosphate raw materials during agglomeration.

The developed[37] mathematical model, which simulates the thermal conditions in an electrothermal reactor, allows one to track visually the main characteristics of the process. The model takes into account the interrelation of thermophysical (thermalphysic) processes in zones with different phase composition and makes it possible to get an idea of the reaction of the object to various kinds of disturbances, such as changes in the charge composition, the dosage of the reducing agent, and the voltage at the electrodes. The mathematical model of the reactor in the approximation of concentrated parameters represents a specific system of nonlinear ordinary differential equations. The system is supplemented with phase transition conditions for zones of different phase states. Special feature of the model is accounting the energy exchange in the charge zone, which makes it possible to track the temperatures under the dome-shaped roof of the ore-smelting furnace. This is very important for maintaining the mode in closed furnaces having the roof, which cannot withstand high temperatures. Besides, the processes in the reactor volume with different phase composition as a whole were considered by means of the correlations accounting the phase transition. The model of a flow reactor was modified in relation to the specificity of these types of chemical and energy-technological redox processes. The model allows one to calculate temperature evolution in different zones of the reactor and track the changes of the structure of zones with different phase composition over time.

5. Physicochemical engineering of electrochemical coating technologies, combined technologies for industrial effluents processing and energy- and resource-efficient technologies for soils purification from petroleum pollutants

The use of a systematic approach made it possible to estimate the scale and internal structure of electroplating production in Russia[38] and abroad.[39] The system analysis of the efficiency and competitiveness of chrome plating technologies was carried out,[40] and a new, modified nonparametric – statistical version of SWOT (‘Strength, Weakness, Opportunities, Treats’) analysis[40] was proposed to compare the effectiveness of two different technologies or enterprises.

As it was stated,[38] there are tens of millions of tons of nonferrous metals involved in technological productions. That is why, the implementation of scientific and technological principles of increasing the efficiency of electroplating plants considering the environmental risks is very important. In order to reduce the environmental impact (EI), new combined resource- and energy-efficient technologies of applying conversion coatings not containing the toxic chromium(VI) compounds have been developed.[41,42]

Taking into consideration the intricate chemistry of chromium compounds,[43,44] complexation reactions, and the kinetics of electrochemical processes,[45] diverse physicochemical[46,47] and mathematical[48] models for selecting the components of resource-saving compositions of technological solutions used to apply protective and functional coatings on various products with chromium and alloys, are proposed.

Comparative analysis of changes in resource-saving indexes [concentrations of metal ions (c) and the total concentration of all components (Σc)] of technological solutions employed in the processes of electrodeposition of coatings has been carried out.[49,50] Quantitative concentration criteria for classifying rational compositions of solutions according to resource-saving indexes ($c < 0.71$ mol dm^{-3}; $\Sigma c < 2.32$ mol equiv. dm^{-3}) and resource intensity ($c > 0.96$ mol dm^{-3}; $\Sigma c > 2.78$ mol equiv. dm^{-3}) are determined. The obtained theoretical and experimental results formed the basis of original infological model of creating a database (DB) for selecting the resource-saving compositions of solutions that allow one to get the protective and functional coatings with specified characteristics. Scientific and technological foundations of physicochemical engineering and improvement of resource efficiency factors of electroflotation of industrial waste waters and extraction of valuable components from them have been developed.[51,52]

A novel logical data model of energy- and resource-saving chemical technology for the recycling of sulfurous components from fuel residues (fuel oil) was proposed.[53] Integration of the processes of electrochemical and microwave synthesis into a combined ‘green’ CPS allows one to obtain useful biologically active organic sulfur compounds. It is shown, that organic disulfides and elemental sulfur can be synthesized using the single-electron oxidizer of thiols and hydrogen sulfide in organic media during waste water cleaning. In comparison with the direct electrochemical process of sulfurous components oxidation, electrosynthesis using the mediators can provide the engineering of high efficiency and low energy consumption cyclic CTP.

The physicochemical and technological foundations of engineering of an energy-efficient electrochemical process of clearing soil of oil and petroleum products have been developed. The main regularities of the chemical unit (CU) operation are determined experimentally and theoretically, options of engineering and hardware design are proposed, and changes in the properties of contaminated soil are analyzed.[54]

A highly efficient electrochemical technology for the disposal of solutions formed during the production of calcium carbonate is proposed. The use of membrane electrolyzers allows one to obtain calcium hydroxide, sodium hydroxide, and hydrochloric acid of required quality.[55] It is shown that electrodialysis systems are also important for the engineering of complex wastewater treatment plants.[56,57]

6. Methods of complex assessment of the energy efficiency of PGCI production facilities; software and information support for the computer-aided synthesis of optimal energy-efficient regenerative heat exchange systems using pinch analysis

Processes integration methods, in particular, thermal integration and pinch analysis approaches, which make up the basis of the pinch methodology, are widely used to increase the energy and resource efficiency of CPS.[58,59] Much more resources and money in the world are being spent on improving the operation and modernization of existing production facilities than on development and construction of new ones. However, powerful tools created for the synthesis of optimal CPS, in some cases, cannot be directly applied for development CPS modernization projects.[60] The task and methods of complex assessment of the energy efficiency of PGCI facilities by means of the method of pinch analysis are described.[58,59]

An assembly equipped by the thermal energy recovery system with a set value of the driving force for vertical heat transfer processes, has been accepted for CPS as an energy efficiency standard. The best available heat transfer technologies shall ensure the values of the composite thermal curves of the initial CPS and the minimum temperature difference of the coolant in the heat exchange equipment. Additionally, the energy efficiency index is calculated under condition of the exclusion of heat losses in EI. For this purpose, a simplified method for estimating heat losses from the heated surfaces of oil refining equipment has been developed.[61] A comparative analysis of energy efficiency of various PGCI plants has been carried out, based on a complex Anselm assessment.

An important stage in evaluation of the energy efficiency of CPS and the synthesis of optimal energy- and resources-efficient regenerative heat exchange system (HES) is the initial data collecting and processing.[59,60] The development of Anselm special software allowed for automation of the process of collecting and processing a large array of initial data.

Approaches for optimal integration of heat in HES were developed.[62] Their application at diesel fuel hydrotreating plants made it possible to reduce the energy consumption by 50%.[63] Methods of heat and power integration between the workshops within vast industrial PGCI sites (total site integration) were described.[64]

7. Methods and algorithms for analysis of the fractal-statistical characteristics of nonstationary gas flows in complex PGCI gas pipelines by means of integral hydrodynamic statistical entropy values

Turbulent gas flows formed in the complex gas pipelines (CGP) during the propagation of high-pressure impulses have oscillatory shock effects on the walls of gas pipelines. It constitutes a dangerous mechanical phenomenon, particularly, when frequency resonances arise between the fluctuations of gas flows and the natural frequency of mechanical vibrations of the gas pipeline structure. These important hydromechanical processes in CGP were studied in detail by the scientific school of Academician of RAS V. P. Meshalkin.[65–68] The problems that play an important role for analyzing and predicting the impact of turbulent pulsations of gas flows onto the walls of CGP should include the task of developing special integral hydrodynamic indices that best characterize the oscillatory shock effect of gas flows on the walls of CGP.

Four classes of integral hydrodynamic statistical entropy values: hydrodynamic, statistical, fractal and potential, are introduced.[65] It is proposed to use fractal dimensions as the main fractal indicators. Effective integral factors based on the Ising and Coulomb potentials[67,69] are also given.

The fractal character of nonstationary turbulent gas flows in CGP is clearly revealed on the wavelet spectra of continuous wavelet transformations of gas flow images. It was shown,[65,66] that there are many similar hydrodynamic components in the wavelet spectra of model gas flows during the pressure pulse propagation in a constrictor (confuser), as an important node in the CGP structure. This indicates the presence of a hierarchical structure and fractal nature of gas flows.[70]

The results of a large number of computational experiments obtained for various photographic images by means of the theory of random fields allowed the authors to propose the method and algorithm for textures generating, based on the nature-inspired algorithms (NIA).[71]

The issues of texture modeling, accounting the influence of genuine physicochemical processes on the formation of textures, are considered in detail in the monograph[72] devoted to the problem of image texture. The work reveals that *binary clusters* are important for assessing the effect of gas flow pulsations on CGP vibration.

Currently, visualization of the texture of gas flows in CGP is a promising field of gas dynamics research. Microphotographic images were obtained by fractal and wavelet analyses and analyzed by spectral methods developed for the study of nanomaterials structure,[73–75] that allowed for predicting the development of high-frequency unsteady turbulence during the propagation of high-pressure pulses in complex gas pipelines.

Thus, it can be concluded that visualization methods are effective digitized tools for studying the turbulent structure of gas flows in CGP. The review[76] presents the latest findings of gas flow analysis conducted by the visualization methods: solving the inverse problem of heat sources in computer models of gas dynamics;[77] problem of 2D modeling of gas flows in unstructured computational grids;[78] modeling of gas flows adjacent to a free surface;[79] computer simulation of advection and convection in gas flows with use of the hydrodynamic model of large vortices.[80]

8. Methods of ecological and economic optimization of production and supply chains of PGSI facilities

The problem of ecological-economic and organizational-structural optimization of PGSI supply chains is mathematically formulated as a problem of mix integer linear programming (MILP) considering the mode of multiperiod functioning of SC (by means of Oracle SNO software package). As a result, the economic feasibility of the construction of the new plant, which processes the wide fraction of light hydrocarbons, in the SC of gas raw materials sector has been justified.

The necessity of finding solutions for the environmental protection (EP) problem and ensuring the environmental safety of CPS has recently generated the rapid growth of publications on the ‘green’ supply chains of PGCI, which include the natural gas (NG) production, its transportation, distribution, and processing into products with high added value.[81]

One of the first articles[82] regarding mathematical modeling and optimization of the organization of functional SC of natural gas using MILP methods dates back to the late 1960s. Thereafter, a number of algorithms have been proposed to accomplish more challenging tasks of SC and CGP optimization, for example: the algorithm of sequential quadratic programming,[83] the method of decomposition[84,85] and piecewise linear linearization in combination with the method of linear programming,[86] the Lagrange algorithm,[87] the method of integer linear programming (ILP).[88] The general mathematical model of gas supply systems has been presented.[89] The algorithm has been introduced and considered[90] for the entire SC of natural gas. The computer model of a nonstationary gas flow in the multilayer insulated, the longest subsea high-pressure gas pipeline has been developed.[91,92]

Optimization methods under conditions of data uncertainty for the PGCI facility operation stage,[93] and the use of the nonlinear programming method for CGP designing[94] were presented. Nonlinear mathematical models,[95] using the algorithm of global extremum search for nonlinear and mix integer nonlinear programming (MINLP)[96] tasks, have been applied for solving the nonconvex optimization problem for distribution CGP. An algorithm for optimal control of CGP under steady and non-steady conditions was described.[97]

The need of accounting for the impact factors on EI has led to the development of new methods of ecological and economic optimization of the conventional CGP optimization problem. Certain fundamental concepts of optimization are proposed,[98,99] and an extensive analytical review on this subject is presented.[100] Specific features of SC in PGCI are described,[101–103] while authors[104] propose to account the life cycle (LC) assessment when describing a complex model of the PGCI supply chain. The statement and methods of solving the optimization problem of ‘green’ SC in PGCI are given.[81] The unique algorithm has been proposed for optimizing the ‘green’ SC of biogas production from farm waste.[105]

Thus, it is necessary to use stochastic programming together with multiple-criteria optimization methods when developing a complex mathematical model for optimizing the structure and multiple-criteria planning of natural gas production for PGCI facilities, taking into consideration the market and environmental factors.

It is established that greenhouse gas emissions have significant impact on global warming. Therefore, for the solution of general problem of SC optimization it is necessary to incorporate the methane leaks data into the general mathematical model of natural gas SC.[106,107] As far as we are aware, this is the first mathematical model allowing one to solve these two interrelated problems in complex, when optimizing the structure and modes of functioning of CGP.

9. Methods for assessment and prevention of the dangerous environmental impact of chemical pollutions of PGCI facilities

One of the organizational tools for implementation of the UN Sustainable Development Goals (SDGs)[108] at PGCI facilities is a world public voluntary program ‘Responsible Care®’[109] [hereinafter (RC)], aimed at encouraging enterprises to apply voluntarily various initiatives and business principles in order to minimize the negative impact on the environment and people.[110] The main instrument to monitor the implementation of the RC program by the facility are key performance indicators (KPI). The gaps in the collected large amount of data make it difficult to evaluate the enterprise efficacy.[111] Unfortunately, a direct comparison of the actual KPI does not provide a reliable estimation of the effectiveness of RC program implementation. Therefore, the research team of Academician V. P. Meshalkin applied the systematic approach[112] to develop a novel algorithm for analyzing large arrays of irregular environmental KPI for companies. Additionally, a complex of digital tools of assessing economic damage based on the data collected during the implementation of the RC program has been proposed.[113]

Methods of system analysis using the digital tools of multivariant visualization were applied to evaluate the compliance of CPS (taking the complex physicochemical processes of chemical immobilization of mercury in waste material as an example) with the SDG indicators and the principles of ‘green’ chemistry.[114] Processes of mercury immobilization are of particular interest because of the attribution of mercury to priority global environment pollutants.[115] The system analysis of the results of multifactor simulation experiments reveals the following: at the initial mercury content in the waste of about 10 wt%, chemical immobilization of metallic mercury (over 95 wt%) in the reaction with elemental sulfur for 90 min results in producing solid, slightly soluble HgS; stable result of mercury immobilization under normal conditions is achieved for the reaction carried out with a sulfur excess of 3 g per 1 g of mercury in a vibration mill; the presence of water (no more than 50 wt% of the total reaction mass) is proven to have a positive effect on the process of immobilization.

One of the hazardous sources of hydrocarbon pollution of subsoil are accidents on oil pipelines, leaks from underground or buried reservoirs and pipelines, unloading and loading operations on oil loading stations, *etc*., which lead to the appearance of technogenic deposits and abnormal geochemical zones.

Various microbiological conditions of polluted soils, lands, and water environments determine the orientation of multistage reactions of transformation of hydrocarbons[116] and complicate the process of identifying the corresponding geochemical anomalies and sources of their formation.

A geochemical modeling approach, based on a universal automated network of observation and injection wells with forced circulation of a suspended mixture of microorganisms, was used to identify and eliminate subsurface oil pollution.[117] The total microbiological activity of the soil, characterized by a gradient in the zone of hydrocarbon pollution distribution, was chosen as a quantitative bioindicator.

The results of multiple-factor geochemical modeling using field experiment data allowed one not only to develop a comprehensive system of knowledge about the nature of the distribution of hydrocarbon pollution of the subsurface, but also to make long-term forecasts and adjust the measures of identification and elimination of this pollution. Biocomposite material is formed by a polymer matrix and a reinforcement (inclusions) of biogenic elements and immobilized strains has been described.[118] These biological inclusions were isolated from contaminated petroleum products. The high activity of the created biocomposite compounds in the processes of cleaning the sea surface from hydrocarbons is shown.

10. Organization and logistics management of business process engineering for improvement of the energy and resource efficiency of PGCI facilities

The main tools of logistics management of engineering of energy- and resource-efficient CPS are functional modeling, computer modeling, which includes a statistical analysis of dynamic series, the method of principal components, production functions, factor analysis. These methods allow us to validate the demand for resource-saving engineering PGCI in the concept of the digital economy.[119,120] An approximation mathematical model of the heat exchange process in a complex heat engineering system consisting of several pipelines, which contain fixed isothermal product, in an insulating casing has been proposed.[121] The relationships between the business processes of digitalization of PGCI facilities and the efficiency of using production resources are studied, the existing mathematical models are updated within the scope of tasks of ensuring sustainable development of facilities.[33,54,122]

An algorithm for calculating resource-saving indicators using independent multicomponent variables (‘digital human capital’ and ‘digital material capital’) has been developed, which allows one to predict the volume of investment in the organization of digital engineering of plants and SC.[123–125]

To provide the personnel needed for solving the tasks of logistics management of business processes of CPS engineering, two models have been developed: a structural model of transformation of the personnel subsystem of production and a labor-saving model of organization of production in the concept of digital economy applying new information technologies.[126,127]

The calculations demonstrated, that implementation of a process approach to the petrochemical enterprise management can lead to the increase in labor productivity factor (determined as the average annual production of added value per employee) by a coefficient from 1.54 to 7.18, depending on the type of production.[128,129]

11. The problem-oriented computer systems, engineering heuristic-computational models and algorithms of intelligent integrated logistics support for the life cycle of PGCI equipment

System analysis of the life cycle of PGCI production equipment was performed using CALS technology tools.[130] The concept of creating a problem-oriented computer system for integrated logistics support of equipment, which includes logistics support for business processes of maintenance and repair, was proposed.[131,132] A special-purpose system of integrated support of equipment at all stages of its LC has been developed (Figure 2), the structure and modes of operation of this system have been described.[133,134] The procedures for data exchange between the integrated logistics support system and various external special information systems are considered.

The procedure for implementing automated data exchange between participants of the life cycle of PGCI equipment is proposed. Built-in graphic editors have been developed, which allow one to create isometric and 3D pipeline diagrams, as well as schematic diagrams of PGCI devices. The relevance of the

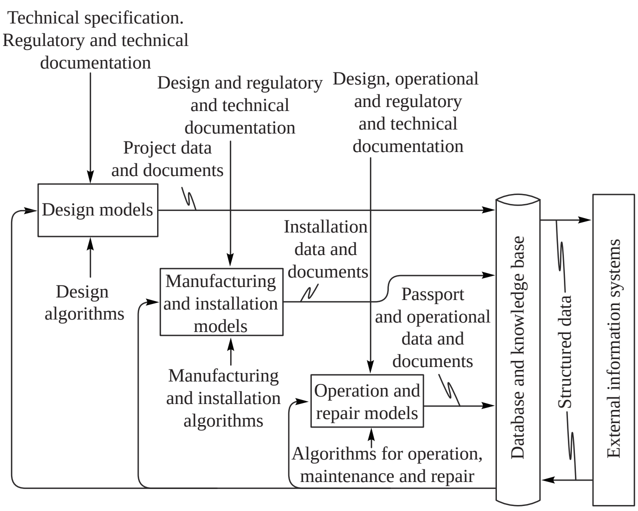

Figure 2 Schematic diagram of a problem-oriented system of integrated logistic equipment support.

practical application of the problem-oriented integrated logistics support system for PGCI facilities was validated.

The problem statement of automation of intelligent decision-making procedures for integrated logistics support of PGCI equipment was formulated.[133,134] Intelligent models of representation[132] knowledge about the equipment design in the form of frames and production rules, as well as heuristic-computational algorithms of automation of determining the characteristics of PGCI equipment are described in detail.[133–135]

12. Theoretical and applied engineering methods in the field of digital transformation of energy- and resource-efficient CPS of the manufacturing of high-quality products

One of the main engineering, organization and management tasks of industrial enterprises is an analytical assessment of the readiness of facilities to planning and organization of the digital transformation of all technological and business processes. Methodology for the development and implementation of projects in the field of data mining (DM) was proposed, and a new method for calculating the readiness index (IR4I) to DM was described.[136] Hence, the use of IR4I index in the forecasting task for the functioning enterprise led to a decrease in daily electricity consumption.[136]

A method for evaluating information assets (IA) has been proposed, the possibility of using this method in practice and the various risks associated with this assessment is proven.[137] Specificity and main characteristics of the IA management process are determined. They require the development of methods and algorithms for solving the following main tasks: classification of IA and their categorization (confidentiality marking), analysis of the life cycle of IA and threats, determination of the criticality level of IA, assessment of damage from the implementation of threats.

New models, methods and algorithms,[138] as well as digital platforms were proposed for the development of applications for intelligent decision-making support in the management of projects,[132] business processes of maintenance, repair and updating of equipment, in order to increase the efficiency of production at all stages of the LC.

A logical-information model is proposed for supporting the process of creating any innovative engineering and organizational and management solutions (or artifacts), such as project proposal, business plan, business solution, report on the research and design development (RDD), *etc*. The model uses high-performance semantic-computational procedures. It allows for checking the extent of innovation of the idea, gives useful recommendations regarding the bibliographic sources, and also generates the research proposals based on this idea.

The plants, manufacturing the high-quality packaging polymer materials (PM) for chemical, pharmaceutical, and food industries at extrusion and calander (ramp roll stack) machines (lines) are complex management objects. The main international trends in the development of PM production in the digital economy are engineering and application of automating computer systems (CS) management. CS help operators to make optimal decisions in order to provide energy and resources saving and production planning. They are based on the collection and processing of large industrial data arrays by means of DM system and optimization algorithms inspired by nature (in particular, genetic algorithms).[140,141]

The task of optimal energy and resource efficient CPS management of the PM manufacture is to determine the optimal values of control actions at the key stages of production. To solve this complex problem, the engineering of flexible reconfigurable problem-oriented CS was performed for CPS. The main subsystems of these CS are the following: the library of DM methods for predicting controlled consumer characteristics of PM and CPS efficacy; the library of physicochemical and empirical mathematical models of the main UO, representing the ‘virtual sensors’, or digital twins, for determination of uncontrollable quality parameters of intermediates (extrudate) and the characteristics of PM.[142]

A library of DM algorithms[143] has been created for predicting the characteristics of PM, it is based on the artificial neural net (ANN) of various types: recurrent, with long short-term memory (LSTM), convolutional (CNN), and combined [CANN (LSTM+CNN)].

A combined algorithm has been proposed for a comprehensive assessment of the performance, residence time, and extrusion process parameters, it considers the extruders equipment (hardware) flexibility, the complex structure of technological flows and the variety of occurring processes.[144] The computer model is based on a cellular model of hydrodynamic processes in various types of partitioned extruders with modular augers consisting of different kinds of elements.[145,146]

Diverse tools of CALS technologies provide digital display of products, equipment units, and PGCI production facilities as a whole, in the form of multiple computer models, drawings and visual 3D images (or digital twins) of industrial objects at all stages of their LC.[5,135,143,147]

Digital twins are very promising digital instruments of analyzing and improving the safety of productions and SC of PGCI and heat power industry (HPI), and they provide a successful solution to the problems of logistics management of end products quality, improving the reliability, and safety of PGCI production cycle.

Most of all, production digital twins are in demand at hazardous PGCI and HPI production facilities, where exothermic chemical reactions, oxidation and high-pressure processes take place. Violation of the optimal technological functioning modes of such CPS and plants can cause emergency situations, not only with significant technogenic and environmental damage, but also with a threat to human life.[148]

Intellectual and computational algorithms for technical diagnostics of the quality of special glass are proposed.[149]

To improve the safety of PGCI production and SC, it is necessary to develop knowledge representation models[143] applying so-called ‘chronicles’ which describe all previous faults of equipment taking into account their cause-and-effect relationships. These models of knowledge representation should be included in the intelligent software and information support of the production digital twin.[150] Troubleshooting of equipment is especially important when starting and stopping CPS technological processes.

Engineering of digital twins of CPS production using CALS technologies is an important operation of the engineering of the production project management information system, it will result in reducing the design time and number of errors and unjustified project decisions. At the stages of establishing the technical task and the feasibility study, the development of the provisional production digital twin will allow one to determine more accurately the parameters of energy consumption, production cycle time, product quality parameters and production safety.

13. Application of methods of reliability indices optimization, digitalized risk management and safety in the energy- and resource-efficient CPS engineering

Implementation of scientifically proven integrated methods in biochemical and chemical-metallurgical industries[152] is of paramount importance for solving the problems of engineering of energy- and resource-efficient environmentally safe CPS. This approach can ensure the optimal reliability and technological safety indices of CPS and territorial gas supply systems,[151] as well as digitalized management and minimization of various types of risks for PGCI production and SC.

Authors[153] worked out the theoretical foundations of analysis and risk assessment, as well as digitalized CPS security management, and proposed the logical-informational, logical and stochastic models of analysis and accident risk assessment for various classes of PGCI objects. A formalized statement of CPS safety management tasks was defined and production rules for decision making[143] regarding the operational CPS safety management, which are based on the prevention of failures and emergencies at CPS,[151] were developed. The procedure of digitalized CPS safety management has been developed by means of modern software and information tools, methods of CPS system analysis, approach and principles of creating intelligent integrated systems of safety management of PGCI facilities.[153]

It was proposed to use a systematic approach to managing the safe handling of chemical products at all stages of the LC and throughout the entire SC of PGCI facilities.[154] To implement this, the functional framework of the information and analytical management system was developed, and algorithm for classifying the types of hazards of chemical products under conditions of uncertainty was offered.

In recent years, the methodology of engineering of reliable and safe chemical-technological systems, which is based on the concept of self-organization, has been proposed. Heuristic algorithm, which includes the order of procedures for initial data processing by a declarative method, is a foundation for suggested main principles and methodology of self-organization of reliability and safety properties of energy- and resource-efficient CPS. The principles of self-organization are based on the logical representation of knowledge in the form of production metadirections. They provide the synthesis of both CPS as a whole and their elements with optimal reliability factors. This synthesis is based on methods of intelligent data processing and the application of the theory of artificial intelligence approach. The initial data describe the factors affecting the CPS and the technical requirements.[125,155]

For the synthesis of CPS with optimal reliability and safety factors, an intelligent instrumental system (IIS) has been developed, which includes an intelligent planner, a multidisciplinary problem solver, knowledge- and databases, ontology, expert systems (ES) and computing modules (CM). This IIS provides self-adaptation and interconnectedness of the structure of ES, CM and DB, relevant to the specific task of synthesizing highly reliable CPS.[155,156]

The intelligent planner implements the self-organization algorithm, while the solver provides a solution of the problem based on the self-organized architecture of the ES, CM and DB. The subsystem of the IIS ontology is intended for the formation of a single semantic information IIS. Production metadirections of self-organization and problem-oriented algorithms for solving problems can be formed and included in the IIS in the process of problems solving on the basis of expert opinions coordination.

Conclusion

In the modern society special attention shall be paid to the successful implementation of the main goals of sustainable development of mankind and the creation of a waste-free, or ‘circular’, digital economy in the context of the industrial revolution ‘Industry 4.0’ and considering the concept of ‘Nano-Bio-Information-Cognitive-Social’ (NBICS) technologies convergence. To achieve this, it is vitally important to conduct fundamental and applied RDD in the field of engineering of high-intensity energy-efficient and environmentally safe CPS. The priority directions, which were recorded in the resolution of the XXI Mendeleev Congress on General and Applied Chemistry, are the following: intensification, combining and miniaturization of UO; digitalized engineering and logistics management of operation of energy- and resource-efficient, environmentally safe, high-tech CPS and SC enterprises, including waste-free, nature-like CPS and UO and engineering of 'green' SC in the real economy sector; multiscale computer modeling of CPS, structure of substances and composite materials; computer optimization and automated synthesis of energy- and resource-efficient CPS and SC, engineering of digitalized robotic-cybernetic intelligent industrial enterprises; assessment of energy and resource efficiency and environmental safety of the LC stages of PGCI products; rational use of natural resources with a wide employment of renewable natural resources; combined energy- and resource-efficient operation and logistics management of environmentally safe handling of industrial and municipal waste and wastewaters; disposal of hazardous waste in natural geophysical formations; digitalized monitoring using drones and other unmanned air vehicles; computer assessment of the environmental impact of technogenic systems; minimization of environmental and production risks for industrial enterprises.

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