CHEMICAL ENGINEERING TRANSACTIONS

VOL. 94, 2022

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Yee Van Fan, Jiří J. Klemeš, Sandro Nižetić

ISBN 978-88-95608-93-8; **ISSN** 2283-9216

DOI: 10.3303/CET2294088

Virtual Model of the Production of Chemical Reagents and High Purity Substances

Arkadiy Bessarabov[a,*], Vasiliy Trokhin[a], Gleb Mindlin[b], Violetta Vasilenko[b]

[b] R&D Centre "Fine Chemicals", Moscow, Russia
[a] Mendeleev University of Chemical Technology of Russia, Moscow, Russia
bessarabov@nc-mtc.ru

Chemical reagents and highly pure substances largely determine the development of the most innovative industries and promising scientific research. One of the main Russian manufacturers of materials of reactive qualification and high purity is the industrial association JSC "EKOS-1". For 30 y, a developed production infrastructure and logistics system has been created. JSC "EKOS-1" supplies products throughout Russia and for export. The dealer network is represented in 14 cities of the Russian Federation. We are developing an information 3D model of the enterprise, including a design 3D model and databases of the model elements. Autodesk Revit, a building information modelling software that implements the building information modelling principle, was chosen as the computer support system. In the first stage, the work was focused on the "Warehouse", which includes 6 warehouses for raw materials and finished products. With the use of Autodesk Revit software, 3D models of warehouses were built, as well as their internal components. All the models are as close as possible to the original objects. 3D models are integrated into the Unity 3D development environment to create a virtual space of the enterprise for its visualization, optimization of logistics and interactive user interaction.

1. Introduction

The transition to a new, digital era and a new technological order leads to the emergence of new technologies, methods, and solutions, while many traditional technologies become obsolete and no longer provide competitive advantages. Of course, the changes taking place in the high-tech industry are of the greatest interest. At the same time, the contribution (weight coefficient) of some technologies in ensuring the global competitiveness of enterprises and even countries is much higher than that of other technologies (Fuller et al., 2020).

The evolution of the manufacturing industry towards automation and digitalization is a consolidated phenomenon. In this direction, Industry 4.0 paradigms are prompting many industrial companies to significantly upgrade their facilities (Vaccari et al., 2022).

Under the Industry 4.0, the scheduling should deal with a smart and distributed manufacturing system supported by novel and emerging manufacturing technologies such as mass customization, Cyber-Physics Systems (CPS), Digital Twin, and SMAC (Social, Mobile, Analytics, Cloud) (Zhang et al., 2019).

Digital twinning is now an important and emerging trend in many applications. A digital twin can be defined as a virtual representation of a physical asset enabled through data and simulators for real-time prediction, optimization, monitoring, controlling, and improved decision making (Rasheed et al., 2020).

The main trends in the usage of information models of various designs are identified, and domestic and foreign experience in implementing Building Information Modelling (BIM) technology is being analyzed. The maturity levels of BIM technologies are considered following Bew Richards BIM implementation model. This helps to analyze the software currently used (Ginzburg et al., 2016).

Currently, practical implementations of digital twins are increasingly used in a variety of areas, including education, construction, healthcare, shipbuilding, automotive, energy, aerospace and chemical industries. In the context of the development of the fifth and the formation of the foundations of the sixth technological order,

Paper Received: 15 April 2022; Revised: 19 May 2022; Accepted: 10 June 2022
Please cite this article as: Bessarabov A., Trokhin V., Mindlin G., Vasilenko V., 2022, Virtual Model of the Production of Chemical Reagents and High Purity Substances, Chemical Engineering Transactions, 94, 529-534 DOI:10.3303/CET2294088

the chemical industry is one of the priorities in the management of innovative processes (Bessarabov et al., 2021).

2. Information 3D model of the industrial enterprise of fine chemistry

Fine chemistry is one of the most important areas in the structure of the chemical industry. Chemical reagents and highly pure substances are a promising class of fine chemical products. They mainly determine the development of the most innovative branches of industry and advanced scientific research (Bessarabov et al., 2015). One of the main Russian manufacturers of materials of reactive qualification and high purity is the industrial association JSC "EKOS-1" (Figure 1).

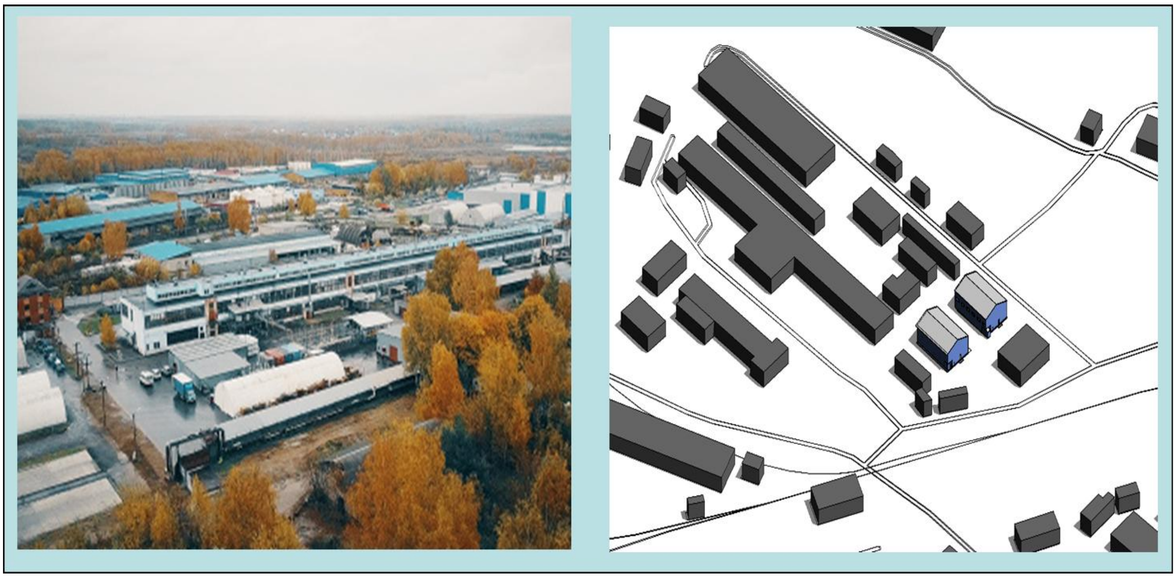

Figure 1: 3D modelling of an industrial enterprise (JSC "EKOS-1")

The stable quality of products of JSC "EKOS-1" is ensured by modern multidisciplinary equipment. The continuous laboratory control from the raw materials supply to the shipment of finished products is organized. The analytical service of JSC "EKOS-1" carries out: the development of general approaches to the analysis of reagents and high-purity substances, identification of methods for the analysis of the main groups of impurities, development of optimal algorithms for the analysis of reagents and high-purity substances, raw materials and intermediate products. Analytical laboratories of the production complex correspond to the requirements of the technical competence of the state system for ensuring the uniformity of measurements MI 2427-2016. The quality management system of JSC "EKOS-1" matches the requirements of the state standard ISO 9001-2011. A developed production infrastructure and logistics system has been created. Products are supplied both throughout Russia and for export.

The enterprise has an integrated modular system for water management. This ecological system allows to reduce water consumption and energy costs, industrial effluents, the negative impact of the enterprise on the environment, as well as improve the efficiency and safety of production (Bessarabov et al., 2018).

The main organizational structures are applied in the enterprise management system. The upper level of the management is a linear-headquarters structure based on the strict subordination of the lower level of management to the highest (rigid hierarchy). Matrix management structures are widely used in JSC "EKOS-1" to carry out the most important projects. The elements of the matrix structure are expressed in the emergence of additional horizontal links between specialists from different departments within the project teams.

Organizational development associated with change management is based on two methods of the Harvard Business School (Michael Beer, Nitin Nohria): "Theory E" and "Theory O" (Beer et al., 2000). The most common in Russia first method (E) is used in the enterprise management system. A rigid “mechanical” approach and top-down implementation of change are at the base of the method. It brings quick financial returns (Rosenzweig et al., 1994). Currently, "Theory O" is beginning to come out on top. It is based on a greater role in the processes of transformation of the human factor, the growth of a corporate culture of management, and the implementation of changes "bottom-up". The divisional organizational structure of management is applied in the supply and distribution services of JSC "EKOS-1" and is focused directly on the most important suppliers and consumers, around which groups that ensure optimal interaction are formed. 3D

warehouse model developed using building information modelling software Autodesk Revit is used in this structure.
The information 3D model of the enterprise (Figure 1), including a design 3D model and databases of the model elements, is being developed. Autodesk Revit, a software package that implements the building information modelling (BIM) principle, was chosen as the computer support system. Building Information Modelling (BIM) is a process of collaborative creation and usage of information about a structure, or building, which forms the basis for all decisions throughout the life cycle of an object (Ginzburg et al., 2016). BIM is based on a three-dimensional information model. BIM is a comprehensive program that uses a common three-dimensional base for the model and tools, which is replenished and improved during the design process. An information model is a digital prototype of an object in which each of its elements is uniquely defined and their logical relationship is provided. Namely, the structure and relationships are the main elements of the information model. The main advantage of this technology is the reduction in the time of creation and implementation of the project by optimizing the schedule and more precise planning.

3. Virtual simulation of warehousing

In the first stage, the work was focused on the "Warehousing" direction, which includes 6 warehouses for raw materials and finished products (Figure 2). All the warehouses belong to the highest class "A" and have the following characteristics: buildings are specially built for warehouse terminals: the material is the high-quality light metal structures; the height inside the terminal allows to lift the pallets to 13 m (seven tiers); the concrete floor can withstand a maximum load of 5 t/m^2 an anti-dust coating is necessarily present; the warehouse is equipped with powerful air conditioning and ventilation devices designed to maintain the specified temperature and humidity conditions; warehouses are equipped with automatic fire extinguishers; an automatic system for accounting for goods and their movement is used; workers use portable scanners, all products have barcodes.

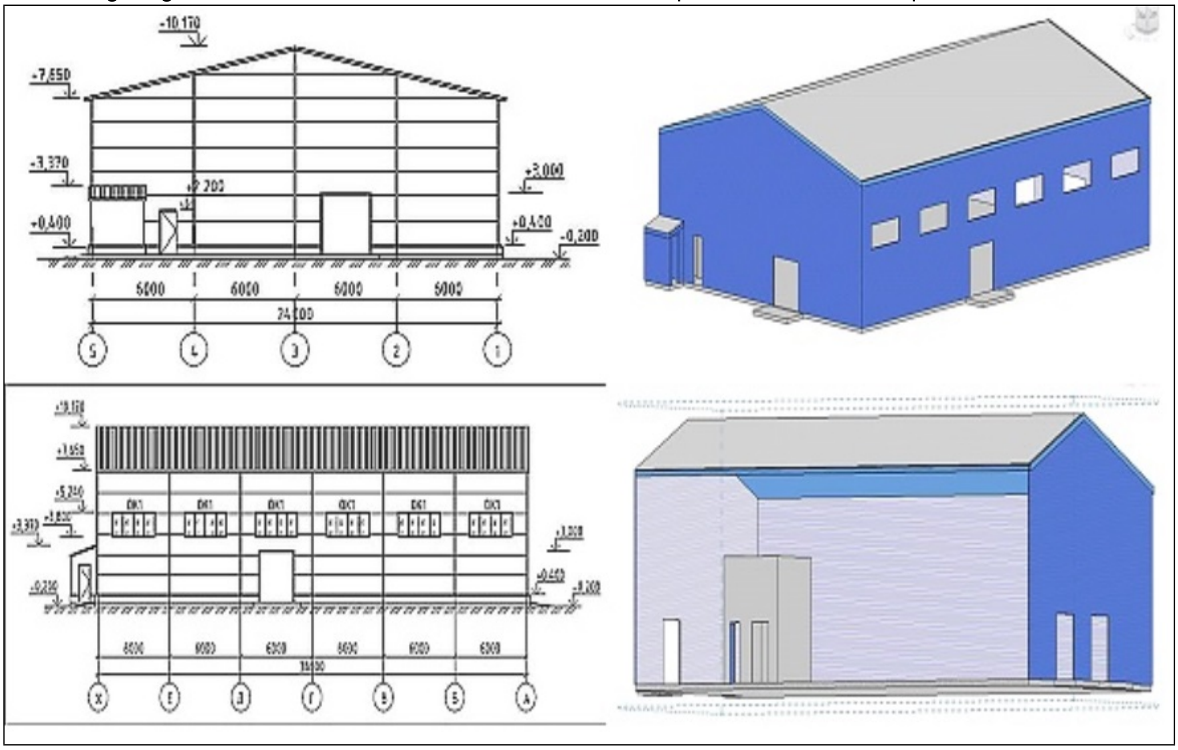

Figure 2: Virtual simulation of warehouse

Warehousing is the most significant element of any logistics chain. At the moment of the development of professional technologies, one can objectively note a high level of demand for specially equipped places to ensure the storage of commodity stocks that are in demand at all stages of the implementation of the corporate commodity flow. This flow begins at the stage of primary formation of raw materials and ends with the stage of purchasing by the end consumer. These objective factors in the functioning of logistics warehouse systems ensured the presence of a wide variety of types of warehouses, and their logistics and management systems.

A modern large warehouse is a complex technical structure that consists of numerous interconnected elements, it has a certain structure and performs a number of functions for the transformation of material flows, as well as the accumulation, processing and distribution of goods among consumers. At the same time, the possible variety of parameters, technological and space-planning solutions, equipment designs and characteristics of a diverse range of goods processed in warehouses classifies warehouses as complex systems. At the same time, the warehouse itself is just an element of a higher-level system - the logistics chain, which forms the basic and technical requirements for the warehouse system, sets goals and criteria for its optimal functioning and dictates the conditions for goods processing. The warehouse should not be considered in isolation, but as an integrated part of the logistics chain. Only this approach will ensure the successful implementation of the main functions of the warehouse and the achievement of a high level of profitability.
In the first stage of the digital twin development of the enterprise JSC "EKOS-1", 3D models of warehouses were designed, as well as their internal components (Figure 2). 3D models designed with the help of Autodesk Revit software make it possible to estimate the volumetric occupancy of the warehouse, predict the optimal shipment routes from the warehouse and rational placement of raw materials or finished products. All the models are as close as possible to the original objects. 3D models are integrated into the Unity 3D cross-platform game engine to create a virtual space of the enterprise for its visualization, optimization of logistics and interactive user interaction.

4. The main 3D models of elements of the internal equipment of the warehouse

At the developing of JSC "EKOS-1" warehouse 3D model, a new set of specialized equipment was created: racks, boxes, pallets, lamps and doors (Figure 3). A real-time rendering and virtual reality plugin Enscape was used to build the exposure and render images. With its help, it is possible to move in the project, create images with a resolution of up to 4 K, special setting for RTX Raytracing and Grass Rendering, creating of videos and virtual tours of the project.

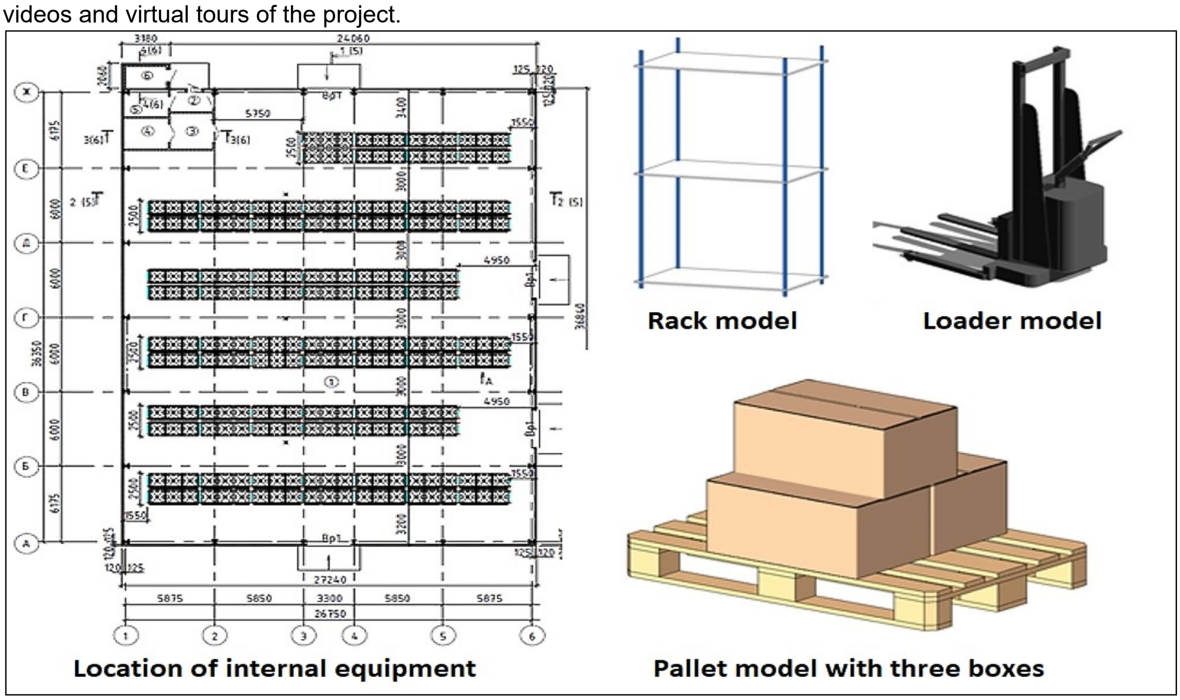

Figure 3: 3D models of the internal equipment of the warehouses of JSC "EKOS-1"

One of the internal elements of warehousing is pallets (Figure 3). They transport reusable containers. This is an independent transport unit designed for transportation, picking, warehousing and storage of the products. Pallets are used to transport heavy or bulky goods. With their help, it is easy to move goods around the warehouse territory and carry out loading and unloading operations. Shelving equipment is mainly used to store products in warehouses. Racks are divided into universal and special. Universal racks are used to store the widest range of goods. The most common type is shelf racks, which are a series of shelves fixed on vertical posts (Figure 3). Universal racks also include checkered, box, frame and gravity racks. Special racks are used to store certain types of goods. Special racks are divided into pillars and consoles.

Loading and unloading machines play an important role in warehouse equipment. They are used for mechanization of loading and unloading operations, intra-warehouse movement and goods warehousing. These include electric and automotive forklifts and electric stackers. Electric forklifts (Figure 3) are powered by batteries and are intended for indoor use. The load capacity of electric forklifts is from 0.5 to 5 t, the lifting height is from 2 to 6 m.
Containers for chemical products include a large list of items that differ in various parameters. Cans, bottles, canisters (Figure 4), etc. can be used to store chemicals. Their volume can vary from 10 mL (small bottles and containers) to 1,000 L (special containers, vats). The most common materials in this segment are glass, metal, polypropylene, etc.

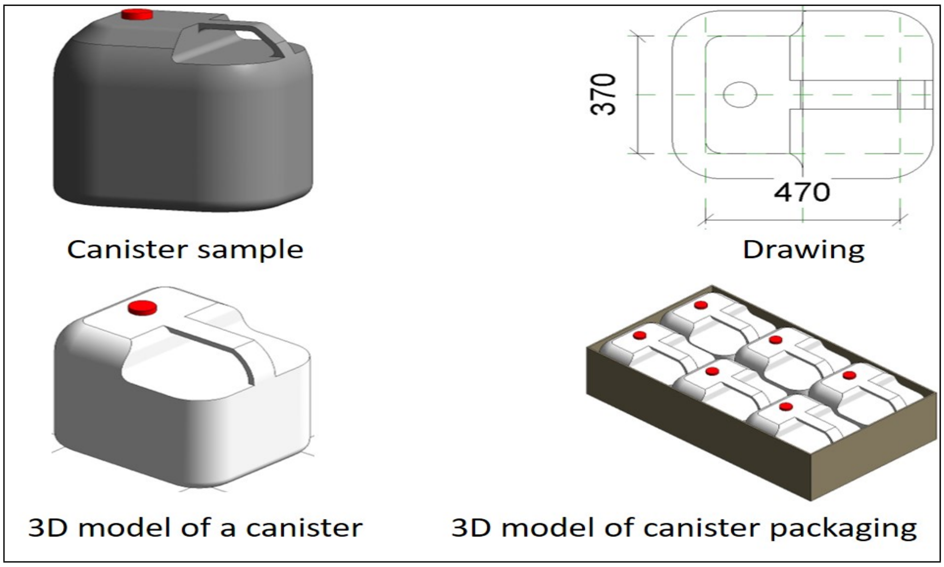

Figure 4: 3D model of a container (canister) for storage of chemical reagents

Containers for chemical reagents and highly pure materials are associated with packaging and labelling processes. The process of chemical reagent packaging under the production conditions consists of the following sequentially performed operations: the actual packaging (weighing or measuring a portion of the reagent); capping filled containers with a stopper or a screw cap; sealing the closure with a collapsible cuff or by the other means; gluing factory brand stickers and labels. Large-tonnage reagents are usually packed using dosing devices, labelling machines and other automatic machines, while fine reagents are mostly manually. After packing and capping, the container is carefully sealed. Sealing of the containers contributes to the quantitative preservation of the reagent. The possibility of evaporation, leakage or spillage of the substance, as well as the preservation of quality, are excluded. The possibility of penetration of ambient air and its harmful effects (moisture, oxygen, etc.) on the substance is excluded. To seal closures, ground glass, cork and polyethene stoppers and plastic screw caps are put on shrinkable caps or cuffs made of polymeric materials, or they are passed over with adhesive tape, or, finally, tied with parchment. To seal jars and flasks with ground stoppers, their heads are also filled with sealing materials.
Each canister (Figure 4), jar, bottle, ampoule and other containers for packaging have to be labelled with the following designations: the name of the enterprise that produced this reagent and its location; name and qualification of the reagent; a mass of the reagent, lot number and date of manufacture; number of the standard or specifications and quality indicators; nomenclature number of the reagent according to the price list; stamp of the technical control department. Depending on the qualification of the reagent, a label of a certain color should be pasted on the container: for a "chemically pure" reagent - red, for "pure for analysis" - blue, for "pure" - green, for "special purity" - yellow.
For all other reagents and preparations, a light brown label is used. The label on bottles with liquid reagents must be protected with polyethylene adhesive tape or other transparent material that protects the label from the chemical attack of the reagent.
Packaging is also important. Sealed and labelled jars and vials should be covered by tight-fitting corrugated paper cases and packed in a transport container. Standard cardboard or thick wooden boxes made of boards or plywood and lined with waterproof paper are used as transport containers. Glass containers with dry reagents are shifted into boxes with corrugated paper and compacted with lignin. Glass containers with liquid reagents are packed in boxes with nests-partitions.

Particular attention is paid to the packaging of reagents intended for export. The transport container must comply with the specific conditions of the country where the products are sent.
The shown container (Figure 4) element is the canister used for packaging chemical reagents containing organic solvents. It is resistant to the permeation of organic solvents and other aggressive environments and has cracking resistance and should not change its appearance. The choice of a polymeric material for the canister manufacture is carried out taking into account the contact admissibility of the packaging material with organic and inorganic reagents.
At 3D modelling of a canister, only its form was taken into account. Materials (polypropylene, polyvinyl chloride or polyacetal) were assigned from the base of the materials. During the model creation, the methods of extrusion along the path and the shift of the profile along the path were applied.

5. Conclusions

Work has been carried out to create a digital twin of the leading Russian manufacturer of materials of reactive grade and high purity JSC “EKOS-1”. With the use of Autodesk Revit software, 3D models of warehouses were designed, as well as their internal components. For many samples of storage equipment and containers specific to the technology of fine chemistry, the corresponding 3D models have been designed for the first time. All the models are as close as possible to the original objects. The developed 3D model of the warehouse is used for marketing and allows to promote finished products. Comparing with the previous warehouse logistics, one can note the new elements of resource saving. The proposed warehouse 3D model allows for a faster search for the necessary information, minimizes the time of warehouse operations and saves labor resources. 3D models are integrated into the Unity 3D cross-platform game engine to create a virtual space of the enterprise for its visualization, optimization of logistics and interactive user interaction. The importance of an integrated approach to the formation of an informational 3D model of JSC “EKOS-1” is shown. The transition to BIM models is effective during working with them at all the stages of the life cycle of an industrial enterprise (Michalski et al., 2022). In this regard, it is proposed to use in the future the digital technology of the "information model of an object life cycle".

Acknowledgements

This work was supported by the Russian Foundation for Basic Research (RFBR) according to the research project № 20-03-00515.

References

Beer M., Nohria N., 2000. Cracking the code of change. Harvard Business Review, 78 (3),133-141.
Bessarabov A., Kvasyuk A., 2015. Cybernetic researches in technology of chemical reagents and high-purity substances. Clean Technologies and Environmental Policy, 17, 1365-1371.
Bessarabov A., Trokhin V., Stepanova T., Vendilo I., 2018. Energy- and resource-saving system of water management for fine chemistry. Chemical Engineering Transactions, 70, 523-528.
Bessarabov A., Trokhin V., Zaremba G., Stepanova T., 2021. System Analysis of the Integration of Innovative Resources of the Leading Enterprises of the Chemical Complex. Chemical Engineering Transactions, 88, 1177-1182.
Fuller A., Fan Z., Day C., Barlow C., 2020. Digital Twin: Enabling Technologies, Challenges and Open Research. IEEE Access, 8, 108952-108971.
Ginzburg A., Shilova L., Adamtsevich A., Shilov L., 2016. Implementation of BIM-technologies in Russian construction industry according to the international experience. Journal of Applied Engineering Science, 14, 457-460.
Michalski A., Głodziński E., Böde K., 2022. Lean construction management techniques and BIM technology – systematic literature review. Procedia Computer Science, 196, 1036-1043.
Rasheed A., Kvamsdal T., San O., 2020. Digital twin: Values, challenges and enablers from a modeling perspective. IEEE Access, 8, 21980-22012.
Rosenzweig P.M., Nohria N., 1994. Influences on human resource management practices in multinational corporations. Journal of International Business Studies, 25, 229-251.
Vaccari M., Bacci di Capaci R., Brunazzi E., Tognotti L., Pierno P., Vagheggi R., Pannocchia G., 2020. Implementation of an Industry 4.0 system to optimally manage chemical plant operation. FAC-PapersOnLine, 53, 11545-11550.
Zhang J., Ding G., Zou Y., 2019. Review of job shop scheduling research and its new perspectives under Industry 4.0. Journal of Intelligent Manufacturing, 30, 1809-1830.