МАТЕМАТИЧЕСКИЕ МЕТОДЫ И ИНФОРМАЦИОННЫЕ СИСТЕМЫ В ХИМИЧЕСКОЙ ТЕХНОЛОГИИ

MATHEMATICAL METHODS AND INFORMATION SYSTEMS IN CHEMICAL TECHNOLOGY

ISSN 2410-6593 (Print), ISSN 2686-7575 (Online)
https://doi.org/10.32362/2410-6593-2023-18-5-482-497
УДК 661.71+51-74

RESEARCH ARTICLE

Principles of creating a digital twin prototype for the process of alkylation of benzene with propylene based on a neural network

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Abstract

Objectives. *To identify the principles of creating digital twins of an operating technological unit along the example of the process of liquid-phase alkylation of benzene with propylene, and to establish the sequence of stages of formation of a digital twin, which can be applied to optimize oil and gas chemical production.*
Methods. *The chemical and technological system consisting of reactor, mixer, heat exchangers, separator, rectification columns, and pump is considered as a complex high-level system. Data was acquired in order to describe the functioning of the isopropylbenzene production unit. The main parameters of the process were calculated by simulation modeling using UniSim® Design software. A neural network model was developed and trained. The influence of various factors of the reaction process of alkylation, separation of reaction products, and evaluation of economic factors providing market interest of the industrial process was also considered. The adequacy of calculations was determined by statistics methods. A microcontroller prototype of the process was created.*
Results. *A predictive neural network model and its creation algorithm for the process of benzene alkylation was developed. This model can be loaded into a microcontroller to allow for real-time determination of the economic efficiency of plant operation and automated optimization depending on the following factors: composition of incoming raw materials; the technological mode of the plant; the temperature mode of the process; and the pressure in the reactor.*

Conclusions. *The model of a complex chemicotechnological system of cumene production, created and calibrated on the basis of long-term industrial data and the results of calculations of the output parameters, enables the parameters of the technological process of alkylation to be calculated (yield of reaction products, energy costs, conditional profit at the output of finished products). During the development of a hardware-software prototype, adapted to the operation of the real plant, the principles and stages of creating a digital twin of the operating systems of chemical technology industries were identified and formulated.*

Keywords: *digital twin, cumene, industrial plant, neural networks, machine learning, ESP8266*

For citation: Kichatov K.G., Prosochkina T.R., Vorobyova I.S. Principles of creating a digital twin prototype for the process of alkylation of benzene with propylene based on a neural network. *Tonk. Khim. Tekhnol. = Fine Chem. Technol.* 2023;18(5):482–497. https://doi.org/10.32362/2410-6593-2023-18-5-482-497

НАУЧНАЯ СТАТЬЯ

Принципы создания прототипа цифрового двойника процесса алкилирования бензола пропиленом на основе нейронной сети

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Аннотация

Цели. *Выявление принципов создания цифровых двойников реально действующей технологической установки на примере процесса жидкофазного алкилирования бензола пропиленом и установление последовательности этапов формирования цифрового двойника, которая может быть применима для оптимизации работы нефтегазохимического производства.*
Методы. *Рассмотрена в целом химико-технологическая система, состоящая из реактора, смесителя, теплообменников, сепаратора, ректификационных колонн и насоса, как система высокого уровня. Выполнен сбор данных, описывающих функционирование установки получения изопропилбензола алкилированием бензола пропиленом путем расчета основных параметров процесса с помощью имитационного моделирования с применением специализированного программного обеспечения UniSim® Design. Разработана и обучена нейросетевая модель, учитывающая влияние различных факторов реакционного процесса алкилирования, разделения продуктов реакции и оценки экономических факторов, обеспечивающих рыночную привлекательность рассматриваемого промышленного процесса. Определена адекватность результатов расчетов оптимальных параметров процесса методами математической статистики. Создан прототип цифрового двойника процесса, реализованной на микроконтроллере.*

Результаты. *Создана прогностическая нейросетевая модель и алгоритм ее построения для процесса алкилирования бензола пропиленом, позволяющая при загрузке ее в микроконтроллер обеспечить в режиме реального времени определение экономической эффективности работы установки и автоматическую оптимизацию работы установки в зависимости от состава поступающего сырья технологического режима системы, температурного режима проведения процесса и давления в реакторе.*

Выводы. *Созданная модель сложной химико-технологической системы производства кумола, откалиброванная на основании промышленных данных длительного пробега технологической установки и результатов расчетов выходных параметров процесса при помощи нейронной сети, реализованной на микроконтроллере, позволяет рассчитать параметры технологического процесса алкилирования (выход продуктов реакции, энергетические затраты, условную прибыль при выпуске готовой продукции). В процессе разработки прототипа программно-аппаратного комплекса управления установкой алкилирования бензола пропиленом на основе данных, адаптированных к работе реальной установки, были выявлены и сформулированы принципы и этапы создания цифрового двойника производственных систем отраслей химической технологии.*

Ключевые слова: *цифровой двойник, кумол, промышленная установка, нейронные сети, машинное обучение, ESP8266*

Для цитирования: Kichatov K.G., Prosochkina T.R., Vorobyova I.S. Principles of creating a digital twin prototype for the process of alkylation of benzene with propylene based on a neural network. *Tonk. Khim. Tekhnol. = Fine Chem. Technol.* 2023;18(5):482–497. https://doi.org/10.32362/2410-6593-2023-18-5-482-497

INTRODUCTION

The petrochemical industry is one of the largest sectors of the world economy. The main trends in the development of modern petrochemistry are aimed at increasing the capacity of petrochemical plants and the selectivity of chemical reactions, reducing the energy intensity of chemical technological processes, processing of new types of raw materials, and environmental safety of production. The key results of these processes will be to increase the efficiency of petrochemical productions.

The modernization and technical re-equipping of operating plants are carried out, as a rule, on the basis of experimental data without the appropriate scientific study. The methods of chemical technological processes optimization applied do not allow us to cover comprehensively the whole range of characteristics and factors affecting the production process. Existing approaches to the selection of the current operating parameters are based primarily on the experience of operators and process engineers, thus limiting the possibility of eliminating shortcomings associated with the human factor [1].

Currently, digital processes using artificial intelligence technologies are being increasingly introduced, in order to resolve urgent production problems and improve the efficiency of industrial enterprises. One of the most effective ways of solving this problem today is mathematical modeling using neural network technologies using modern hardware and software systems.

The use of neural networks based on Big Data provides a unique opportunity to establish the hidden relationships of the qualitative and quantitative characteristics of feed streams, fuel, cooling water, and electricity consumed by cumene with production efficiency indicators. In the conditions of existing production, this enables the potential for increasing energy saving in a short time to be identified and the number of measures needed to optimize industrial technological processes to be significantly reduced: redistribution of feed streams, fuel, water, and electricity [2].

At the same time, the application of intelligent systems in the industrial sector is often implemented with the use of cloud data storage and distributed computing. The use of external cloud systems poses certain difficulties and risks:

– high cost of ownership of cloud services infrastructure;

– the possibility of unauthorized access by the provider's personnel due to insufficient data protection;

– temporary loss of access to information may occur as a result of network equipment failures[1].

Industrial companies are concerned about the uninterrupted operation of all plant facilities and services. The risks associated with the transfer of data and calculations for the management of existing production to external cloud resources are a potential threat to the safety of operation of existing fire and explosion hazardous facilities. In this regard, embedded solutions based on industrial controllers and supervisory control and data acquisition (SCADA) systems are currently a fault-tolerant alternative to external cloud services.

The basic unit of a digital intelligent system at an industrial petrochemical enterprise is a digital twin (DT). This is a digital (virtual) model of industrial facilities, systems and processes of an enterprise which accurately reproduces the characteristics and actions of the original and is synchronized with it. The DT is used to simulate events which occur with the original under certain conditions, significantly reducing the time and material costs for testing complex and expensive equipment, thus preventing possible emergencies and ensuring the safety of existing production[2].

Classification of DTs by levels of integration with a real production facility[3,4]:

– DT prototype is a virtual analogue of the facility, including all the data for reproducing the original object;

– DT instance is a database of all characteristics, operational properties, and information about the operation of a physical facility, including its three-dimensional model and functioning in parallel with the original;

– DT aggregate is a collected intelligent cyber physical system including DTs and real facilities, controlled from a single center and exchange data with each other online.

The development of new digital technologies has marked the arrival of the fourth industrial revolution (Industry 4.0) [3] and the trend towards the re-profiling of all sectors of industrial production. Using supply chain management-marketing systems as an example, [4] enabling technologies that enable the transition to Industry 4.0 were identified: advanced manufacturing, additive manufacturing, augmented reality, simulation, cloud computing, industrial Internet of Things (IoT), cyber security, and Big Data analytics and customer profiling. Among these, the most used digital technologies are mobile and cloud computing, IoT, big data analytics, and blockchain [5].

Digital transformation is profoundly changing our way of living, rendering obsolete not only products or services, but also the way in which firms organize their business processes along with how they create and capture value. Thereby, reinventing a business model is mandatory for incumbents in their attempt to survive in the changing digital world [6].

At the same time, [7] notes that information on available assistive technologies and trends is scarce and limits the ability to make appropriate decisions.

The concept of Digital Transformation itself is multifaceted [8]. In [9], the different types of digital transformation impacts on innovation processes are classified, and barriers to integrating digital competencies into traditional companies are described. It should be noted that research on the relationship of digital transformation to innovation processes and innovation management is at an embryonic stage. The concept of DT is analyzed in [10]. It was shown that DTs of technological processes may be used for monitoring.

The effectiveness of digitalization is clear: it enables industry processes to be automated, a variety of information to be stored and data analyzed. It can also predict future incidents and system states [11]. 2021 has been a year of growth in the active involvement of global oil and gas companies in business transformation from upstream to downstream,

[1] "We risk losing data and breaking the law" – why companies are afraid of the clouds. VC.ru. 2021. Available from URL: https://vc.ru/promo/246963-riskuem-poteryat-dannye-i-narushit-zakon-pochemu-kompanii-opasayutsya-oblakov. Accessed January 5, 2022.

[2] Zuykova A. What are digital twins and where are they used. RBC. 2021. Available from URL: https://trends.rbc.ru/trends/industry/6107e5339a79478125166eeb. Accessed January 5, 2022.

[3] Prokhorov A. Digital twins. The concept is evolving. C-News. 2018. Available from URL: https://data.cnews.ru/articles/2018-04-18_tsifrovye_dvojniki_kontseptsiya_razvivaetsya. Accessed January 5, 2022.

[4] Digital twin technology. Future2Day. 2019. Available from URL: https://future2day.ru/texnologiya-cifrovyx-dvojnikov/. Accessed January 5, 2022.

with the re-engineering of production strategies and operating models taking the lead. Ceipek *et al*. [12] conducted an analysis of a 10-year US panel dataset showing that underperforming firms are more willing to engage in the emerging digital transformation, while a superior level of prior performance make firms less inclined to engage in such digital technologies. As a rule, the management of large successful companies is not willing to change and upgrade resources to include digital technologies, because they are inert and inflexible, and the volume of production is high. Such companies lack incentives to adopt advanced digital technologies [13]. Therefore, company boards of directors are often the inhibitor of digital change in this case. Managers also need to actively combat myopia, inertia, or rigidities that ensue from an established product and business logic to ensure the exploration of cutting-edge solutions for future product development [12]. This inertia is partly explained by the fact that according to estimates made by [14], 66% to 84% of digital transformation projects fail, 13% of which is a sizable share considering the costs, both monetary and otherwise, of putting these projects in place.Nevertheless, more and more business leaders have recently begun to understand the importance of using digital data and analytics to improve business performance[5].

Digital transformation can lead to notable advantages for firms, such as helping to create products and services that are more efficient and consistent with customer needs, thus providing a shorter innovation process and time to market, and creating related digital ecosystems [15].

In 2002, Michael Greaves gave a lecture in which he formulated the world's first concept of DTs [16].

Digital twinning in industry was first applied in the aerospace industry [17], but the oil industry has long used only traditional modeling and optimization techniques. Nowadays, in oil and gas chemistry, the use of DTs is becoming increasingly important [18, 19].

The classification of data from the literature on the use of DTs of production systems has shown that three options for their use are possible:

1) modeling the reliability of systems, the ability to plan their maintenance by monitoring anomalies, deformations, fatigue cracks, diagnosis of the state of the existing physical object;

2) study of system behavior at each stage of life cycle and prediction of its characteristics by digital simulation of physical object and control of its life cycle using the IoT concept;

3) optimizing the behavior of the system at the design stage prior to the creation of the physical object, or optimizing and predicting the characteristics of the product life cycle based on its past and present states [17].

In [20], information on various factors enabling the application of DTs in industry and creating barriers to their implementation is systematized. Currently, there are two approaches to describing DTs [21]:

– a full equivalent of a cyber-physical system;

– only one, key and fundamental, component of a cyber-physical system out of several possible ones [22]. This also stresses the opinion that a true DT provides an automatic bidirectional data transfer between the digital and the physical counterparts [23]. This distinguishes DTs from digital models with manual information transfer and from digital shadows, in which the collection of information from the physical object to the digital analogue is automatic and the reverse data transfer is done manually [24].

The authors [25] provide information on existing methods for designing DTs, based on data from a real object[6], or from a real physical system [26], or a combination of these approaches, resulting in the greatest added value and functionality of the twin.

Although Industry 4.0 proposes the use of DTs in industry for predictive maintenance and aftermarket analysis, there are few applications in this area. This is due to imperfect methodology for developing real-time DT models, limited synchronization capabilities between the digital and physical object [27], problems with Big Data collection and processing, a lack of highly accurate models for multilevel object representation, and difficulties in implementing them in production, including due to companies' resistance to change. New generation information technology [28], which provides a continuous exchange of information between DT and production facilities [29], can help to resolve this problem.

There are successful examples of application of DTs for solving problems of optimization of industrial plants. These include the optimization of the reactor unit of styrene production in the Tabriz petrochemical complex using an artificial neural

[5] Booth A., Patel N., Smith M. Digital transformation in energy: Achieving escape velocity. 2020. Available from URL: https://www.mckinsey.com/industries/oil-and-gas/our-insights/digital-transformation-in-energy-achieving-escape-velocity#. Accessed January 5, 2022.

[6] Steve Miller. Predictive Maintenance Using a Digital Twin. 2019. Available from URL: https://www.mathworks.com/company/newsletters/articles/predictive-maintenance-using-a-digital-twin.html. Accessed January 5, 2022.

network and an adaptive neuro-fuzzy inference system [30], improving the energy efficiency of furnace equipment using a DT integrated into the SCADA system [31] and coke formation prediction at a catalytic cracking unit [32].

In this regard, it is thus pertinent to identify the principles of creating a DT of the process of liquid-phase alkylation of benzene with propylene, a prototype of an intelligent industrial process control system.

MATERIALS AND METHODS

Chemical process description

The method of coproduction of phenol and acetone by oxidation of cumene obtained by gas-phase alkylation of benzene with propylene over $AlCl_3$ catalyst, was first developed and introduced into industrial production in the Soviet Union by a group of chemists (P.G. Sergeev, R.Yu. Udris, and B.D. Kruzhalov). At present in global industry, cumene is mainly produced on zeolite catalysts (licensors of the modern alkylation process are such companies as BADGER[7], UOP[8], LUMMUS[9], and IFP[10]) [33, 34]. Processes for the production of cumene, phenol, and acetone from cumene are constantly being improved. Various methods for intensifying the process have been proposed, for example by optimizing the recycle flows in the alkylation process or introducing ozone as an initiator in the cumene oxidation process [35].

Works are known in which the optimization of the alkylation process was carried out by means of traditional technological methods (carrying out the process using a reactive distillation column [36], the introduction of additional separation columns [37]). Other authors have proposed ways of intensification based on the results of mathematical modeling using conventional approaches. Thus, the authors of [38] applied a computer model written in Borland Delphi and defined the optimal parameters of the alkylation process to increase product yield and decrease catalyst consumption. In previous studies [39], we proposed a model of the reactor block in Aspen® HYSYS (*Aspen Technology, Inc.*, USA)[11], which enables the cumene yield in the alkylator to be calculated with sufficient accuracy and optimal parameters of the process conditions to be selected depending on the required productivity. At the same time, the results of such modeling are "idealized", since it is not possible to take into account all the factors of real production. Therefore, the optimal operating parameters calculated on the basis of such models cannot be directly applied in real faculties and require additional clarification. The regulation of technological mode parameters is performed by means of the SCADA, based on the laws of proportional–integral–derivative regulation. However, the main responsibility for making decisions on the choice of operating parameters lies with operators. This can lead to errors due to human factor, including suboptimal process management and loss of profit share.

Application of DTs based on neural network modeling technologies not only allows all the factors affecting the equipment (including hidden ones) to be taken into account, but also plant operation to be reproduced as accurately as possible and continuously synchronized. As a result, it is possible to regulate process mode parameters by applying a new type of controllers integrated into intelligent cyberphysical systems and automatically to optimize plant operation online without operator intervention. This approach is currently the first step towards the creation of smart manufacturing, or more correctly called intelligent manufacturing.

In [40], for the liquid-phase alkylation process, modeling was performed using two-layer neural networks. The optimum values were calculated for temperature and pressure in the reactor, as well as its length, allowing the maximum yield of cumene to be obtained. The authors [41], simulated the yield and selectivity of benzene alkylation reaction products formation with propylene using two-layer neural networks and compared the calculated data with the experimental results with an average relative error ranging from 3.7% to 7.7%.

However, there is no information in the literature regarding the creation of DTs of the process of liquid-phase alkylation of benzene with propylene based on neural networks, in which the output parameter is the profit of the process unit.

Creating a database of raw data

The creation of a DT of the cumene production process implies the development of a virtual model which enables not only the process conditions to be reliably repoduced, but also, as a result of continuous analysis of stream data, to regulate the process faster than the operator can react to the event.

[7] Badger Licensing LLC. 2021. Available from URL: https://www.badgerlicensing.com/. Accessed January 5, 2022.

[8] UOP. 2022. Available from URL: https://uop.honeywell.com/. Accessed January 5, 2022.

[9] Lummus Technology. 2022. Available from URL: https://www.lummustechnology.com/. Accessed January 5, 2022.

[10] IFP Energies nouvelles (IFPEN). 2022. Available from URL: https://www.ifpenergiesnouvelles.com/. Accessed January 5, 2022.

[11] Aspen Technology, Inc. 2022. Available from URL: https://www.aspentech.com/en. Accessed January 5, 2022.

In order to develop such a virtual model of a chemical technological process, the operation of a complex multiparameter system must be reproduced.

The first step in creating a DT is simulation using data, obtained from the factory set. In order to show the possibility of developing a model of a DT of the process, despite the lack of data from a real process unit, we created our own initial database by simulating the process unit in the Honeywell UniSim® Design[12] software .

The reactor was modeled according to the method described in [39]. In order to form a detailed model of the alkylation reactor, 13 chemical reactions (1 main and 12 side) were used, the kinetic parameters of which are given in Table 1. As part of the creation of a DT model, it was assumed that the kinetic parameters of the reactions were constant in the range of the selected values of temperature and pressure.

In a continuation of studies of the alkylation process, the reactor model was supplemented with a separation system using commercial-grade cumene production.

The design scheme includes three blocks: raw materials preparation, reaction block, and a separation system. The process equipment consisted of a reactor for alkylation and transalkylation reactions, two columns—atmospheric column for extracting benzene from the reaction mass and a vacuum column for separating a mixture of cumene and diisopropylbenzenes, a separator for separating off-gases, six heat exchangers, a mixer, and a pump.

Figure 1 shows a simplified scheme for the production of cumene.

In the feed preparation unit, the initial benzene and propylene are mixed with recycled diisopropylbenzenes (Dcumene) in the mixer M-1, then heated to 60 °C. This mixture is fed to the reaction unit, modeled on the basis of the equilibrium reactor R-1 and the separator SK-1. From here unreacted off-gases (propane, ethane) are released. This reactor is characterized by complete conversion of propylene into reaction products. The selectivity for cumene is about 99%.

The separation system is a system of columns RC-1 and RC-2. Column RC-1 is designed to extract benzene from the reaction mass which returns

Table 1. Kinetic parameters of the reactions of the alkylation of benzene with propylene at a temperature of 122 °C and a pressure of 1.6 bar

Reaction	A_0, c^{-1}	E_a, kJ/mol	k, c^{-1}
1	2	3	4
$C_6H_6 + C_3H_6 \rightarrow i\text{−}C_6H_5CH(CH_3)_2$	$1.58 \cdot 10^5$	150.94	$3.74 \cdot 10^{-12}$
$C_6H_5CH(CH_3)_2 + C_3H_6 \rightarrow C_6H_4(CH(CH_3)_2)_2$	$2.26 \cdot 10^5$	128.81	$1.47 \cdot 10^{-9}$
$C_6H_4(CH(CH_3)_2)_2 + C_3H_6 \rightarrow C_6H_3(CH(CH_3)_2)_3$	$1.80 \cdot 10^4$	140.64	$5.81 \cdot 10^{-12}$
$C_6H_6 + C_3H_6 \rightarrow n\text{−}C_6H_5C_3H_7$	$1.28 \cdot 10^5$	130.41	$5.53 \cdot 10^{-10}$
$2C_3H_6 \rightarrow C_6H_{12}$	$1.97 \cdot 10^5$	116.20	$6.68 \cdot 10^{-13}$
$2C_2H_4 \rightarrow CH_2{=}CH\text{−}C_2H_5$	$1.65 \cdot 10^6$	166.98	$7.64 \cdot 10^{-10}$
$2\ C_2H_4 \rightarrow CH_3\text{−}CH{=}CH\text{−}CH_3$	$2.92 \cdot 10^6$	141.47	$2.00 \cdot 10^{-9}$
$2C_2H_4 \rightarrow CH_2{=}C(CH_3)_2$	$3.95 \cdot 10^6$	138.86	$3.13 \cdot 10^{-8}$
$C_6H_6 + CH_2{=}CH\text{−}C_2H_5 \rightarrow C_6H_5CHCH_3C_2H_5$	$5.45 \cdot 10^6$	159.90	$1.33 \cdot 10^{-11}$
$C_6H_6 + CH_2{=}C(CH_3)_2 \rightarrow C_6H_5C(CH_3)_3$	$5.65 \cdot 10^5$	158.23	$2.11 \cdot 10^{-12}$
$C_6H_6 + CH_2{=}CH\text{−}C_2H_5 \rightarrow C_6H_5C_4H_9$	$1.42 \cdot 10^6$	147.95	$7.18 \cdot 10^{-11}$
$C_6H_6 + C_2H_4 \rightarrow C_6H_5C_2H_5$	$7.16 \cdot 10^5$	37.40	$5.15 \cdot 10^{-10}$
$C_6H_5C_2H_5 + C_2H_4 \rightarrow C_6H_4(C_2H_5)_2$	$2.90 \cdot 10^4$	129.58	$1.55 \cdot 10^{-10}$

Note: A_0 is the pre-exponential factor or Arrhenius equation, E_a is the activation energy for the reaction, k is the rate constant.

[12] Honeywell International Inc. 2022. Available from URL: https://honeywell.com. Accessed January 5, 2022.

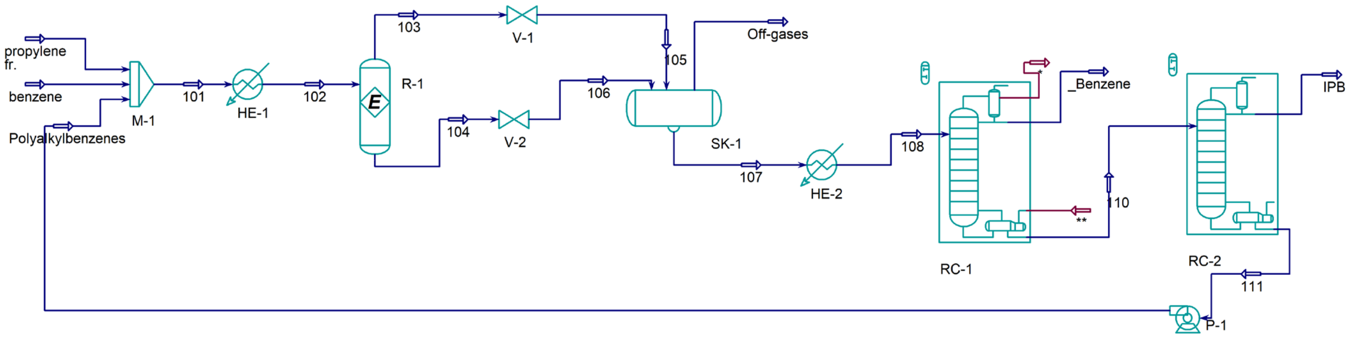

Fig. 1. Simplified scheme for the production of cumene:
M-1 – mixer; HE-1, HE-2 – heat exchangers; R-1 – reactor; SK-1 – separator; RC-1, RC-2 – distillation columns.

to the feed preparation unit (not shown in the diagram). The column has 56 valve trays, the top and bottom temperatures are 108.5 and 186.0 °C, respectively. A mixture of cumene and Dcumene is fed into the RC-2 vacuum separation column, where they are separated at a column top pressure of 200 mm Hg. Column RC-2 consists of 23 valve trays, top and bottom temperatures are 134.0 and 189.0 °C, respectively. From above, commercial-grade cumene is obtained, and Dcumenes are removed from the cube, which are sent for mixing with the initial benzene and propylene.

The temperature (from 128 to 147 °C) and pressure (0.15 to 0.24 MPa) of the process in the reactor, the ratio of benzene to propylene (from 3:1 to 4:1), corresponding to the operating ranges of the installation under consideration were selected as input parameters of the neural network. The output parameter, in contrast to the works of other authors, is the principle profit from the process.

The values of the principal profit from the sale of cumene *PP*, RUR/h, were calculated by Eq. (1), taking into account the income from the sale of cumene and the cost of energy resources of the installation.

$$PP = C \cdot i \cdot P_i - a \cdot P_a - b \cdot P_b - c \cdot P_c, \quad (1)$$

where C is the cumene concentration in a commercial product, i is the amount of cumene produced, kg/h, a is the water vapor consumption, kg/h, b is the circulating water consumption, kg/h, c is the electricity consumption, kW/h, is the calculated data obtained from the model. Constant values: P_i is the price of commercial cumene, accepted at 4.7825 RUR/kg, P_a is the price of water vapor, accepted at 1.19 RUR/kg, P_b is the price of circulating water, accepted at 7.11 RUR/kg, P_c is the price of electric power, accepted at 2.50 RUR/kW.

The energy requirements are determined using the UniSim® Design cumene production plant model. Steam is used as a heat carrier in reboilers of columns RC-1 and RC-2, heat exchangers of propylene fraction and benzene (HE-1, HE-2), and a feed preheater in front of the reactor. Recycled water is used in the condensers of the columns RC-1, RC-2, in order to reduce the temperature in the reactor and cool the bi-Dcumenes after the column RC-2. The P-1 pump consumes electric power.

Selection of the topology and learning algorithm for the neural network

The data obtained as a result of modeling the technological unit in the UniSim® Design software was used to create a predictive neural network model of the process. Based on the structural approach, this enables the principal profit of the unit to be established depending on the feedstock composition, the temperature of the process, and the pressure in the reactor.

We used a two-layer direct communication network with sigmoidal transfer functions (2) of neurons in the hidden layer:

$$\sigma(x) = \frac{1}{1 + e^{-x}} \quad (2)$$

and linear transfer functions in the output layer of neurons (Fig. 3). The choice was due to the fact that such a neural network configuration takes into account the non-linear effects of the original process model. However, at the same time, the computational complexity of the sigmoid function allows it to be used in devices with limited performance (embedded solutions, microcontrollers, etc.). The two-layer network was chosen because in the paper [41], when solving a similar problem, reliable results were obtained.

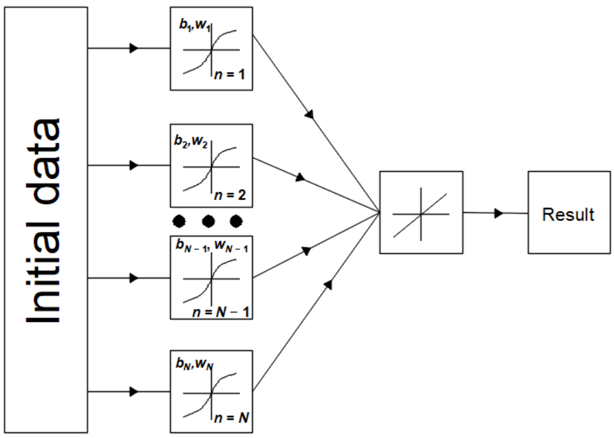

Fig. 3. Model of the used neural network. $b_1 \ldots b_N$ are bias terms of each perceptron, $w_1 \ldots w_N$ are weight vectors of each perceptron, n is the index, N is the number of perceptions in model.

All data was divided into 3 groups: learning curve (70%), training sample (15%), and data for testing the network (15%).

The learning curve is used to train the neural network, after which the neural network is trained in one iteration. Then the learning curves and training samples are mixed and the process is repeated until the minimum value of the standard deviation of the training sample is found. Subsequently the neural network is tested with the calculated values of weights and biases on the data for validation.

We used the Levenberg–Marquardt algorithm (backpropagation algorhythm), Bayesian regularization algorhythm and scaled conjugate gradient algorhythm in the MATLAB® software package[13] (*MathWorks*, USA). The choice of the neural network training algorithm was made by comparing the regression coefficient R.

CALCULATION OF TRANSFER FUNCTIONS COEFFICIENTS

When creating a DT based on a neural network model, the process of continuous receipt at the input of the neural network model of the initial process parameters needs to be organized (in this case, temperature, pressure, reagent ratio) along with their transformation into the output data of the model (in this case, principal profit). In order to produce the model in the form of a computational module of the DT of the process, calculation of transfer functions coefficients is required. This was performed using a program written in Python programming language using the NumPy[14] and Pandas[15] libraries.

When calculating the coefficients, the network topology and the learning algorithm selected in the previous stage in MATLAB® software were used.

RESULTS AND DISCUSSION

After modeling, we obtained a database for creating a DT. Database includes 2100 values by varying the input parameters (temperature, pressure in the reactor and the benzene/propylene ratio) in the operating ranges of the plant under consideration. At each step, UniSim® Design performed calculation of the entire model, the costs of commercial-grade cumene and energy resources were determined, and then the principal profit was calculated.

The model created in UniSim® Design is three-parameter. The assessment of the reliability of the data obtained was carried out by comparing one-factor calculations and known theoretical laws.

With a benzene/propylene ratio equal to 3:1 (Fig. 2a), an increase in the principal profit is observed with an increase in pressure from 0.15 to 0.24 MPa and an increase in temperature from 128 to 140 °C. Fluctuations of the principal profit values are explained by the multifactorial influence of energy consumption in the columns of the separation system. Increasing the temperature in the reactor increases the process rate, but is thermodynamically disadvantageous due to the exothermicity of the process. Despite the increase of energy consumption in the reactor and a decrease in the selectivity of the target reaction, with an increase in the process temperature, costs are compensated by reducing the consumption of steam in the separation columns and growth of the principal profit.

An increase in pressure leads to an increase in the principle profit by increasing the product yield from the reactor, reducing steam and cooling water consumption, even though the circulating pump's power consumption increases.

Carrying out the process with a benzene ratio of 4:1 (Fig. 2b) is economically unprofitable for any combinations of temperature and pressure (negative principal profit), since, although feeding more benzene into the reactor leads to greater process selectivity, the cost of benzene separation in the K-1 column exceeds the effect of higher cumene yield.

[13] MATLAB. 2022. Available from URL: https://www.mathworks.com/products/matlab.html Accessed January 5, 2022.

[14] NumPy. 2022. Available from URL: https://numpy.org/. Accessed January 5, 2022.

[15] Pandas. 2022. Available from URL: https://pandas.pydata.org/. Accessed January 5, 2022.

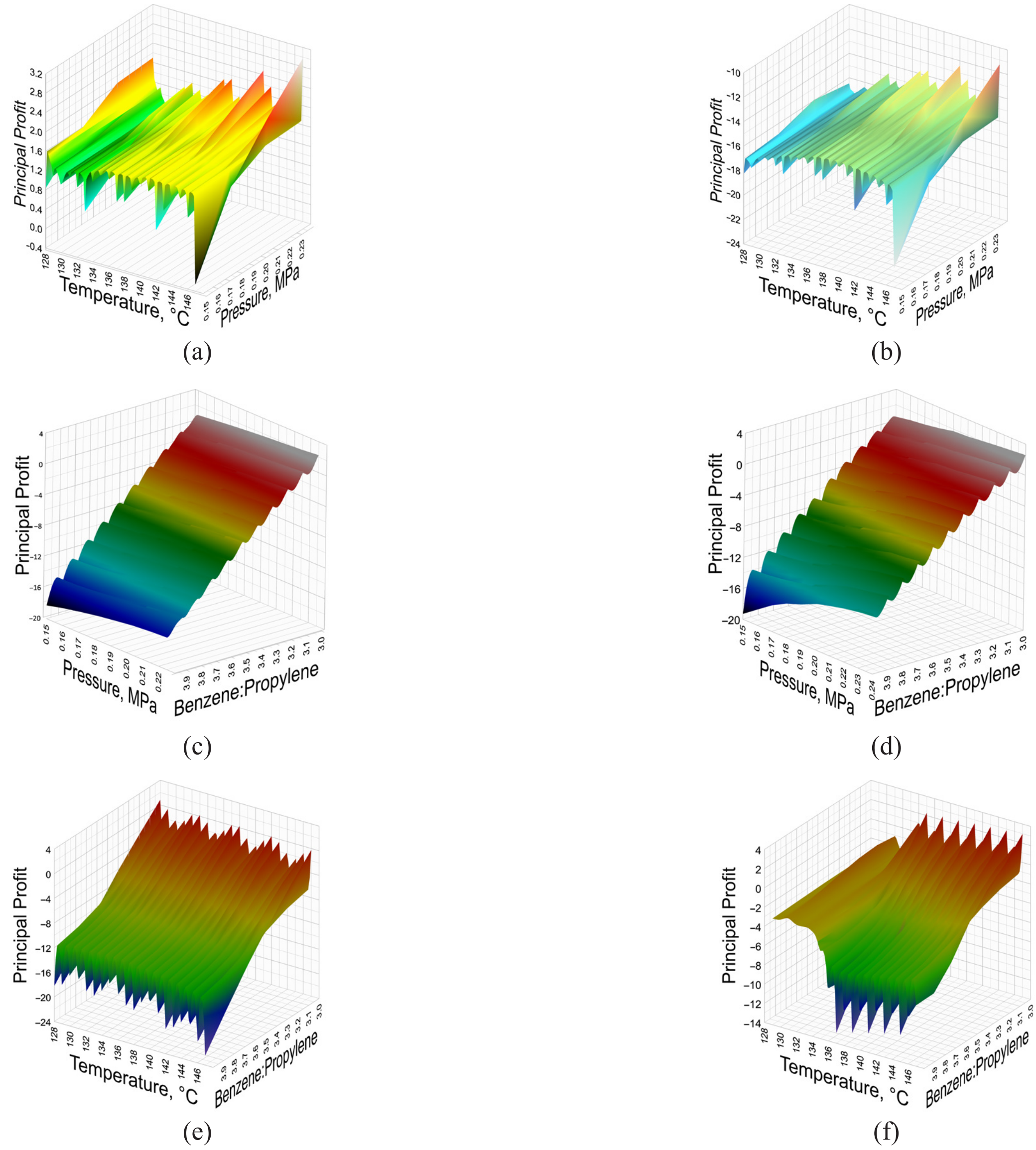

Fig. 2. Dependence of the principal profit on the parameters of the technological process at fixed values: The benzene/propylene ratio = 3:1 (a), 4:1 (b), temperature in the reactor 128 °C (c), 140 °C (d), pressure in the reactor 0.15 MPa (e), 0.24 MPa (f).

At a fixed temperature of 128 and 140 °C (Figs. 2c and 2d), the pressure increase does not lead to a significant increase in the principal profit. At the same time, increasing the amount of fed benzene in relation to propylene significantly reduces the principle profit due to the growth of costs of benzene separation in the column RC-1.

At a minimum fixed pressure of 0.15 MPa (Figs. 2e and 2f), the increase in temperature does not significantly affect the principal profit, while at a pressure of 0.24 MPa, a slight increase in the principal profit is observed.

Thus, the maximum principal profit is achieved with a minimum benzene/propylene ratio of 3:1 and temperatures and pressures of 140 °C and 0.25 MPa, respectively. This corresponds to the known theoretical laws.

Nevertheless, in a real process unit, the process is not carried out at the maximum parameter limit (due to triggering of interlocks, the need to ensure the safety of the technological process). Within the ranges, the influence of process parameters on the principal profit is non-linear, therefore, the selection of regression equations describing the process accurately enough is extremely difficult in this case, Optimization requires methods to be used which describe non-periodic series with a trend other than linear, such as neural networks.

The choice of neural network training algorithms (Levenberg–Marquardt algorithm (backpropagation algorhythm), Bayesian regularization algorhythm and scaled conjugate gradient algorhythm) was made by comparing the regression coefficient R. The smallest standard deviation corresponds to the back-propagation algorithm with 12 neurons in the first hidden layer. In this case, the neural network is trained for 54 epochs (Table 2, Fig. 4).

The program allows for the continuous refinement of the transfer functions coefficients, while taking into account the possible arrival of new initial data from production plants (Table 3).

Development of the DT prototype

We chose the ESP8266 microcontroller developed by *Espressif Systems* (Chine) as a prototype of an industrial ACS (automatic control system) controller with an implemented DT: one of the leaders in the development of hardware solutions for the IoT.

The advantages of ESP8266 as a model tool in comparison with other microcontrollers are: prevalence, low price, standard programming language "C", open-source program code, libraries, availability of sensor expansion boards, input-output devices, availability of standard input-output ports (with I2C, SPI, UART, GPIO interfaces), an analog-to-digital converter, which allows for data acquisition and demonstration platform processing, as well as easy integration with industrial controllers. Also, the microcontroller has sufficient computing and communication capabilities for it to be used in solutions for the IoT (single-core 32-bit LX6 microprocessor, up to 160 MHz, program memory 4 MB, ROM 2.4 MB, RAM 32 KB, WiFi module) [43], [44].

This device is programable using specialized software: compiler, linker, and programmer. We used the PlatformIO integrated development environment to create a program [45] to calculate the principal profit of the production unit based on technological parameters. The program was loaded into a microcontroller which will independently receive the initial data from the sensors and produce the result.

Thus, we were able to create a prototype of a DT based on a microcontroller, allowing for the operation of a cumene production unit to be simulated and the process mode optimized. When training a neural network based on data from a real operating plant, the neural network can automatically take into account the specific features of the technological process.

Table 2. Results of neural network modeling

Number of neurons in the hidden layer	Algorithm								
	Backpropagation			Bayesian regularization			Scalable conjugate gradients		
	Number of epochs	Standard deviation MSE	Regression value *R*	Number of epochs	Standard deviation MSE	Regression value *R*	Number of epochs	Standard deviation MSE	Regression value *R*
1	24	1.37	0.9905	48	0.92	0.9926	57	0.76	0.9934
2	94	0.18	0.9986	50	0.12	0.9991	63	0.72	0.9935
3	71	0.23	0.9982	170	0.18	0.9985	200	0.23	0.9982
4	18	0.20	0.9985	72	0.31	0.9976	112	0.55	0.9958
5	45	0.18	0.9986	240	0.11	0.9991	79	0.10	0.9991
6	22	0.36	0.9972	126	0.20	0.9985	66	0.15	0.9989
7	50	0.43	0.9969	258	0.19	0.9986	84	0.36	0.9972
8	17	0.09	0.9993	538	0.31	0.9975	140	0.38	0.9970
9	27	0.37	0.9972	684	0.29	0.9976	62	0.73	0.9940
10	20	0.07	0.9995	673	0.18	0.9985	191	0.42	0.9969
11	43	0.29	0.9977	323	0.08	0.9994	48	1.70	0.9886
12	**54**	**0.03**	**0.9998**	**353**	**0.17**	**0.9986**	**235**	**0.17**	**0.9986**
13	80	0.06	0.9995	1000	0.48	0.9963	211	0.21	0.9982
14	48	0.31	0.9975	1000	0.35	0.9973	222	0.76	0.9940
15	13	0.05	0.9997	803	0.17	0.9985	240	0.27	0.9980

Note: MSE is a mean squared error.

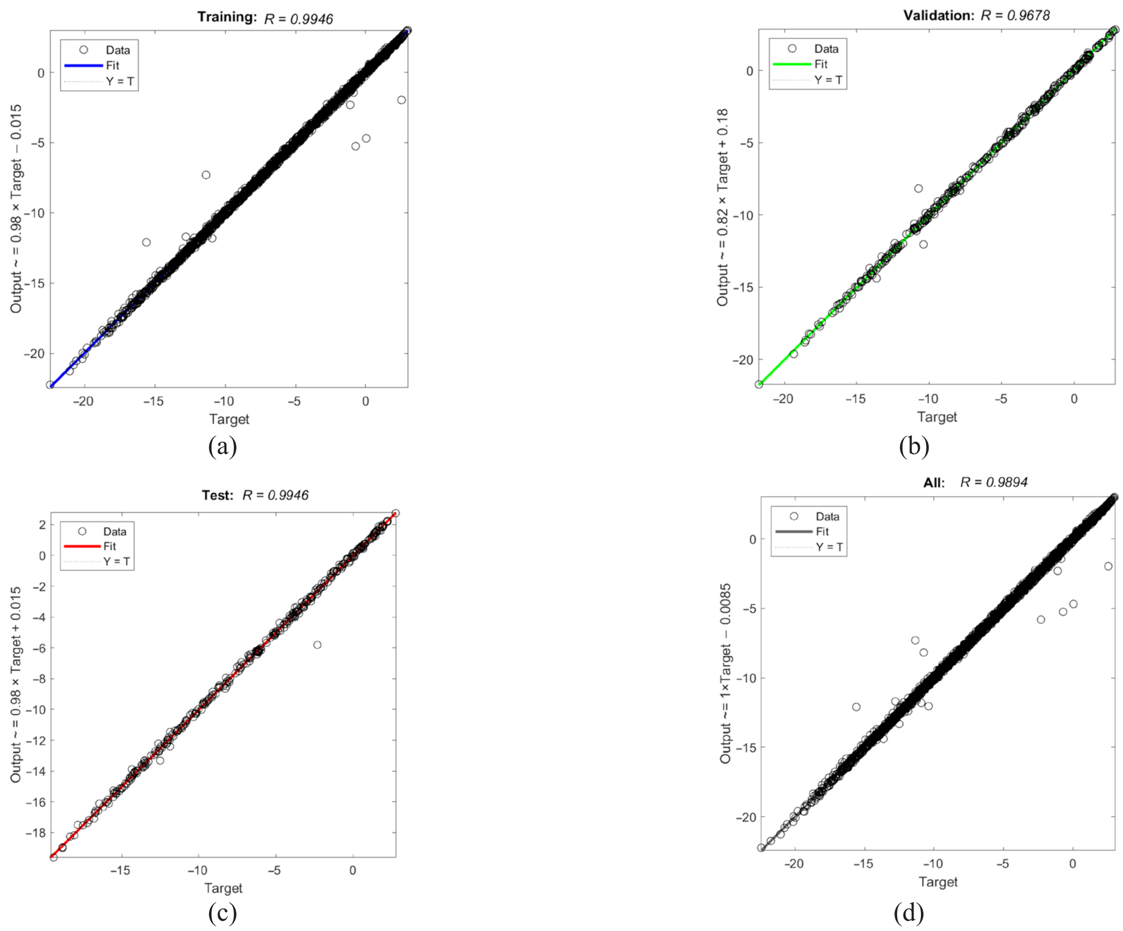

Fig. 4. The results of the selection of the neural network configuration: (a) on the learning curve (70% of the data), (b) on the test set (15% of the data), (c) on the control sample (15% of the data), (d) on all the data (100% of the data). Target is the target value of the principal profit, Data is the calculated points, Fit is the result of the neural network, Y = T (Output = Target) is the perfect match line.

Table 3. Coefficients of the transfer function of the neural network

First hidden layer					Second hidden layer		
Neuron number	Coefficients				Neuron number	Coefficients	
	b	w_1	w_2	w_3		b	w
1	2.388	−1.982	−1.258	0.410	1	−0.381	−0.020
2	−2.198	1.085	−1.129	−2.321			0.027
3	−1.643	0.623	−0.406	0.549			−1.196
4	2.214	−2.470	0.227	−0.473			−0.027
5	0.186	−0.254	0.028	−1.003			0.223
6	0.168	0.531	0.207	−0.315			0.547
7	0.338	1.550	−1.577	−1.462			0.023
8	−1.475	−0.512	−0.040	−0.480			0.905
9	1.997	0.659	−2.912	0.074			−0.009
10	1.417	0.409	−0.742	−0.903			0.186
11	−1.433	−1.565	−2.107	1.744			−0.010
12	−2.498	−1.126	−0.720	1.040			−0.145

Note: b is the bias term of each perceptron, w_1, w_2, w_3, w are weight vectors of each perceptron.

Based on the prototype, it is planned to create simulators for training production personnel, as well as integrated solutions for optimizing the operation of process units.

The production of cumene is large-scale, so the implementation of the results of this work in terms of the use of new digital technologies may be associated with certain difficulties due to lack of motivation, inertia and lack of obvious need to change the technological base.

Also the promotion of DTs in industry is strongly influenced by the shortage of integrated circuits and financial crises, during which the management seeks to maintain production, while avoiding risks associated with the introduction of innovative technologies and approaches in production. An important factor when creating DTs based on big data from manufacturing, is that the data generated must be professionally and efficiently processed and filtered for subsequent analysis; otherwise the results will be unreliable. There may also be uncertainties associated with errors in the operation of instrumentation, controllers, and actuators of the control system. A partial solution of this problem may be the involvement of a group of qualified specialists, consisting of programmers, technologists, and scientists for screening, classifying and filtering the meaningful data from the database.

A DT obtained using big data, based on a simulation model, cannot in principle take into account all the factors which impact a real plant. Therefore, the DT obtained in this way must be adapted to each specific industrial plant, training it further on data from a real plant.

Our proposed DT prototype can be used in the future to create simulators, useful for training personnel of cumene production.

Further research will be directed towards the creation of an aggregated cumene production twin. This is a cyberphysical system and is characterized by a continuous two-way data exchange with real plants [44]. Data exchange within a cyberphysical system can be organized using a blockchain platform which can serve as a data management tool within the company. With the ever-increasing need for connectedness and security, especially in the petrochemical industry, blockchain may provide the backbone of the manufacturing future [45].

DT creation principles

Based on our research, using the example of the process of liquid-phase alkylation of benzene with propylene, we established the following stages in creating a DT, also applicable for any petrochemical process:

1. The formation of database of information about the functioning of a technological object, which can be performed in two ways:

– collection of process parameters by processing mode sheets of production operators, or collecting data directly from SCADA of a technological facility;

– calculation of the basis process parameters (pressure, temperature, reaction time, reflux ratio, energy consumption, etc.) by modeling the process using specialized software.

2. Defining the preferred algorithm for training a neural network model and calculation of its basic parameters (number of neurons and layers, types of transfer functions, etc.).

3. Assessment of the adequacy of the chosen neural network model using statistical methods criteria.

4. Calculation of the parameters of transfer functions required to predict the optimal parameters of technological modes of production facilities.

5. Selection of an intelligent system (IC) for industrial process control: a prototype of a DT, taking into account the scope and parameters of the application.

6. Programming of an intelligent industrial process control system, testing, pilot tests at an industrial plant.

7. Performing stages 1–6 for all technological objects and production processes.

8. Creation of an aggregated production twinon, including the developed DTs of related technological objects and their continuous data exchange with real installations, in order to clarify the functioning parameters.

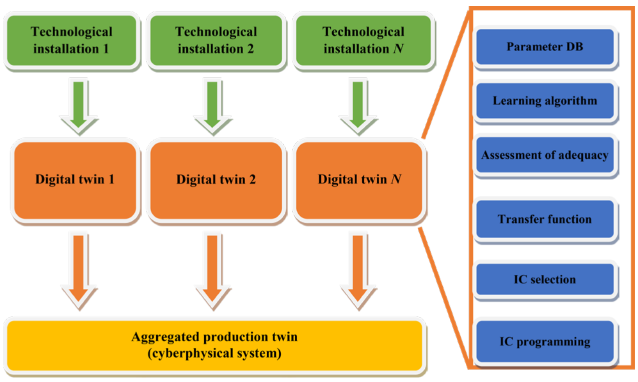

Fig. 5. Cyberphysical system creation algorithm.

CONCLUSIONS

The process of liquid-phase alkylation of benzene with propylene is one of the main large-scale petrochemical processes. At the same time, there is a need to create a cyber-physical system to control and continuously optimize production.

In this article we demonstrated an algorithm aimed at developing a digital production twin as the first step in creating a cyber-physical system. Using the results of the UniSim® Design simulation of the real plant a set of technological data was created and a neural network was built. This allows the economically optimal technological mode of the plant to be defined in online mode. In the process of forming the neural network. the principles of creating a digital duplicate of the process were established, and a prototype of the intelligent process control system was developed.

Given the importance of digital transformation, including the application of DTs and cyber-physical systems in industrial enterprises, the methodology developed to create a DT for the production of cumene by alkylation of benzene with propylene is also significant. The paper systematizes the principles of creating a DT production, as a comprehensive expert system of predictive analysis of production processes.

The practical application of the results of our study is to create a prototype of a DT based on a microcontroller for cumene production unit. A microcontroller control program based on neural network technology was created to enable online optimization of technological mode parameters to be carried out under continuous conditions.

It was shown that it is possible to form a technological database for training of DT in two ways. The first way consists in the processing of technological parameters, acquired from production. In the case of a lack of technological data, they can be obtained simulating the plant, for example, using UniSim® Design.

The implementation of the digital intelligent system will significantly reduce the response time of the operator or control system to changes in technological parameters. It will contribute to reduced costs and the number of measures required to optimize industrial technological processes, as well as improved efficiency and enhanced environmental friendliness of oil and gas chemical production.

Authors' contributions

K.G. Kichatov – writing and editing the text of the research article, methodology, hardware management, microcontroller programming (communication interface, neural network optimization).

T.R. Prosochkina – conceptualization, formal analysis, writing and editing.

I.S. Vorobyova – UniSim® Design simulation, neural network building and training, microcontroller programming.

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this document.

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Поступила: 30.09.2022; получена после доработки: 29.01.2023; принята к опубликованию: 09.10.2023.
The article was submitted: September 30, 2023; approved after reviewing: January 29, 2023; accepted for publication: October 09, 2023.

The text was submitted by the authors in English
Edited for English language and spelling by Dr. David Mossop