IRSTI: 27.35.21 **https://doi.org/10.58805/kazutb.v.1.30-1409**

DEVELOPMENT OF MATHEMATICAL MODELS OF THE MAIN UNITS OF THE SULFUR PRODUCTION UNIT BASED ON SYSTEM ANALYSIS

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A methodology has been proposed for constructing a package of models for technological systems composed of interconnected units, based on diverse available information. This methodology is demonstrated through the development of models for the main units of the sulfur production block. The models describing the relationship between sulfur yield at the reactor outlets and their input and operating parameters were identified as a system of multiple regression equations, using aggregated experimental, statistical, and expert data, along with the sequential inclusion of regressors approach. Models assessing the sulfur quality at the Claus reactor outlet were constructed as fuzzy regression equations. Parametric identification of the regression coefficients was performed using the least squares method in the REGRESS software package, while fuzzy regression coefficients were determined using modified least squares and α-level sets within the framework of fuzzy set theory. As a result, mathematical models of the thermoreactor and Claus reactor at the Atyrau refinery's sulfur production unit were developed.

Keywords: sulfur production unit, mathematical model, system analysis, fuzzy information, fuzzy model, structural and parametric identification.

КҮКІРТ ӨНДІРУ БЛОГЫ НЕГІЗГІ АГРЕГАТТАРЫНЫҢ МАТЕМАТИКАЛЫҚ МОДЕЛЬДЕР КЕШЕНІН ЖҮЙЕЛІК ТАЛДАУ НЕГІЗІНДН ҚҰРУ

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Өзара байланысқан агрегаттар кешенінен тұратын технологиялық жүйенің модельдер пакетін әртүрлі қолжетімді ақпараттар негізінде және жүйелік талдау тәсілдерін қолдану арқылы құру методикасы әзірленіп, оны күкірт өндіру блогы мысалында жүзеге асыру көрсетілген. Жинақталған және өңделген эксперименталдық-статистикалық деректер мен эксперттік ақпараттар негізінде, сондай-ақ регрессорларды тізбектей қосу тәсілінің идеясын пайдалана отырып, реакторлар шығысындағы күкірт көлемін сипаттайтын модельдер құрылымы көп регрессиялық теңдеулер жүйесі түрінде идентификацияланған. Клаус реакторының шығысындағы күкірт сапасын бағалайтын модельдер айқын емес регрессиялық теңдеулер түрінде жасалған. Регрессиялық коэффициенттерді параметрлік идентификациялау ең кіші квадраттар әдісі арқылы REGRESS бағдарламалық пакетінде жүзеге асырылған, ал айқын емес коэффициенттерді анықтау α-деңгейлі жиындар негізінде айқын емес жиындар теориясының тәсілдері арқылы орындалған. Нәтижесінде, Атырау МӨЗ күкірт өндіру блогының термо және Клаус реакторларының математикалық модельдері құрылған.

Түйін сөздер: күкірт өндіру блогы, математикалық модель, жүйелік талдау, айқын емес ақпарат, айқын емес модель, құрылымдық, параметрлік идентификациялау.

РАЗРАБОТКА МАТЕМАТИЧЕСКИХ МОДЕЛЕЙ ОСНОВНЫХ АГРЕГАТОВ БЛОКА ПРОИЗВОДСТВА СЕРЫ НА ОСНОВЕ СИСТЕМНОГО АНАЛИЗА

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Разработана методика построения пакета моделей технологической системы, состоящей из взаимосвязанных агрегатов, на основе различных доступных данных с использованием методов системного анализа, и реализована на примере блока производства серы. На основе агрегированных и обработанных экспериментально-статистических данных и экспертной информации, а также с использованием идеи последовательного включения регрессоров, были идентифицированы модели, описывающие объем серы на выходе реакторов, в виде системы многорегрессионных уравнений. Модели, оценивающие качество серы на выходе Клаус-реактора, построены в форме нечетких регрессионных уравнений. Параметрическая идентификация регрессионных коэффициентов выполнялась с применением метода наименьших квадратов через программный пакет REGRESS, а нечеткие коэффициенты определялись с использованием методов теории нечетких множеств и преобразования на основе α-уровней. В результате были построены математические модели термо- и Клаус-реакторов блока производства серы Атырауского НПЗ.

Ключевые слова: блок производства серы, математическая модель, системный анализ, нечеткая информация, нечеткая модель, структурная и параметрическая идентификация.

Introduction. In oil refining production, for example at the Atyrau Oil Refinery, the existing sulfur production unit is a complex facility, that is, a system consisting of interconnected units influenced simultaneously by many different parameters [1]. The main units of the sulfur production block include reactors, namely the Claus reactor (R-001), thermal (SWS) reactors (R-002, R-003); condensers (E-001, E-002, E-004); a furnace (F-002); separators (D-001, D-004); and pumps (B-001, B-002) [2]. An analysis of approaches to developing mathematical models of such complex technological facilities has shown that issues related to constructing mathematical models of complexes consisting of interconnected technological units under conditions of insufficient initial information, as well as system modeling of their operation, remain insufficiently studied [3-8].

When developing mathematical models of industrial technological facilities and systems, problems arise due to the lack of initial information required for their construction.

Under conditions of uncertainty arising from the randomness of the initial information, it is recommended to apply probabilistic modeling or simulation modeling approaches [9-12].

However, if uncertainty arises due to the vagueness of the initial information-which is common in industrial practice-these approaches cannot be applied. In such cases, statistical data are insufficient or completely unavailable, and because the information is vague, it is impossible to collect quantitative statistical data. As a result, the axioms of probability theory (such as statistical stability of the object, repetition of experiments under identical conditions, etc.) are not satisfied, and therefore there is no basis for applying probabilistic approaches. Conducting active experiments for the purpose of collecting statistical data is either impossible or economically inefficient [13, 14]. Thus, in these situations, the main available information consists of vague information expressed in the form of words, statements, opinions, and judgments based on the knowledge, experience, and intuition of human decision-makers and expert specialists. In such cases, it is undoubtedly possible to compensate for the missing part of the information required for model development by using vague (fuzzy) information. That is, it is necessary to organize and conduct expert evaluation [15-17] and to process its results using methods of fuzzy set theory [18]. If the indicated sources of fuzzy information are reliable-namely, if the decision-makers and expert specialists are competent and the expert evaluation and its results are processed correctly-then on the basis of such information it is possible to construct models that take into account all complex interrelations between various parameters of complex, non-quantifiable industrial facilities and processes and that most closely correspond to real production conditions. The obtained fuzzy models, as a rule, describe real industrial facilities

and problems with higher adequacy than models constructed using traditional approaches (if such models can be constructed at all). Therefore, the development of mathematical models of technological systems in industry based on various available types of information, including fuzzy information, using the methodology of systems analysis, is a highly relevant task for both science and industry.

The aim of this work is to develop a methodology for constructing a complex of mathematical models for technologically complex units with difficult quantitative characterization, using the main units of the sulfur production block as an example, based on systems analysis, as well as to develop models of the main reactors of the sulfur production block.

Materials and Methods. It is necessary to formulate a methodology for constructing a system of mathematical models of industrial technological facilities that operate under conditions of insufficient initial information and uncertainty and are difficult to describe using quantitative data. Using the Claus reactor and thermal reactors as examples-where part of the available initial information is characterized by uncertainty-it is required to construct mathematical models of reactors R-001, R-002, and R-003 for the purpose of their optimal control, employing statistical data and fuzzy information [19]. Let us formulate the problem of developing mathematical models of the Claus and thermal reactors using statistical methods, expert evaluation, and approaches based on fuzzy set theory. As a result of collecting and processing the available initial information, it has been established that the statistical data required to estimate the sulfur yield (output) at the outlets of these reactors can be obtained experimentally. That is, statistical models determining the sulfur output at the reactor outlets can be constructed in the form of regression equations. Since quantitative information for assessing the quality of the produced sulfur is insufficient and cannot be collected, models for evaluating sulfur quality should be developed based on additional fuzzy information.

Thus, through an interconnected internal (parametric) and external (structural) cyclic process, the problem is formulated of identifying mathematical models of the sulfur production reactors under study in the form of the following set of regression and fuzzy regression equations:

$$y_j = a_{0j} + \sum_{i=1}^{n} a_{ij}x_{ij} + \sum_{i=1}^{n}\sum_{k=i}^{n} a_{ijk}x_{ij}x_{kj} + ...+, j = 1,2$$

$$\widetilde{y_j} = \tilde{a}_{0j} + \sum_{i=n+1}^{m} \tilde{a}_{ij}x_{ij} + \sum_{i=n+1}^{m}\sum_{k=i}^{m} \tilde{a}_{ijk}x_{ij}x_{kj} + ...+, j = 3,4.$$

The constructed models should adequately describe the sulfur yield at the outlets of the thermal reactors and the Claus reactor ($y_j,\ j = 1,2$) , as well as the fuzzy indicators characterizing sulfur quality, namely the mass fraction of sulfur and the mass fraction ($\tilde{y}_j,\ j = 3,4$) of water in the product obtained from the Claus reactor.

Solution approaches and results. The results of this work include a methodology for constructing mathematical models of technological facilities based on various types of information using systems analysis, as well as models of the Claus and thermal reactors. The units of the sulfur production block are interconnected, and changes in the operating parameters of one unit lead to changes in the parameters of others, thereby affecting the sulfur production process. Therefore, to optimize and control the sulfur production process, a system of models of the main units of the technological complex is required, constructed on the basis of systems analysis and taking into account the influence of technological parameters of each unit on the intermediate and final products of the entire complex. In order to develop such a system (package) of models, this work employs systems

analysis methods, probabilistic and experimental-statistical approaches, as well as expert evaluation and fuzzy set theory methods [20].

Let us formulate a methodology for constructing a complex of mathematical models of complex industrial technological facilities based on systems analysis. The model of each facility within a technological system can be developed using various approaches and methods; that is, for each unit of the sulfur production complex, a set of models may be obtained, for example deterministic, statistical, fuzzy, or structured models.

In order to integrate such diverse models into a single complex (model package) for the purpose of system-level modeling of the technological complex, a systems analysis of the advantages and disadvantages of each model to be constructed is required. This involves defining criteria that evaluate characteristics such as the costs required to develop the model, its accuracy, adequacy, applicability for the intended purpose, and so on, as well as establishing principles for combining the constructed models into a single package.

For this purpose, the various possible types of models for the main units of the sulfur production block have been systematically analyzed. Based on the study of the features of the sulfur production complex and process [21], experimental and expert evaluation data, and an analysis of modeling approaches for these or similar complex units, the possible model types for the main units of the sulfur production block have been assessed. The results of this analysis (model evaluation) are presented in Table 1. The main criteria used to compare the different types of models for evaluation are: the availability of information required to construct the model; the cost (complexity) of model development; the accuracy (adequacy) of the model; the applicability of the model for the intended purpose (in our case, solving multi-criteria optimization and control problems under conditions of uncertainty); and the possibility of integrating the model into a single system (package) for the purpose of system-level modeling of the entire facility.

Table 1 presents the evaluations of the possible models for the main units of the sulfur production block, obtained based on the processing of the results of the systematic analysis. Based on the information provided in the table, it is possible to select the most effective types of models for the main units of sulfur production according to the chosen criteria.

The construction of regression models for the reactors of the sulfur production block at the Atyrau Oil Refinery is complicated due to the lack or insufficiency of proper statistical information, the absence of specialized industrial instruments, and the low reliability of the available instruments. Therefore, as an effective tool to supplement the missing information with additional qualitative data-such as the knowledge, experience, and judgment of expert specialists-it is recommended to use expert evaluation methods, while the modeling approach should involve models and composite methods based on fuzzy set theory.

The accuracy of the constructed fuzzy or composite models is generally lower compared to other considered models; however, under conditions of uncertainty, they are fully sufficient for modeling, optimizing, and controlling sulfur production processes.

In practice, when information is insufficient, it is necessary to use all available types of data to construct a model. A model built on such diverse information is called a *composite model*. However, constructing a composite model can be inefficient, as it requires organizing and conducting various types of experiments and studies, as well as preprocessing the collected data.

Mathematical Models of the Sulfur Production Block Reactors. As determined from the results of the systematic analysis above, the models of the Claus and thermal reactors are constructed based on various types of information, including aggregated and processed statistical data, results of expert evaluations processed using fuzzy set theory methods, and material and heat balance equations.

Table 1 - Results of the Systematic Analysis of Possible Model Types for the Main Units of the Sulfur Production Block

№	Main units of the sulfur production block	Criteria	Types of Models			
			Deterministic	Statistical	Fuzzy	Composed
1	2	3	4	5	6	7
1.1	**Reactors** (R-001, R-002, R-003)	Availability of required information	2.5	4.5	4.5	5.0
1.2		Cost of model development	1.0	4.0	3.5	3.0
1.3		Model accuracy	4.5	3.0	2.5	4.0
1.4		Applicability to the need	3.5	4.0	3.5	5.0
1.5		Possibility of integration into one package	4.0	3.5	3.5	3.5
1.6		Model adequacy	3.0	3.5	3.5	4.0
		Sum of prices	**18.5**	**22.5**	**21.5**	**24.5**
2.1	**Capacitors** (E-001, E-002, E-004)	Availability of required information	3.5	4.5	4.0	4.0
2.2		Cost of model development	1.5	4.0	3.5	3.0
2.3		Model accuracy	4.5	3.5	3.5	3.5
2.4		Applicability to the need	4.0	4.0	4.0	4.5
2.5		Possibility of integration into one package	4.5	4.0	4.0	4.0
2.6		Model adequacy	3.5	3.5	3.5	3.5
		Sum of prices	**21.5**	**23.5**	**22.5**	**22.5**
3.1	**Oven** (F-002)	Availability of required information	4.0	5.0	4.5	4.0
3.2		Cost of model development	3.0	5.0	4.0	4.0
3.3		Model accuracy	4.5	4.5	3.5	4.0
3.4		Applicability to the need	4.0	4.0	4.0	4.0
3.5		Possibility of integration into one package	4.0	4.5	4.0	5.0
3.6		Model adequacy	4.0	4.5	4.5	5.0
		Sum of prices	**23.5**	**27.5**	**24.5**	**25.0**
4.1	**Separators** (D-001, D-004)	Availability of required information	4.5	5.0	4.0	4.5
4.2		Cost of model development	3.0	5.0	4.0	2.5
4.3		Model accuracy	4.5	4.5	2.0	4.0
4.4		Applicability to the need	4.0	4.5	4.5	4.5
4.5		Possibility of integration into one package	3.5	4.0	3.5	4.0
4.6		Model adequacy	4.0	4.0	3.5	4.0
		Sum of prices	**23.5**	**27.0**	**21.5**	**23.5**

5.1	**Extractors** (B-001, B-002)	Availability of required information	4.5	4.0	4.0	4.5
5.2		Cost of model development	5.0	4.5	4.0	4.0
5.3		Model accuracy	5.0	4.0	4.0	4.5
5.4		Applicability to the need	4.5	4.5	4.0	4.5
5.5		Possibility of integration into one package	4.5	4.0	4.0	4.0
5.6		Model adequacy	4.5	4.0	4.0	4.5
		Sum of prices	**28.0**	**25.0**	**24.0**	**26.0**

Note: The evaluation (ranking) uses a score scale (1-5), where 1 represents the lowest score and 5 the highest. The scores may be fuzzy, i.e., expressed as fuzzy numbers.

To identify the mathematical models of the reactors as multiple structural and fuzzy regression models, the approach of sequentially adding regressors [22] is used, while a modified form of the least squares method is employed for parametric identification [23].

Thus, using the mentioned approach of sequentially adding regressors, the structure of the mathematical models of the reactors was obtained in the form of the following multiple and fuzzy regression equations:

$$y_{TR} = a_0 + \sum_{i=1}^{4} a_i x_i + \sum_{i=1}^{4}\sum_{k=1}^{4} a_{ik} x_i x_k \quad (1)$$

$$y_{RC} = a_0 + \sum_{i=5}^{7} a_i x_i + \sum_{i=5}^{7}\sum_{k=i}^{7} a_{ik} x_i x_k \quad (2)$$

$$\tilde{y}_S = \tilde{a}_0 + \sum_{i=5}^{7} \tilde{a}_i x_i + \sum_{i=5}^{7}\sum_{k=i}^{7} \tilde{a}_{ik} x_i x_k \quad (3)$$

$$\tilde{y}_W = \tilde{a}_0 + \sum_{i=1}^{7} \tilde{a}_i x_i + \sum_{i=5}^{7}\sum_{k=i}^{7} \tilde{a}_{ik} x_i x_k \quad (4)$$

where: y_{TR} - sulfur yield at the outlet of the thermal reactor; y_{RC} - sulfur yield at the outlet of the Claus reactor; qualitative indicators of the produced sulfur: $\tilde{y}_S$ - fuzzy estimate of the sulfur mass fraction (depending on grade, from 99.20% to 99.98%); $\tilde{y}_W$ - fuzzy estimate of the mass fraction of water in the product (depending on grade, from 1.0% to 0.2%); input and operating parameters of the reactors affecting the sulfur production process (x_i, $i = \overline{1,4}$; x_i, $i = \overline{5,7}$;): x_1 - feed to the thermal reactor (26–28 t/h); x_2 - temperature in the thermal reactor (1000–1413 °C); x_3 - temperature at the outlet of the thermal reactor (180–350 °C); x_4 - flow rate of combustion air in the thermal reactor (200–700 Nm³/h); x_5 - feed to the Claus reactor (6–8 t/h); x_6 - temperature at the inlet of the Claus reactor (180–290 °C); x_7 - temperature at the outlet of the Claus reactor (300-345 °C); a_0, a_i, a_{ik}, $i = \overline{1,4}$, $k = \overline{i,4}$; and $\tilde{a}_0, \tilde{a}_i, \tilde{a}_{ik}$, $i = \overline{5,7}$, $k = \overline{i,7}$; - regression coefficients to be identified (with crisp and fuzzy notations): constant term affecting the reactor outlet parameters $(a_0, \tilde{a}_0)$; linear effects (x_i) ; quadratic and interaction effects (x_{ik}).

The obtained models (1)-(4) had their regression coefficients identified using the REGRESS software package based on the modified least squares method.

Thus, the results of the parametric identification of the models describing the relationship between the sulfur yield at the reactor outlets and their input and operating parameters are as follows:

$$\begin{aligned} y_{TR} = f_1(x_1, x_2, x_4) =& 0.686792x_1 + 0.012480x_2 + 0.052000x_3 + 0.260000x_4 \\ &+ 0.025917x_1^2 + 0.0000090x_2^2 + 0.0002080x_3^2 + 0.00005200x_4^2 \\ &+ 0.000471x_1x_2 + 0.000589x_1x_4 + 0.0000250x_2x_4 + 0.000104x_3x_4 \end{aligned}$$

$$\begin{aligned} y_{RC} = f_2(x_5, x_6, x_7) =& 0.6712330x_5 + 0.0171430x_6 + 0.0129230x_7 \\ &+ 0.0788140x_5^2 + 0.000058x_6^2 + 0.00003x_7^2 \\ &+ 0.000035x_5x_6 + 0.000589x_5x_7 + 0.0000250x_6x_7 \end{aligned}$$

The unknown fuzzy regression coefficients $\tilde{a}_0, \tilde{a}_i,\ i = \overline{5,7}$ and $\tilde{a}_{ik},\ i = \overline{5,7},\ k = \overline{i,7}$; of models (3) and (4), which describe the sulfur quality at the Claus reactor outlet, are evaluated using α-level sets with α = 0.5, 0.75, and 1.

As an example, we present $\tilde{y}_S$ - the identified fuzzy estimate of the sulfur mass fraction in the product at the Claus reactor outlet:

$$\begin{aligned} \tilde{y}_S = f_3(x_5, x_6, x_7) =& (0.5/0.037008 + 0.75/0.037020 + 1/0.037033 + 0.75/0.037045 + 0.5/0.037057) \\ &\cdot x_5 + (0.5/0.076885 + 0.75/0.076900 + 1/0.076915 + 0.75/0.076930 \\ &+ 0.5/0.076945)x_6 - (0.5/0.169430 + 0.75/0.169455 + 1/0.169475 \\ &+ 0.75/0.169495 + 0.5/0.169520)x_7 + (0.5/0.000010 + 0.75/0.000020 \\ &+ 1/0.000027 + 0.75/0.000034 + 0.5/0.000044)x_5^2 + (0.5/0.000093 \\ &+ 0.75/0.000108 + 1/0.000118 + 0.75/0.000128 + 0.5/0.000143)x_6^2 \\ &- (0.5/0.000007 + 0.75/0.000057 + 1/0.000574 + 0.75/0.000157 \\ &+ 0.5/0.000207)x_7^2 + (0.5/0.000050 + 0.75/0.000070 + 1/0.000080 \\ &+ 0.75/0.000090 + 0.5/0.00011)x_5x_6 - (0.5/0.000045 + 0.75/0.000065 \\ &+ 1/0.000075 + 0.75/0.000085 + 0.5/0.000105)x_5x_7 \\ &- (0.5/0.000174 + 0.75/0.000199 + 1/0.000209 + 0.75/0.000219 \\ &+ 0.5/0.000244)x_6x_7 \end{aligned} \tag{5}$$

Results and Discussions. From the results of the systematic analysis of the possible model types for the main units of the existing sulfur production block at the Atyrau Oil Refinery, it is evident-from the sum of the criteria values (18.5, Table 1)-that due to the complexity of the reactors and the processes occurring within them, the difficulty of their study, and the impossibility of obtaining theoretical information and necessary data, constructing deterministic models for the reactors is practically infeasible or economically inefficient.

According to the evaluation results, statistical (stochastic) and fuzzy models for the reactors of the sulfur production block received relatively high scores (21.5; 22.5). However, based on the sum of the criteria values, the most effective type of model for the reactors is the composite model (24.5). In other words, it is necessary to construct composite models for the reactors.

For the pumps, based on the criteria scores, constructing a deterministic model is more advantageous (28.0) compared to other model types, meaning that a deterministic model is the most

efficient choice for them (Table 1). As shown in the table constructed on the basis of systems analysis, for the condensers, furnace, and separators, building statistical models is the most optimal solution (23.5; 27.5; 27, respectively).

In constructing models of the units included in a technological complex, a decomposition approach is often used, in which the models of each unit are developed individually, without considering the integration of the obtained models into a single system. Solving system-level modeling tasks in this isolated manner does not yield the desired efficiency or positive outcomes. Since the operation of an individual unit in a technological system is interconnected with the operations of other units, modeling and optimizing a single unit alone cannot fully improve the performance of the entire system. Therefore, to comprehensively address the issues of modeling and optimizing a technological system, it is necessary to create a package of interconnected models that accounts for the relationships between units. By using such a model package, it is possible to perform system-level modeling of the technological complex. Systemic modeling of the technological complex allows for the identification of “bottlenecks” that limit its operation, and addressing these issues can significantly increase the capacity and efficiency of the technological complex and its processes.

The integration of individual unit models into a single system (package) must be carried out in accordance with the operation of the technological complex process. In this case, the output of one model (the modeling results) serves as the input for another model (the initial data required for modeling), and this output may in turn be the input for a previous or another model. For example, in the sulfur production complex, the output of the E-001 condenser model - that is, its modeling results - serves as the input for the E-004 condenser model, and the results of modeling this condenser are then used as the input for the R-001 Claus reactor. In turn, the outputs of the Claus reactor models are required as input data for modeling the parallel-connected R-002 and R-003 reactors and the E-002 condenser.

The model describing the product of the Claus reactor, that is, the sulfur yield, was identified as a multiple regression model using experimental–statistical methods, while the models for assessing sulfur quality were constructed as fuzzy regression equations based on fuzzy information obtained from experts.

Conclusion. Based on the results of the systems analysis, a methodology for constructing mathematical models of technological facilities using various types of information has been formulated. According to the proposed methodology, the model of each unit of a technological complex is selected from among the possible types of models based on comparison and selection criteria, identifying the most effective model for that unit. The possible models of the main units of the sulfur production block were systematically analyzed, and the most efficient type of model to be constructed for each unit was determined.

Based on the conducted systems analysis and research results, the structure and parameters of the mathematical models of the reactors in the sulfur production block at the Atyrau Oil Refinery were identified using aggregated and processed information.

The model describing the relationship between the sulfur yield at the outlets of the thermal and Claus reactors and their input and operating parameters was identified in the form of multiple regression equations. The qualitative indicators of sulfur: the mass fractions of sulfur and water in the product at the outlet of the Claus reactor - were structurally identified as multiple fuzzy regression equations. Thus, in this work, using the example of the sulfur production block, a methodology for constructing a package of models for technological complexes consisting of interconnected units is presented, along with the results of its implementation.

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