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RESEARCH ARTICLE

A Systematic Approach to the Model Development of Reactors and Reforming Furnaces With Fuzziness and Optimization of Operating Modes

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ABSTRACT The paper studies the problems of developing interconnected models of aggregates of complex chemical-technological systems (CTS) in conditions of scarcity and fuzziness of the initial information. Since the known methods of model development do not allow for solving these problems, we propose a systematic method that allows the development of a package of models of interconnected aggregates of complex CTS using the available information of a different nature. In the proposed method, formal and informal methods of system analysis are jointly used. Due to synergy and emergence, the proposed system allows the synthesis of the most adequate and effective CTS models using the knowledge, experience, and intuition of experts and other available data. Using the method, we have developed a package of models of interconnected reactors and used it in a case study for a reforming reactor and furnace of the Atyrau refinery catalytic reformer based on available statistical and fuzzy information. To study and optimize the operating modes of the reformer unit, a system of computer simulation and optimization of the reformer unit was created. Comparison of the obtained results of computer modeling and optimization with the results of known deterministic models shows the advantages of the proposed approach in the face of scarcity and fuzziness of the initial information. The importance and novelty of the proposed method lie in the possibility of developing a package of models of interrelated CTS units based on various types of available information. This allows one to systematically simulate and optimize the operating modes of the CTS. The practical significance of the results is that this case study can be successfully applied in the development of models of various technological units for oil refining, petrochemistry, and other industries.

INDEX TERMS Decision maker, fuzzy information, model package, system approach.

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I. INTRODUCTION

Currently, one of the urgent tasks of oil refining and the economy of the Republic of Kazakhstan is to increase the production of high-quality motor fuels. The importance and relevance of this task are justified by the great demand for

high-quality motor fuels in both the domestic and foreign markets. In connection with the increase in environmental requirements for motor fuels, the relevance of the production of high-quality gasoline that meets stringent environmental requirements and standards is now even higher. The most effective approach to solving the problem under consideration is the use of mathematical modeling and optimization methods, which allow optimizing the processes of oil refining and the production of high-quality motor fuels [1], [2].

Currently, catalytic reforming process units are used in all refinery plants to produce high-quality gasoline that meets all modern environmental requirements. The catalytic reforming unit, like other technological refinery plants, belongs to a complex chemical-technological system (CTS), consisting of many interconnected technological units, such as a reactor, column, furnace, etc. [3], [4], [5].

The operating modes of the catalytic reformer are influenced by many technological parameters and production indicators, which are characterized by uncertainty due to the random and/or fuzzy nature of their values. At the same time, the fuzziness of the value of some indicators of the production of high-quality gasoline is due to the fact that such important quality indicators of the produced gasoline as octane level, sulfur composition, knock resistance and other measuring instruments are not measured. Such parameters are usually determined with the participation of specialists in laboratory conditions and are described by fuzzy terms of the “not less” type. “no more”, “low”, “medium”, “high”, etc.

This situation makes it difficult to develop mathematical models and optimize the operating modes of a catalytic reforming unit using traditional mathematical methods [6]. In this regard, in order to develop mathematical models and optimize the operating modes of interconnected CTS units, characterized by uncertainty, deficiency, and fuzziness of the initial information, it is necessary to develop new methods based on a systematic approach and experimental statistical methods and the mathematical apparatus of fuzzy set theories [7], [8]. Thus, there is a need to use fuzzy information, which is the experience, knowledge, and intuition of a decision maker (DM), or domain expert expressed in natural language. Currently, methods of expert assessments and fuzzy set theories [9], [10], [11] are effective means of collecting, formalizing, and using such fuzzy information. All this makes it possible to substantiate the relevance of the task of developing a package of models of interconnected aggregates of complex CTS, which are characterized by uncertainty, randomness, and fuzziness of the initial information.

In this regard, the main goal of this study is to develop a new systematic method for synthesizing models of interconnected CTS aggregates in conditions of scarcity and fuzziness of initial information based on available information of a different nature. In addition, the goal is to produce a case study by optimizing the operating modes of the reactors and the reforming furnace of the catalytic reforming unit by computer simulation based on the developed package of their models.

To achieve this goal, the following research tasks have been identified and are being solved:

- on the basis of a systematic approach, develop a method for developing a package of models of interrelated CTS units under conditions of uncertainty using available information of a different nature;
- to develop a package of models of reactors and a reforming furnace of the LG-35–11/300–95 unit of the Atyrau refinery based on available statistical and fuzzy information as a case study;
- computer simulation and optimization of the reformer modes of the LG-35–11/300–95 catalytic reformer of the Atyrau refinery.

Known methods for developing mathematical models make it possible to develop models of individual objects based on initial information of the same type. In contrast to known methods, the proposed system makes it possible to develop a package of models of interrelated CTS aggregates based on various types of information (deterministic, stochastic, fuzzy). This makes it possible to develop more efficient models of complex CTS under conditions of uncertainty and lack of initial information and optimize their modes of operation based on system simulation on a computer. The use of knowledge, experience, and intuition of DM and experts, the apparatus of fuzzy theories in the proposed method allows one to effectively simulate and optimize the modes of operation of fuzzy CTS. The fuzzy results for implementation on a computer can be converted into clear results based on the defuzzification methods of fuzzy set theories.

Here is a clear statement of the main contribution of the conducted research. Based on the methodology of systems analysis, a new system method integrating deterministic, stochastic and fuzzy approaches and their various combinations, which allows to develop a system of models of interrelated units of complex CTS of various industries. The proposed system method makes it possible to develop effective models of CTS aggregates under conditions of uncertainty, combined into a single system of models. In this case, the obtained system of models due to the effect of synergy and the property of emergence allows to systematically simulate CTS and optimize the modes of their work. The proposed method is implemented by the example of developing a system of models of the main units (reactors and furnace) of the reforming unit and can be exported to other technological units of oil refining, petrochemical and other industries.

II. RELATED WORK

Issues of mathematical modeling of various CTS technological units, including catalytic reforming and cracking units, have been studied in various works. Mohaddec et al. [8], Kafarov and Dorohov [9], and Jorov [13] in their studies developed deterministic models of typical processes occurring in CTS technological units, including installation of catalytic reforming and the kinetics of processes.

The proposed deterministic models in these works of individual units and elementary processes of chemical technology are based on the laws of conservation of mass and energy and are theoretically justified and universal, which are their advantages. But the problem is that the models of individual aggregates in these works are built without taking into account the mutual influences of the CTS aggregates and the fuzziness of the initial information. Therefore, the development of such models under conditions of uncertainty, lack of information, and fuzziness of the initial information is impossible, and such models are unsuitable for system modeling of a CTS operation. The adoption of various assumptions and the idealization of real processes in order to apply these models in conditions of scarcity and fuzziness of the initial information leads to a decrease in their adequacy and their unsuitability in practice.

Pinheiro C.C. and others investigated the issues of modeling and control of the catalytic cracking process in the production of high-quality gasoline [14]; however the reactor models were considered without taking into account connection with other units of the cracking unit, such as furnaces, columns, etc. Although the proposed model is suitable for optimizing the operating modes of the reactor, it does not allow for system modeling and optimizing the operating modes of the catalytic reforming unit as a whole.

Control methods for technological units based on the stochastic approach were studied in the work of Coleman and Babu [15], while Bequette [16] investigated the problems of managing technological processes occurring in various CTS units based on their statistical models. Such statistical models are suitable for the optimization and management of complex objects. To develop such models, it is necessary to have an array of reliable statistical data on the state and operation of objects and to conduct multiple experiments to collect and process statistical data. But for a number of CTS units like the Atyrau Refinery catalytic reformer under study, such experiments are not possible due to the lack of instrumentation to measure some of the important production parameters needed for model development.

Grinchuk in his work [17] investigated the issues of mathematical physical modeling of thermal modes of operation of electric furnaces based on probabilistic methods.

Arutyunov et al. in [18], as well as Lisienko and Volkov in [19] proposed methods for modeling thermal work and heat transfer in furnaces. However, these works also do not take into account the relationship of furnaces with reactors, columns, and other CTS units, which reduces their practical value. In addition, when applying the methods proposed in [17], [18], and [19] in practice, there are problems associated with the lack of statistical data and the fuzziness of available information. Moreover, even with the theoretical possibility of collecting and processing the necessary statistical information, in practice, under production conditions, this may turn out to be economically inexpedient and unprofitable. In this regard, it is necessary to develop mathematical models of industrial furnaces, taking into account

their relationships with other main CTS units and the scarcity and fuzziness of the initial information.

There are various control systems developed on the basis of models that allow you to optimize the modes of operation of objects. For example, one can create a catalytic process control system that allows solving problems of optimal temperature distribution at the inlet of cracking reactors [20], while Gumen [5] proposed a gasoline quality control system in the stabilization unit of a catalytic reformer.

The application of situational control of the reforming process based on models is considered by Pospelov [21]. These control systems allow one to optimize the processes and modes of operation of objects only in deterministic or stochastic conditions, while the proposed models and control systems are not effective or not suitable at all in conditions of fuzzy initial information.

The studies of Matveykin et al. [22], Keller and Gorak [23], and Aliev et al. [24] considered approaches to the development of models and management of objects based on them in the conditions of fuzziness of some part of the initial information. The proposed methods make it possible to develop fuzzy models based on the level set under conditions of clear values of the input, mode parameters, and fuzzy values of the object's output parameters. But in such methods of developing fuzzy models, the problems of developing linguistic models with fuzzy values and input, regime, and output parameters of the object remain unresolved. In addition, papers [22], [23], and [24] do not consider the development of a package of models of interconnected CTS technological units.

The well-known methods for synthesizing, modelling and optimizing individual CTS units are based on traditional deterministic and statistical methods and do not solve the problem of developing complex models of interconnected units in a fuzzy environment and system modeling of CTS.

In practice, the catalytic reformer and other CTS of oil refining is a good case study, as it consists of many interconnected and mutually influencing vaguely described technological units such as reactors, furnaces, columns, etc. In production, experienced production operators, i.e. DMs, can make effective decisions on choosing the optimal mode of operation of fuzzy CTS based on their preferences, knowledge, and experience, taking into account the current situation in the production. Based on expert evaluation methods and fuzzy set theories, it is possible to formalize the knowledge, experience, and intuition of DM experts, expressed in the form of fuzzy information, and apply for the synthesis of efficient models, and optimization of CTS operating modes in a fuzzy environment. This work is aimed at solving this system problem, developing a package of models of interconnected aggregates, and optimizing CTS using the available fuzzy information.

In contrast to the known methods for developing models of individual technological objects, the proposed system method allows the development of a package of models of interrelated CTS technological units based on available information of

a different nature. The advantage of the proposed method is that, based on a systematic approach, it makes it possible to synthesize a package of models of interrelated CTS technological units in conditions of scarcity and fuzziness of the initial information. In addition, the proposed system method makes it possible to synthesize various known types of mathematical models, as well as linguistic, hybrid models of complex, fuzzy CTS.

III. MATERIALS AND METHODS

A. OBJECT OF THE STUDY AND PROBLEM DESCRIPTION

The object of this case study is the LG-35–11/300–95 Atyrau refinery catalytic reforming unit and its main interconnected technological units designed for the production of high-quality gasoline [25]. LG-type catalytic reformers are available in almost all domestic and foreign refineries [3], [5], [26], [27]. The reforming process is the most important technological process of modern oil refining and petrochemistry.

The capacity of the LG-35–11/300–95 plant for raw materials is 300.0 thousand tons per year, it uses catalysts UOP - S-12T (hydrotreating unit) and UOP - R-56 (reforming unit [25]). The target product of the installation is a high-octane component of commercial gasoline (with an octane rating of up to 95 points according to the research method) and liquefied household gas [28]. reforming unit designed to clean raw materials from sulfur and other harmful compounds and to improve the quality of gasoline.

Figure 1 shows the flow diagram of the block under study, i.e., the reforming block of the LG-35–11/300–95 Atyrau refinery. The reforming unit of the LG unit is intended for carrying out processes for the conversion of naphthenes and paraffin into hydrocarbons with higher octane numbers, i.e. into aromatic hydrocarbons. The resulting aromatic hydrocarbons, since they have high octane numbers, are further used as high-quality commercial gasoline. The catalytic process is based on the reaction of dehydrogenation and dehydroisomerization of naphthenic hydrocarbons, and isomerization of alkane hydrocarbons on a platinum catalyst under high hydrogen pressure. As a result of the above reactions in gasoline fractions, the number of aromatic hydrocarbons increases, which have high octane characteristics.

The main units of the reforming unit include the reforming reactors R-2, R-3, R-4, and R4a. In addition, the reforming process is affected by the reforming furnaces F-1 and the reforming separators S-7, and S-9 (Figure 1). Therefore, for system simulation of the operation of the reforming unit of the LG-35–11/300–95 catalytic reformer, it is necessary to develop a system of mathematical models of these main units. In this work, a package of models of interconnected reactors R-2, R-3, R-4, R4a, and a reforming furnace F-1 is being developed.

Technological units, including the reactor and the reforming furnace of the reforming unit, as can be seen in Figure 1, are interconnected. Changes in the regime parameters of one of them lead to a change in the parameters of others, which

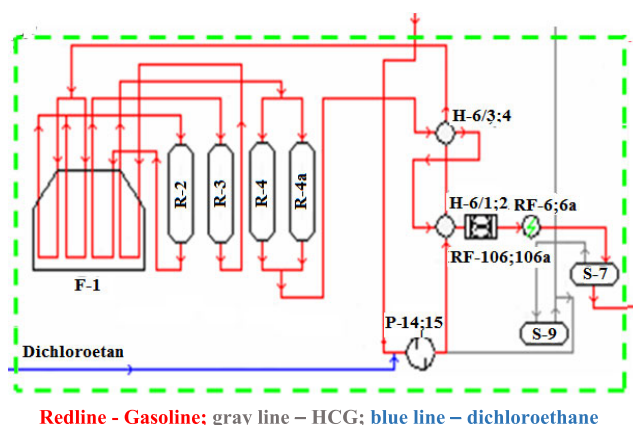


FIGURE 1. Process diagram of the LG-35-11/300-95 catalytic reforming unit.

affects the reforming processes. In this regard, in order to optimize and control the reforming process in the optimal mode, it is necessary to build a package of interconnected mathematical models of these units, compiled on the basis of a systematic approach.

Since the LG-35–11/300–95 Atyrau refinery has been in operation for more than 50 years, there are certain problems associated with wear and low reliability of measuring instruments. Therefore, there are problems with the measurement of information and there is a shortage of quantitative information about the state and operation of the object. In addition, some important parameters characterizing the quality of gasoline (octane number, fractional composition) are evaluated qualitatively with fuzzy expressions with the participation of a human operator and factory laboratory assistants. All this complicates the development of mathematical models of reforming reactors based on traditional mathematical methods.

Experienced technologists work on the object under study, they are the DM, who makes the decision to control the operating modes of the units of the catalytic reformer. DMs and domain experts can describe the operation of reactors and vaguely evaluate product qualities based on their knowledge, experience, and intuition in natural language. At the same time, DM experts describe the state of the reactors and product quality with fuzzy expressions such as “a lot”, “little”, “high”, “medium”, “no more”, “no less”, etc.

The modern achievement of the mathematical apparatus of theories of fuzzy sets and methods of system analysis makes it possible to formalize, process, and apply fuzzy information to solve problems of uncertainty in the development of mathematical models of complex fuzzy CTS [7], [11], [12], [29]. In this regard, it became necessary to develop a method for synthesizing a package of various models of interconnected aggregates of complex fuzzy CTS based on available information of a different nature using formal and informal methods of system analysis [6], [10], [11], [12], [13], [20], [26], [30], [31], [32], [33], [34]. In these works, the issues of the integrated use of these various methods for developing models under conditions of uncertainty and fuzziness of the

initial information have not yet been sufficiently studied and resolved.

This paper proposes a method for developing a package of models of CTS aggregates under conditions of uncertainty based on information of a different nature, which makes it possible to comprehensively use various methods for developing models.

B. THE PROPOSED METHOD FOR DEVELOPING A PACKAGE OF MODELS UNDER CONDITIONS OF UNCERTAINTY

On the basis of a systematic approach, we developed a systematic method for constructing mathematical models of interconnected CTS units using the LG-35–11/300–95 installation as an example, based on available information of a different nature. Available initial information can be experimental and statistical data, theoretical information, and expert evaluation results in the form of fuzzy information. A block diagram of the proposed method for developing a package of models of CTS aggregates under conditions of uncertainty based on information of a different nature, which allows the complex use of various modeling methods, is shown in Figure 2.

Let us describe the main blocks of the proposed method for developing a package of models of CTS aggregates under conditions of scarcity and fuzziness of the initial information based on the available information of a different nature.

In block 2, for the development of a package of models, the main input, and operating parameters of the CTS units are determined, which affect the output parameters that evaluate their performance quality. In this case, the vector of input, mode parameters used to control the modes of operation of the CTS can be crisp $\mathbf{x} = (x_1, \dots, x_n)$ or fuzzy $\tilde{\mathbf{x}} = (\tilde{x}_1, \dots, \tilde{x}_n)$. Estimated output parameters, which are usually considered as criteria, can also be crisp $\mathbf{y} = (y_1, \dots, y_m)$ or fuzzy $\tilde{\mathbf{y}} = (\tilde{y}_1, \dots, \tilde{y}_m)$.

In blocks 3 and 4, a systematic analysis of the operation of CTS units and the relationship between them is carried out, and the purpose of modeling and criteria for choosing an effective type of model for each unit are determined. Based on the expert assessment and the selected criteria, taking into account the purpose of the simulation, the most effective type of model is selected for each CTS unit.

Starting from block 5, one or another type of CTS aggregate model is constructed depending on the results of an expert assessment, according to the maximum value of the integrated criterion (IC) and the nature of the available information.

In conditional blocks 6, 8, and 10, the conditions are checked, depending on the results of which a deterministic model (block 7), a statistical model (block 9), and a fuzzy model (block 11) are developed. Moreover, if, as a result of checking in block 10, the vector of input, regime parameters are clear (measured), which in practice can take place, then fuzzy models are developed $\tilde{y}_j =$

$f_j(x_1, \dots, x_n, \tilde{a}_0, \tilde{a}_1, \dots, \tilde{a}_n), j = \overline{1, m}$, for example, based on the FM method (block 11) proposed in [35].

If both the input, regime, and output parameters of the aggregate are fuzzy, then, based on the logical rules of conditional inference, linguistic models are synthesized *IF* $\tilde{x}_1 \in \tilde{A}_1 \vee \tilde{x}_2 \in \tilde{A}_2, \dots, \vee \tilde{x}_n \in \tilde{A}_n$ *THEN* $\tilde{y}_j \in \tilde{B}_j$. (block 12).

In block 11, when developing fuzzy models, clear input, mode parameters of the unit $\mathbf{x} = (x_1, \dots, x_n)$, are selected, and output fuzzy parameters $\tilde{y}_j \in \tilde{B}_j, j = \overline{1, m}$, describing the quality of operation of CTS units are determined. Then the structure of fuzzy models $\tilde{y}_j = f_j(x_1, \dots, x_n, \tilde{a}_0, \tilde{a}_1, \dots, \tilde{a}_n), j = \overline{1, m}$, is determined, i.e. the problem of structural identification of models is solved. Often the structure of the model can be identified based on the method of successive inclusion of regressors [36] in the form of fuzzy equations of multiple regression:

$$\tilde{y}_j = \tilde{a}_{0j} + \sum_{i=1}^n a_{ij}x_{ij} + \sum_{i=1}^n \sum_{k=i}^n a_{ikj}x_{ij}x_{kj}, j = \overline{1, m}.$$

After structural identification, the problem of parametric identification of fuzzy parameters is solved, i.e. estimation of fuzzy regression coefficients $\tilde{a}_0, \tilde{a}_1, \dots, \tilde{a}_n$. This problem can be solved on the basis of the level α modified with the help of the set and the method of least squares.

When developing linguistic models, fuzzy input, regime parameters $\tilde{x}_i \in \tilde{A}_i, i = \overline{1, n}$, are first chosen, affecting the output $\tilde{y}_j \in \tilde{B}_j, j = \overline{1, m}$ fuzzy parameters of CTS aggregates. These parameters required to build the model are linguistic variables: $\tilde{A}_i \in X, \tilde{B}_j \in Y$ are fuzzy subsets, X, Y are universal sets of input and output parameters. Then, based on expert evaluation methods involving DM, the term sets $T(X, Y)$ are determined that describe the fuzzy parameters of aggregates and the membership functions of fuzzy parameters and indicators are constructed: $\mu_{\tilde{A}_i}(\tilde{x}_i), \mu_{\tilde{B}_j}(\tilde{y}_j), i = \overline{1, n}, j = \overline{1, m}$.

Based on the experience of modeling technological objects of oil refining production in a fuzzy environment, we can recommend the following adaptable structure of the membership function, for example, for output parameters:

$$\mu_{\tilde{B}_j}(\tilde{y}_j) = e^{\left(Q_{B_j}^t \left| (y_j - y_j^{m_t})^{N_{B_j}^t} \right| \right)}$$

where $\mu_{\tilde{B}_j}(\tilde{y}_j)$ – membership function describing the output fuzzy parameters to the fuzzy set \tilde{B}_j ; t – term number; $Q_{B_j}^t$ – parameter (coefficient) that determines the level of fuzziness, which is determined when identifying the membership function of a term t ; $N_{B_j}^t$ – coefficients that determine the scope of the membership function of the term t of the fuzzy parameter, allowing you to change the shape of the graph of the membership function; $y_j^{m_t}$ fuzzy the variable that most closely matches the given term t . This variable is determined from the following condition $\mu_{\tilde{B}_j}(y_j^{m_t}) = \mu_{B_j}(y_j)$. After that, the links between the input and output linguistic variables are determined, i.e. fuzzy mappings \tilde{R}_{ij} between \tilde{x}_i and \tilde{y}_j are constructed. For the convenience of using a fuzzy mapping,

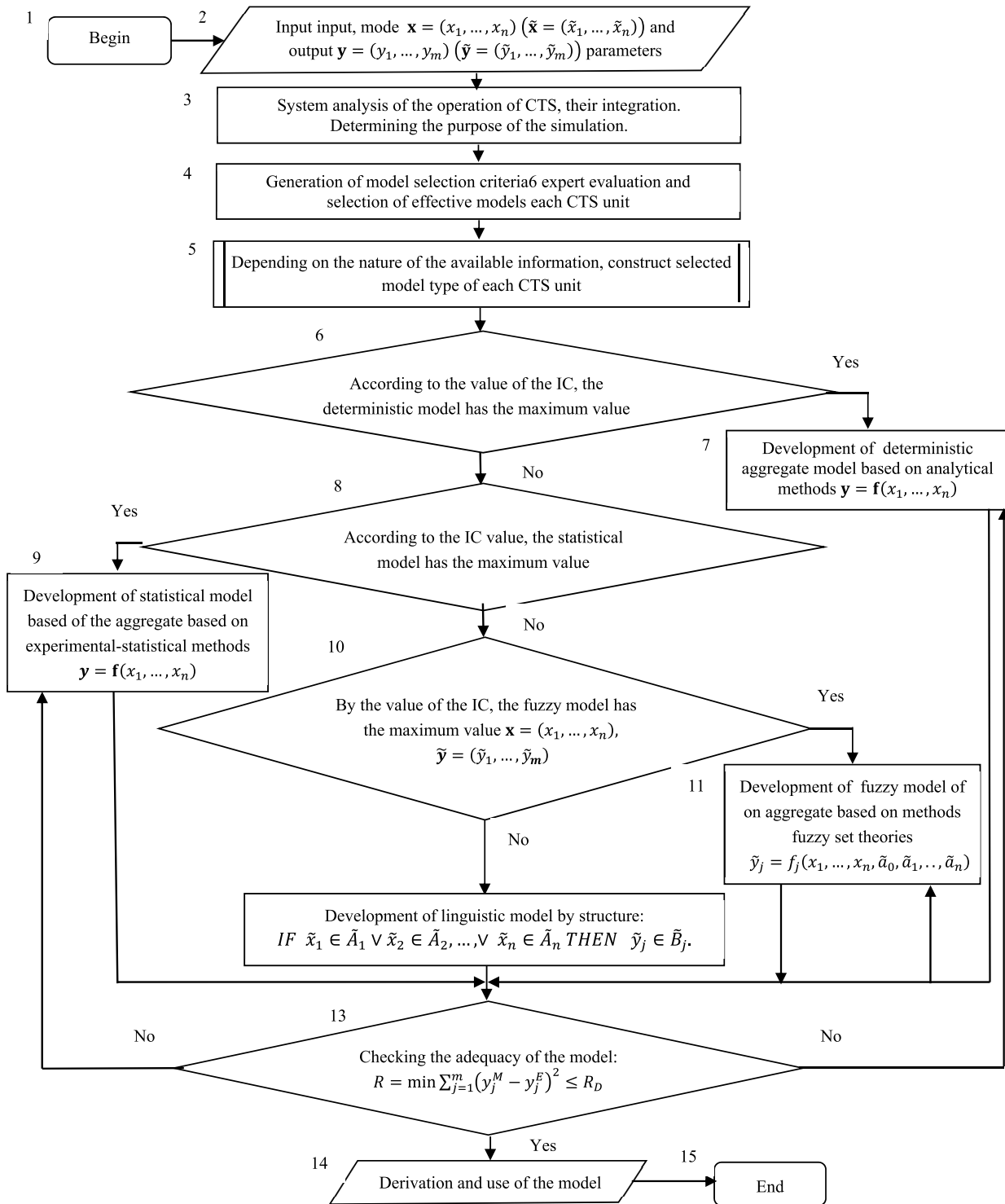


FIGURE 2. Block diagram of the proposed method for developing a system of models of interconnected CTS units under conditions of uncertainty based on information of different nature.

a matrix of connections with membership functions is defined in the calculation:

$$\mu_{\tilde{R}_{ij}}(\tilde{x}_i, \tilde{y}_j) = \min [\mu_{\tilde{A}_i}(\tilde{x}_i), \mu_{\tilde{B}_j}(\tilde{y}_j), i = \overline{1, n}, j = \overline{1, m}].$$

Then the linguistic model can be built on the basis of the logical rules of conditional inference, which have a common

structure:

$$IF \tilde{x}_1 \in \tilde{A}_1 \vee \tilde{x}_2 \in \tilde{A}_2, \dots, \vee \tilde{x}_n \in \tilde{A}_n THEN \tilde{y}_j \in \tilde{B}_j, j = \overline{1, m},$$

where \vee – is the “and” sign, meaning the fulfillment of all logical conditions of the conditional part of the logical model.

Based on the compositional inference rule $\tilde{B}_j = \tilde{A}_i \circ \tilde{R}_{ij}$, fuzzy values of the output parameters of the CTS aggregate under study are determined, then numerical values of the output parameters can be determined from fuzzy solutions. At the same time, using the compositional inference rule, the output parameters of the object are determined, which determine the qualities of its work, for example, using the maximin product.

Let \tilde{x}_i^* be the values of the input fuzzy parameters of the object, estimated by experts. Then the set of current values of the input parameters is defined as a fuzzy set in which the membership functions of the input parameters will be maximum: $\mu_{\tilde{A}_i}(\tilde{x}_i) = \max(\mu_{\tilde{A}_i}(\tilde{x}_i^*))$. In this case, the fuzzy values of the output variables are determined in the form of a membership function, expressing the maximin product:

$$\mu_{\tilde{B}_j}(\tilde{y}_j) = \max \left\{ \min_{\tilde{x}_i \in X} \left[\mu_{\tilde{A}_i}(\tilde{x}_i^*), \mu_{\tilde{R}_{ij}}(\tilde{x}_i^*, \tilde{y}_j) \right] \right\}.$$

Clear (numerical) values of the output parameters can be determined using the following expression: $y_j^c = \arg \max_{\tilde{y}_j} \mu_{\tilde{B}_j}(\tilde{y}_j^*)$ parameters, in which the membership functions reach the maximum values.

If both theoretical and statistical data, and fuzzy information describing the operation of the CTS aggregate are insufficient or their collection is not economically feasible, and the integrated criterion for the combined model has the maximum estimate using the hybrid method, a combined (hybrid) model can be built [29]. In this case, the combined model is developed on the basis of available information of various nature (theoretical, statistical, fuzzy). To do this, to describe a specific parameter of the object, various combinations of the above blocks of the proposed method are used.

In block 13, the adequacy of the developed models is checked. The following criterion is used to assess adequacy:

$$R = \min \sum_{j=1}^m (y_j^M - y_j^E)^2 \leq R_D,$$

where y_j^M are the calculated values of the output parameters obtained using the model, and y_j^E are the experimental (real) values of the object's output parameters, R_D - is the allowable deviation value.

If the adequacy condition is met, then the model is recommended for modeling and determining the optimal modes of operation of the CTS, in our case, the catalytic reformer. Otherwise, the reason for the inadequacy of the model is determined and the transition is processed into the appropriate blocks of the described methodology to eliminate the causes of inadequacy and increase it. In this case, the reason for the inadequacy of the model can be: not including in the model some parameters that significantly affect the process; incorrect structural and/or parametric identification of the model, etc.

The catalytic reforming unit of the LG-35-11/300-95 unit is a complex, fuzzy CTS consisting of interconnected units,

which are simultaneously affected by a large number of different parameters. As can be seen from the scheme shown in Figure 1, the main units of the reforming unit include the reforming reactors R-2, R-3, R-4 and R4a, the reforming furnace F-1 and the reforming separators S-7, S-9.

Blocks 3, 4 of the CTS modeling method under uncertainty show that under uncertainty, based on the available information of a different nature, models of each CTS unit can be built using different initial information and appropriate modeling methods. As a result, various types of models can be built, for example, statistical, fuzzy or combined. In addition, the central part of the code can be developed towards an Application Programming Interface (API) which allows two or more applications to communicate with one another in a fast simple way.

IV. RESULTS

A. REACTOR AND REFORMER MODEL PACKAGE FOR THE LG-35-11/300-95 UNIT OF THE ATYRAU REFINERY BASED ON AVAILABLE STATISTICAL AND FUZZY INFORMATION

In the reforming unit of the LG-35-11/300-95 unit, the technological reforming process takes place. To optimize the operating modes of the reforming unit, we developed mathematical models of the reactors of the interconnected reforming reactors R-2, R-3, R-4, R-4a and the reforming furnace F-1.

In practice, to build models with a lack of information, it is necessary to use available information of any nature. Models of technological units obtained based on such data can be called *combined* or *hybrid* [29]. They can be generated using various combinations of available data and are designed to take into account the merits of different types of models. However, the development of combined models can be difficult due to the fact that the stage of organizing, conducting research and experiments of a different nature, as well as pre-processing the collected data is necessary.

To develop models of CTS units based on the proposed method and combine them into a single package of models for system modeling and optimization of system operation modes, it is necessary to analyze the advantages and disadvantages of the models being developed. For this purpose, criteria for comparison and selection of the optimal type of model for each unit of the reformer unit (CTS) need to be defined.

Based on the results of studies of the specifics of the process and units of the catalytic reforming unit, experimental data and an expert survey, and analysis of approaches to modeling similar objects, possible types of models of the main units of the reforming unit of the LG-35-11/300-95 catalytic reformer were evaluated. The result of the conducted system analysis, evaluation of models is presented in the form of Table 1.

A five-point scale was used to evaluate (rank) the types of models. Peer review was carried out using the Delphi method with the participation of 10 DM experts in the subject area.

TABLE 1. Units for magnetic properties results of analysis and expert assessment of the types of models of the main units of the catalytic reforming unit of the Ig-35-11/300-95 installation.

| Aggregates catalytic reforming unit (main) | Criteria | Model types | | | |
|--|--|---------------|------------|-------|--------------|
| | | Deterministic | Statistics | Fuzzy | combinations |
| Reactors: R-2, R-3, R-4.4a | Availability of ne-cessary information | 2 | 4 | 4 | 5 |
| | Development cost | 1 | 4 | 3 | 3 |
| | Degree of adequacy | 4 | 3 | 4 | 4 |
| | Suitability for the intended purpose | 3 | 3 | 4 | 5 |
| | Possibility of bundling | 4 | 3 | 3 | 3 |
| | Integrated criteria (IC) | 14 | 17 | 18 | 20 |
| Furnace reforming F-1 | Availability of ne-cessary information | 3 | 5 | 4 | 5 |
| | Development cost | 2 | 4 | 4 | 4 |
| | Degree of adequacy | 5 | 4 | 4 | 4 |
| | Suitability for the intended purpose | 4 | 5 | 4 | 4 |
| | Possibility of bundling | 4 | 4 | 4 | 4 |
| | IC | 18 | 22 | 20 | 21 |
| Reforming separators: S-7, S-9 | Availability of ne-cessary information | 4 | 5 | 4 | 5 |
| | Development cost | 3 | 4 | 4 | 4 |
| | Degree of adequacy | 5 | 4 | 4 | 4 |
| | Suitability for the intended purpose | 4 | 5 | 4 | 4 |
| | Possibility of bundling | 4 | 4 | 4 | 4 |
| | IC | 20 | 22 | 20 | 21 |

Table 1 contains the results of the 5th round of peer review, when the values of the concordance coefficient reached $W = 0.95$, i.e. after reaching the required level of agreement among experts. Since local criteria are evaluated in points, integrated criterion (IC) values are determined by summing the value of local criteria.

As the main criteria for comparing different types of models by which they are evaluated, the following were chosen: the availability of the necessary information to build a model of the corresponding type, the cost of developing a model, the level of model adequacy, the applicability of these models for their intended purpose (in our case, to optimize the operating modes of the reforming unit under conditions uncertainties) and the possibility of combining a model of this type into a single package of models for the purpose of system simulation of the operation of the unit as a whole

Combining individual models of units into a single package is carried out in accordance with the flow of the technological process of reforming on the block under study. The outputs of one model are the inputs of another. For example, in the catalytic reformer, the simulation results of the R-2 reactor are

the input data for simulating the operation of the 2nd stage of the F-1 multi-chamber furnace, the simulation results of the furnace are the input data for the R-3 reactor models. And the output results of the R-3 models are the input data for the 3rd stage of the F-1 furnace, the output results are the input data for the reactors R-4, R-4a (see Figure 4 below). Therefore, when choosing the types of unit models, in addition to the adequacy and efficiency of their application, it is necessary to take into account the possibility of their integration into a single system and applicability for optimizing the operating modes of the reactor system and reforming furnace based on modern computers.

As a result of system analysis and evaluation of possible types of model, as can be seen in Table 1, the most optimal type of model for reforming reactors R-2, R-3, R-4, R-4a is a combined (hybrid) model.

In the conditions of the Atyrau refinery, the collection of reliable statistical information for building regression models of reactors for building regression models of the product quality of reforming reactors R-2, R-3, R-4 and R-4a is complicated by the lack of special industrial instruments. In this regard, as more effective tools that complement the missing data based on fuzzy information (knowledge of DM, specialist experts), expert assessments were chosen, and methods based on fuzzy set theories and combined methods were chosen as methods for building models.

1) MATHEMATICAL MODELS OF REFORMING REACTORS

As a result of processing experimental-statistical and expert data and applying the idea of the method of successive inclusion of regressors, based on the method of synthesizing mathematical models in a fuzzy environment [the following structures of the combined models of the studied reactors R-2, R-3, R-4, R-4a have been identified:

$$y_1^{R-2} = a_0 + \sum_{i=1}^5 a_i x_i + \sum_{i=1}^5 \sum_{k=1}^5 a_{ikj} x_i x_k, \quad (1)$$

$$y_1^{R-3} = a_0 + \sum_{i=1}^5 a_i x_i + \sum_{i=1}^5 \sum_{k=1}^5 a_{ikj} x_i x_k, \quad (2)$$

$$y_1^{R-4, R-4a} = a_0 + \sum_{i=1}^5 a_i x_i + \sum_{i=1}^5 \sum_{k=1}^5 a_{ikj} x_i x_k, \quad (3)$$

$$y_j = a_{0j} + \sum_{i=1}^5 a_{ij} x_i + \sum_{i=1}^5 \sum_{k=1}^5 a_{ikj} x_i x_k, \quad j = 2, 3 \quad (4)$$

$$\tilde{y}_j = \tilde{a}_0 + \sum_{i=1}^5 \tilde{a}_{ij} x_i + \sum_{i=1}^5 \sum_{k=1}^5 \tilde{a}_{ikj} x_i x_k, \quad j = \overline{4, 6}, \quad (5)$$

where $y_1^{R-2}, y_1^{R-3}, y_1^{R-4, R-4a}$ are output parameters, volumes of catalyzate from reactors R-2, R-3, R-4, R-4a; y_2, y_3 —volumes of hydrogen-containing gas (HCG) and dry gas; $\tilde{y}_j, j = \overline{4, 6}$ are the main quality indicators of the catalyzate,

namely the octane number (\bar{y}_4), fractional composition: 10% distillation (\bar{y}_5) and 50% distillation (\bar{y}_6). These qualitative indicators are determined with the participation of a person (DM, experts) and are expressed in fuzziness. The octane number must be «at least», i.e. $\lesssim 86$ according to the motor method, and the fractional composition should be «not higher, ≥ 70 °C» (for 10% distillation) and ≥ 115 °C (for 50% distillation). Through $x_i, i = \overline{1, 5}$ - input, operating parameters of reforming reactors are indicated: x_1 - consumption of supplied raw materials; x_2 - space velocity in reforming reactors; x_3 and x_4 - temperature and pressure in reforming reactors; x_5 - hydrogen/feedstock ratio; a_{0j}, a_{ij}, a_{ikj} and $\tilde{a}_{0j}, \tilde{a}_{ij}, \tilde{a}_{ikj}$ are, respectively, clear and fuzzy parameters of models (1)-(5) subject to identification.

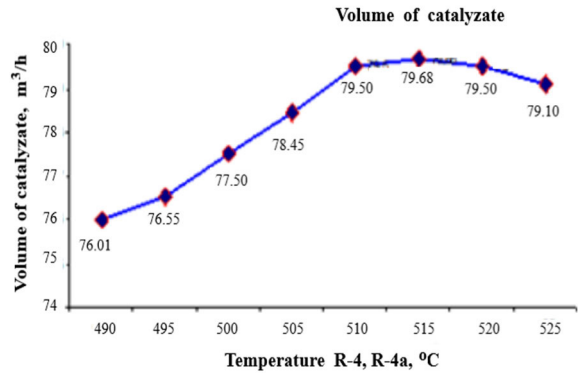
From the results of the structural identification of the reformer models, it can be seen that the models describing the product yields (catalyzate, dry gas and HCG) (1)-(4) are built by experimental-statistical methods in the form of multiple regression equations. And the models that evaluate the quality of the catalyzate (gasoline) are identified in the form of fuzzy equations of multiple regression based on the methods of synthesizing fuzzy models using fuzzy information from DM, experts.

Parameters, i.e., regression coefficients of models (1)-(4) are identified using the REGRESS software package in which the least squares method is implemented. As a result, the dependence of the yield of catalyzate and HCG on the input, regime parameters $x_i, i = \overline{1, 5}$ is determined in the form of the following models (6)-(9):

$$y_1^{R-2} = 0.398481x_1 + 12.153846154x_2 - 0.032113821x_3 - 0.983750x_4 + 0.019750x_5 + 0.0049375x_1^2 + 9.349112426x_2^2 - 0.000065272x_3^2 - 0.0379200x_4^2 + 0.00049375x_5^2 + 0.2278846x_1x_2 + 0.0001004x_1x_3 + 0.0375441x_2x_3 - 0.486153846x_2x_4 - 0.00064276x_3x_4, \quad (6)$$

$$y_1^{R-3} = 0.39500x_1 + 12.107692308x_2 - 0.01862348x_3 - 0.9758800x_4 + 0.01967500x_5 + 0.00504406x_1^2 + 8.95470880x_2^2 - 0.00006450x_3^2 - 0.04989583x_4^2 + 0.000049187x_5^2 + 0.2388874x_1x_2 + 0.0000101x_1x_3 + 0.0020835x_1x_4 + 0.000517207x_1x_5 + 0.035873247x_2x_3 - 0.504487179x_2x_4 - 0.000663799x_3x_4 \quad (7)$$

$$y_1^{R-4, R-4a} = 0.398984x_1 + 11.186923x_2 - 11.1869231x_2 - 0.031589537x_3 - 1.02391304x_4 + 0.0253700x_5 + 0.005069676x_1^2 + 9.289940828x_2^2 - 0.000058560x_3^2 - 0.044517958x_4^2 + 0.0000491x_5^2 + 0.2301828x_1x_2 + 0.0001003x_1x_3 + 0.0001003x_1x_3$$



x_1 - raw material input - 80 m³/h;
 x_2 - volumetric velocity - 1.3 hour⁻¹;
 x_4 - pressure in the reactor R-4, R-4a - 24, kg/cm²;
 x_5 - ratio H₂/raw material - 400 nm³

FIGURE 3. Change of catalyst volume as a function of reformer temperature R-4, R-4a at constant values x_1, x_2, x_4, x_5 .

$$+ 0.0021684x_1x_4 + 0.0004987x_1x_5 + 0.0364495x_2x_3 - 0.5250836x_2x_4 - 0.0006867x_3x_4, \quad (8)$$

$$y_2 = 500.000x_1 + 7142.8571x_2 + 10.10100x_3 - 1458.3333x_4 + 25.000x_5 + 6.2500x_1^2 + 5102.0408x_2^2 + 0.0204x_3^2 - 60.7639x_4^2 + 0.0625x_5^2 + 178.5714x_1x_2 + 0.2525x_1x_3 - 15.625x_1x_4 + 15.6345x_1x_5 - 297.6190x_2x_4 - 2.5252x_3x_4 - 0.05051x_3x_5 - 1.0417x_4x_5 \quad (9)$$

Since in practice there are no special requirements for the dry gas yield (y_3), the model for calculating the dry gas yield is not presented in this paper.

Based on the simulation results, on the basis of the obtained models, a plot of the dependence of the volume of catalyzate from the output of the R-4, R-4a reactors on the temperature in these reactors was plotted (Figure 3). But, at the same time, the quality indicators of products were not taken into account.

For the purpose of parametric identification of fuzzy regression coefficients $\tilde{a}_{ij}, i = \overline{0, 5}, j = \overline{4, 6}$ and $\tilde{a}_{ikj}, i = \overline{0, 5}, k = \overline{i, 5}, j = \overline{4, 6}$ models (5) fuzzy sets describing the quality indicators of products are divided into the following level sets $\alpha = 0.5; 0.75; 1$. Then, based on the methods of fuzzy set theory, the values of qualitative indicators of catalyzate \bar{y}_4, \bar{y}_5 and \bar{y}_6 are determined for each level α . Thus, fuzzy models (5) can be represented as the following system of conventional regression models for each slice $\alpha = 0, 5; 0, 75; 1$, describing the quality indicators of gasoline:

$$y_j^{\alpha_l} = a_{0j}^{\alpha_l} + \sum_{i=1}^5 a_{ij}^{\alpha_l} x_{ij} + \sum_{i=1}^5 \sum_{k=1}^5 a_{ikj}^{\alpha_l} x_i x_k, j = \overline{4, 6}, \quad (10)$$

where $l = \overline{1, 3}$ - levels α slices.

Then the problem of identifying the parameters $a_{ij}^{\alpha_l}, l = \overline{1, 3}, i = \overline{1, 5}, j = \overline{4, 6}$, of the obtained system of ordinary

regression models, can be solved as well-known identification problems multiple regression options, such as using the least squares method. To identify the parameters $a_{ij}^{\alpha_l}$, the REGRESS software package was used, which makes it possible to identify the nonlinear regression coefficients based on the modified least squares method.

The identified regression coefficients of the regression $a_{ij}^{\alpha_l}$ of the model (5) are then combined in order to estimate the values of fuzzy coefficients based on the following rule of fuzzy set theories:

$$\tilde{a}_{ij} = \bigcup_{\alpha \in [0, 0.5 \div 1]} a_{ij}^{\alpha_l} \text{ or } \mu_{\tilde{a}_{ij}}(a_{ij}) = \sup_{\alpha \in [0, 0.5 \div 1]} \min \left\{ \alpha_l, \mu_{a_{ij}^{\alpha_l}}(a_{ij}) \right\}, \quad (11)$$

where $a_{ij}^{\alpha_l} = \left\{ \tilde{a}_{ij} \mid \mu_{\tilde{a}_{ij}}(a_{ij}) \geq \alpha \right\}$

Based on the above results and using the REGRESS program, parametric identification of models describing the fuzzy dependence of quality indicators of catalyst $\tilde{y}_j, j = \overline{2, 4}$ on input, mode parameters $x_i, i = \overline{1, 5}$ at levels $\alpha = [0.5; 0.85; 1; 0.85; 0.5]$. After combining the identified regression coefficients on the levels by formula (11), the following models for the octane number of gasoline (\tilde{y}_4) and 10% of distillation (\tilde{y}_5) were obtained:

$$\begin{aligned} \tilde{y}_4 = & 00.43557x_1 - 20.076921x_2 + 0.052837x_3 - \\ & - 0.7200x_4 + 0.42445x_5 + 0.005435x_1^2 + 15.44394x_2^2 + \\ & + 0.000107x_3^2 - 0.030135x_4^2 + 0.00015x_1x_3 + \\ & + 0.00027x_1x_5 - 0.557695x_2x_4 + 0.00007x_3x_5; \end{aligned} \quad (12)$$

$$\begin{aligned} \tilde{y}_5 = & 0.40627x_1 - 9.285911x_2 + 0.06925x_3 - \\ & - 0.541663x_4 - .016045x_5 + 0.00511x_1^2 + \\ & + 6.6326535x_2^2 + 0.000137x_3^2 - \\ & - 0.02255x_4^2 - 0.000015x_5^2 + 0.386907x_2x_4 - \\ & - 0.01145x_2x_5 - 0.000665x_4x_5. \end{aligned} \quad (13)$$

Similarly, 50% distillation (\tilde{y}_6) is determined, which also characterizes the quality of the catalyzate.

2) MATHEMATICAL MODELS OF THE REFORMING FURNACE F-1

The multi-chamber reforming furnace F-1 is designed to restore the temperature in the reaction zone to a temperature of 490–530 °C. The main technological parameters of the reforming furnace, which are regulated and affect the process, include: loading; inlet and outlet temperature; furnace pressure. As a result of the analysis of the available data, the study of the operating modes of these units and expert evaluation (see Table 1), experimental-statistical methods for building models were chosen to develop models of the reforming furnace.

The mathematical description, which is the basis of the model, should reveal the relationship between the parameters of the thermal operation of the furnace. The main drawback

of the previously existing methods for calculating furnaces is that they are focused on assessing only the integral characteristics of heat transfer, which do not exclude the case of pipe burnout. Recently, a zonal modeling method has been developed that makes it possible to estimate the local characteristics of heat transfer [18].

In the mathematical aspect, the essence of zonal methods for calculating furnaces is to replace the integral-differential equations describing heat transfer by approximating a finite system of algebraic equations. Then, from the solution of the resulting system of algebraic equations, the energy characteristics of heat transfer are determined - the temperatures and the resulting flows of individual zones of the system. The zone method provides a more accurate calculation result (with increasing number of zones), but is complex and requires data that is usually difficult to access in an industrial environment. At the same time, to simulate the operation of industrial furnaces in an interactive mode and to quickly obtain information, it is necessary to have a fairly simple mathematical model. Therefore, in this work, an experimental-static approach to the development of furnace models was chosen.

To calculate the output parameters of the furnace based on experimental and statistical data, regression equations are included in the model. At the same time, it is assumed that the form of the distribution law of random measurements ε_j is close to normal, i.e.:

$$M[\varepsilon_j] = 0, D[\varepsilon_j] = G^2 = const, \quad j = \overline{1, m}.$$

Then, based on the method of sequential inclusion of regressors, the structure of regression models that determine the volume y_1 and the temperature y_2 of the outlet stream of furnace F-1 can be identified as:

$$\begin{aligned} y_j = & a_{0j} + a_{1j}x_1 + a_{2j}x_2 + a_{3j}x_3 + a_{4j}x_1^2 + a_{5j}x_2^2 + \\ & + a_{6j}x_3^2 + a_{7j}x_1x_2 + a_{8j}x_1x_3 + a_{9j}x_2x_3 + \varepsilon_j, \end{aligned} \quad (14)$$

where $a_{ij}, i = \overline{0, 9}, j = 1, 2$ - regression coefficients, identifiable least squares method; x_1, x_2, x_3 - accordingly, the inlet flow, temperature and pressure in the furnace, changing which the optimal values are found $y_j, j = 1, 2$.

As a result of processing the data of regime sheets and other experimental and statistical data by the methods of regression analysis and using the REGRESS program package, we identified the parameters of the models (14):

$$\begin{aligned} y_1 = & 0.495553x_1 + 0.017727x_2 + 0.866667x_3 + \\ & + 0.006297x_1^2 + 0.000040x_2^2 + 0.032098x_3^2 + \\ & + 0.000676x_1x_2 + 0.007342x_1x_3 + 0.000657x_2x_3, \end{aligned} \quad (15)$$

$$\begin{aligned} y_2 = & 0.662420x_1 + 0.597701x_2 - 5.777778x_3 + \\ & + 0.008438x_1^2 + 0.001374x_2^2 - 0.213991x_3^2 + \\ & + 0.004568x_1x_2 + 0.049068x_1x_3 + 0.004427x_2x_3. \end{aligned} \quad (16)$$

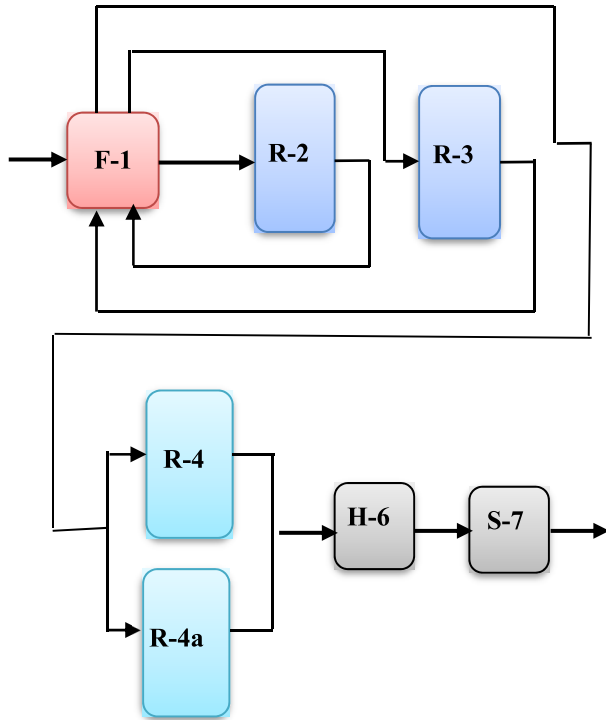


FIGURE 4. Scheme of combining the developed models of the main units of the LG-35-11/300-95 reformer into a system of models.

To simulate the operating modes of the heat exchanger H-6 and separator S-7 of the reformer unit, it is possible to use well-known deterministic and statistical models [18], [19].

Based on the results of research and analysis of the operation of interconnected systems of reactors R-2, R-3, R-4 and R-4a, furnace F-1, heat exchanger H-6 and separator S-7 of the reformer unit and in accordance with the course of the reforming process, the developed models combined into a single package of models. The scheme of combining these models into a single package of models is shown in Figure 4.

In the above scheme of combining individual models of CTS elements into a single package of models (Figure 4), through F-1, R-2, R-3, R-4, R-4a, software-implemented models of the main units of the LG-35-11/300-95 unit reforming unit are designated. For convenience, the designations of the programs are taken in accordance with the designations of the simulated main units of the reformer unit discussed above. Using the resulting software package on a computer, it is possible to systematically simulate various operating modes and determine the optimal operating modes of the reformer unit, which provide significant economic benefits and environmental safety of production.

B. COMPUTER MODELING AND OPTIMIZATION OF THE OPERATING MODES OF THE REFORMER UNIT OF THE CATALYTIC REFORMER LG-35-11/300-95 ATYRAU REFINERY

In production conditions, when managing the modes of operation of fuzzy CTSs, a DM often finds himself in a difficult situation related to making the best decision, which requires

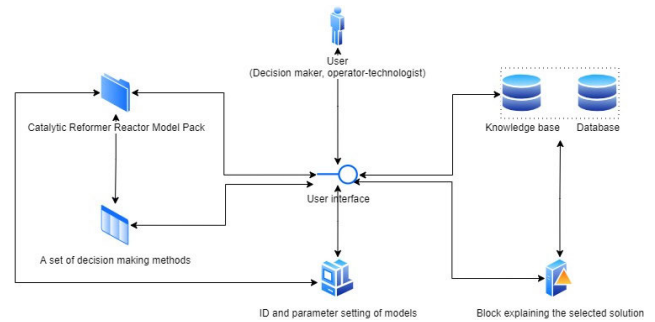


FIGURE 5. IDSS structure for optimization of reforming unit operation modes LG-35-11/300-95.

analyzing a large amount of information, comparing many alternatives according to a vector of criteria. This task is further complicated by the fact that the criteria are still controversial, and the DM needs to evaluate the consequences of the decision made under conditions of uncertainty.

The most effective approach to solving such complex, difficult to formalize tasks is the creation and application of intelligent decision support systems (IDSS) for choosing the optimal CTS operation mode based on modern computers. Such systems make it possible to combine the achievements of modeling, optimization and decision-making methods with the ability of DM to solve fuzzy problems and the capabilities of modern computers. Such a symbiosis of formal and informal methods, computer technologies makes it possible to improve and speed up the procedure for making the best decision by a person while optimizing CTS operating modes.

The structure of the IDSS, which includes CTS models developed taking into account the fuzziness of the initial information, the knowledge base accumulating the knowledge of DM, specialist experts, and other necessary blocks of the system, can be represented as in Figure 5.

The main IDSS blocks shown in Figure 5 are connected through information flows and each of them performs certain functions in the system, and together, due to the synergy and emergence properties of the system, they can effectively implement the decision-making process for choosing the optimal CTS operation mode.

In the given IDSS structure, the functional block “Package of models of reactors and furnaces of the LG-35-11/300-95 reforming unit” includes a system of interconnected models of reactors (6)-(9), (12), (13) and furnace (15), (16) of the LG-35-11/300-95 reformer unit developed above. These models are developed on the basis of various methods depending on the nature of the initial information and are combined into a single package in accordance with the flow diagram of the reforming process.

The functional block “Decision-making methods for optimizing the operating modes of the reforming unit” is intended for setting and solving decision-making problems for multi-criteria optimization of the operating modes of reactors and a reforming furnace, taking into account the fuzziness of the initial information. This block uses heuristic methods for solving decision-making problems based on the modification

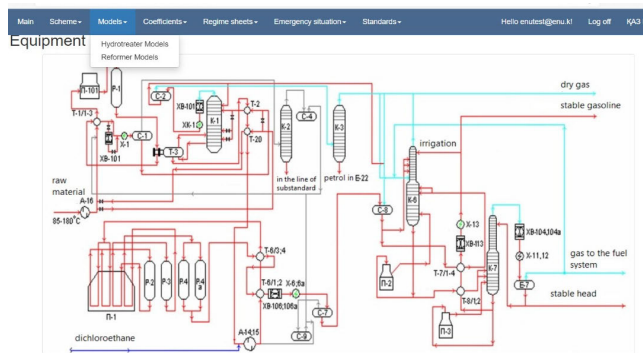


FIGURE 6. IDSS interface when selecting the Models menu.

of various optimality principles for working in a fuzzy environment [37]. Based on a package of models, a knowledge base and data, and, if necessary, other blocks of the system, these methods make it possible to determine and select the DM of the optimal operating mode for the LG-35–11/300–95 reformer unit according to the selected criteria with the issuance of recommended values of input and operating parameters.

The “User interface” block is designed to ensure efficient exchange of information between the DM-system in the process of solving the decision-making problem to optimize the operating modes of the reactors and the furnace of the reformer unit.

“Identifier and setting of model parameters” is a program that, based on parametric identification algorithms, if necessary, identifies model parameters. This block, as necessary, checks the adequacy of the models and, if inadequacy is detected, recalculates, i.e., identifies the parameters of the models.

Let us consider the process of computer simulation in order to optimize the operating modes of the reformer unit of the LG-35–11/300–95 Atyrau refinery. In this work, on the basis of the models of reactors and the reforming furnace developed above in paragraph III-A, a computer simulation subsystem IDSS was created, which makes it possible to optimize the operating modes of the reforming unit of the LG-35–11/300–95 unit.

Selecting the «Models» menu from the IDSS main page opens the «Hydrotreater Models» and «Models of the reformer unit», i.e. the main catalytic reformer units in which the plant products are produced (Figure 6).

By selecting the item “Models of the reforming unit” (Figure 7), it is possible to carry out system modeling and optimization of the operating modes of the reforming unit based on the package of mathematical models developed above in paragraph III-A.

As can be seen from Figure 7, in the interface that opens as a result of selecting the submenu “Models of the reformer unit”, information is provided on the current values of the input, operating parameters of the reformer unit, which were entered during previous simulations, indicating the date and time of their input.

| Date | x1– feedstock consumption, m3/hour | x2 – space velocity in reforming reactors, m3/h |
|------------------------|------------------------------------|---|
| 5/2/2022 8:13:47 AM | 1 | 2 |
| 5/3/2022 9:27:14 AM | 11 | 22 |
| 5/4/2022 1:25:00 PM | 65 | 1.25 |

| x3 – temperature in the reforming reactor, °C | x4 - pressure in the reforming reactor, kg/cm2 | x5 – hydrogen/feedstock ratio, nm3 | |
|---|--|------------------------------------|----------------|
| 3 | 3 | 4 | Edit Delete |
| 33 | 44 | 55 | Edit Delete |
| 507.5 | 22 | 400 | Edit Delete |

FIGURE 7. IDSS interface for viewing, deleting or editing the input values of the reformer unit to calculate (simulate) the operating modes of the reformer unit.

During the simulation, it is possible to change the values of input, mode parameters and display the simulation results in a form convenient for DM. This information can be edited or deleted by clicking on the «Edit» or «Delete» actions provided at the end of each entry (see Figure 7).

For computer simulation of the operating modes of the reformer unit, it is necessary to click on the “Create a new calculation” button. At the same time, the window “Calculation of the reformer block model” is displayed on the screen, which, in a form convenient for DM, allows you to enter the values of the input and operating parameters of

the reformer block: x_1 is the flow rate of the feedstock (hydrogenate) in m^3/h ;

x_2 – space velocity in reforming reactors, m^3/h ; x_3 – temperature in reforming reactors in $°C$;

x_4 is the pressure in the reforming reactors, kg/m^3 ; x_5 is the hydrogen/feedstock ratio in nm^3 .

In the right part of these input, mode parameters in the boxes, by default, their average values are entered. DM can change and introduce other values of input, mode parameters $x_i, i = \overline{1, 5}$ of the block from the area of acceptable values to carry out other computer operating modes of the reforming block.

FIGURE 8. IDSS interface for modeling the operation modes of a catalytic reforming unit LG -35-11/300-95.

Entering or changing the values of the input, operating parameters of the reformer unit $x_i, i = \overline{1, 5}$ for computer simulation and displaying the simulation results with these values of the input operating parameters, you must click on the «Calculate» button. At the same time, the main results of computer simulation are displayed in the lower part of the window (Figure 8), namely the following values of the output parameters of the reformer unit: y_1 – volume of gasoline (catalyst) from reactors R-4, R-4a, in m³/h; y_2 – is the volume of HHG from the reformer unit, in m³/h; y_3 – octane number of catalysate, not less than 94; y_4 - fractional composition of the catalyzate - 10% distillation, i.e. distilled at a temperature not exceeding; y_5 - is the content of actual resins according to GOST 8489-85, in mg. per 100 ml. gasoline, no more.

Here, the output parameters y_1 and y_2 determine the quantitative values of the target products from the reformer, i.e. gasoline and hydrogen-containing gas. The remaining output parameters y_3, y_4 and y_5 are fuzzy quality indicators of gasoline obtained after defuzzification.

The following is a fragment of the C# program for creating the HttpPost method for calculating the results of computer simulation.

As a result of computer simulation of various modes of operation of reactors and a reforming furnace, on the basis of their models constructed above, the optimal mode was determined that allows increasing the yield of the catalyzate and improving its quality indicators, i.e., maximizing the octane number and minimizing the temperature of its distillation and the content of actual resins in the catalyzate.

The results of computer simulation and optimization of the operation of the reactors and the reforming furnace and their comparison with the results of modeling and optimization of other known reforming models, as well as real data obtained from the LG-35–11/300–95 Atyrau refinery unit are shown in Table 2.

```

Creation of HttpPost method for getting
[HttpPost]
[OnlyAjaxAllowed]

public async Task<ActionResult>
ModelDeepCatalysisEvaluationCount(decimal x1,
decimal x2, decimal x3, decimal x4, decimal x5)
{
    var kr =
db.KatalizReactVolume.FirstOrDefault();
    var eg =
db.ExitGazFromRiformingBlock.FirstOrDefault();
    var qk =
db.QualityKatalizIndicator.FirstOrDefault();
    var fk =
db.FractKatalizCompound.FirstOrDefault();
    var cf =
db.ContenFactSmol.FirstOrDefault();
    var y1 =
GetModelDeepCatalysisCoefficient(kr, x1, x2, x3,
x4, x5);
    var y2 =
GetModelDeepCatalysisCoefficient(eg, x1, x2, x3,
x4, x5);
    var y3 =
GetModelDeepCatalysisCoefficient(qk, x1, x2, x3,
x4, x5);
    var y4 =
GetModelDeepCatalysisCoefficient(fk, x1, x2, x3,
x4, x5);
    var y5 =
GetModelDeepCatalysisCoefficient(cf, x1, x2, x3,
x4, x5);
    return Json(new
    {
        y1, y2, y3, y4, y5,
    }, JsonRequestBehavior.AllowGet);
}

private async Task<ActionResult>
GetModelDeepCatalysisCoefficient(IQueryable<T>
cf, decimal x1, decimal x2, decimal x3, decimal
x4, decimal x5)
{
    /* it's a main formulas
    Y = +/-A1 + A11*X11 +/- A21*X21 +
A31*X31 + A41*X41 - A51*X51
    + A111*X11*X11 + A221*X21*X21 +
A331*X31*X31 + A441*X41*X41 - A551*X51*X51 +
A121*X11*X21 + A131*X11*X31 + A141*X11*X41 -
A151*X11*X51
    +/- A231*X21*X31 +/- A241*X21*X41 -
A251*X21*X51 +/- A341*X31*X41 - A351*X31*X51 -
A451*X41*X51*/
    return cf.CoeffPoprav +
cf.CoeffLinearDependencyX1 * x1 +
cf.CoeffLinearDependencyX2 * x2 +
cf.CoeffLinearDependencyX3 * x3 +
cf.CoeffLinearDependencyX4 * x4 +
cf.CoeffLinearDependencyX5 * x5 +
cf.CoeffSquareDependencyX1 * x1 * x1 +
cf.CoeffSquareDependencyX2 * x2 * x2 +
cf.CoeffSquareDependencyX3 * x3 * x3
+cf.CoeffSquareDependencyX4 * x4 * x4 +
cf.CoeffSquareDependencyX5 * x5 * x5 +
cf.CoeffRelativeDependencyX1X2 * x1 * x2
+cf.CoeffRelativeDependencyX1X3 * x1 * x3 +
cf.CoeffRelativeDependencyX1X4 * x1 * x4 +
cf.CoeffRelativeDependencyX1X5 * x1 * x5 +
+cf.CoeffRelativeDependencyX2X3 * x2 * x3 +
cf.CoeffRelativeDependencyX2X4 * x2 * x4 +
cf.CoeffRelativeDependencyX2X5 * x2 * x5
+cf.CoeffRelativeDependencyX3X4 * x3 * x4 +
cf.CoeffRelativeDependencyX3X5 * x3 * x5 +
cf.CoeffRelativeDependencyX4X5 * x4 * x5;
}

```

As can be seen from the data given in Table 2, the results of computer simulation and optimization based on the developed models, built taking into account the fuzziness of some

TABLE 2. Results of computer modeling and optimization based on known models [43], models developed by us taking into account fuzzy information and experimental data from the Ig-35–11/300–95 unit of the atyrau refinery.

| Output parameters evaluating the quantity and quality of products | Known, deterministic models | Developed models taking into account fuzzy information | Experimental data |
|--|-----------------------------|--|---------------------------------------|
| Target product output, % (mass) | 94.7 | 95.3 | 95.0 |
| Content of aromatic hydrocarbon _A , % (mass) | 68.9 | - | - |
| Output of high-quality gasoline (volume), m ³ /h | 77.1 | 77.9 | 77.7 |
| The octane number of gasoline by the motor method | - | 87 | (86) ^l |
| Fractional composition of gasoline, °C: 10% distillation Content of actual resins, in mg. per 100 ml. gasoline | - - | 67 4,7 | (68) ^l (5) ^l |

Note: the input and operating parameters of the process are taken approximately the same, (.)^l means that the data were determined in the laboratory.

part of the initial information, are better than the results of modeling using deterministic models, and so make it possible to determine a more efficient mode of operation of the reactors. The effectiveness of this mode is that the percentage of output of the target product from the reactors increases and more accurately corresponds to the values of real data. The output volume of high-quality gasoline is increased by 1.03 m³/h. In addition, the developed models make it possible to determine quality indicators, i.e., the octane number of gasoline, its fractional composition and the content of actual resins, in mg. per 100 ml. gasoline, which are characterized by fuzziness.

Based on these comparisons, we can conclude that the developed models are more adequate than deterministic models and allow us to evaluate fuzzy quality indicators of the produced target products.

V. DISCUSSION OF THE RESULTS

The proposed method for developing a package of models of interrelated CTS aggregates under uncertainty based on various available information uses a systematic approach, methods of expert assessments and fuzzy set theories. At the same time, the joint use of methods of system analysis, peer review, fuzzy set theories, as well as traditional methods of model development allows one to obtain the effect of synergy and provides the proposed system method with the effect of synergy and the property of emergence. Taking into account the flow of the process on the CTS, the developed models of its individual elements are combined into a single package of

models, which allows one to systematically simulate the CTS and select the optimal operating modes of the system.

In order to determine the most suitable type of model for each CTS unit, it is necessary to conduct a system analysis, and an expert assessment of each type of model according to pre-selected criteria for evaluating and selecting an effective type of model. The following criteria are recommended as such criteria: the availability of initial information for the development of the appropriate type of model; development cost; adequacy of the model, etc. Since the developed models of individual CTS units must be combined into a package of models for system simulation of the CTS operation, the possibility of combining the selected type of model into a single package of models should be taken into account. In the general case, a fuzzy expert assessment can be carried out, i.e. using fuzzy estimates, for example, fuzzy scores. In this case, to process the results of expert evaluation, one should apply the methods of fuzzy set theories, i.e., the membership functions of fuzzy estimates are built, and the integrated criterion is determined by combining these functions. This approach can be effectively used in the development of mathematical models of complex fuzzy CTS, which are often characterized by uncertainty. At the same time, the condition for the applicability of the proposed method is the availability of experienced experts, which in practice, as a rule, are available. The mathematical apparatus for collecting, formalizing and applying fuzzy information from DM experts is the methods of peer review and fuzzy set theory.

As shown by the simulation results using the constructed models based on the proposed method, taking into account the fuzziness of a part of the initial information, they are the best in comparison with the known results of deterministic modeling (Table 2).

As a result of modeling, taking into account fuzzy information, a more efficient mode of operation of the reactors was determined, which provides an increase in the yield of catalyze by 0.7 m³/hour. In addition, this result is more consistent with the real data obtained from the operating installation, i.e., the developed models are more adequate.

The advantages of the proposed approach to modeling, taking into account the fuzziness of the initial information, is also the possibility of determining fuzzy quality indicators - octane number, temperature of 10% distillation and the content of actual resins, in mg. per 100 ml. catalyze. These indicators are not determined in known deterministic models, but in practice they are determined with the participation of a person, through laboratory analysis. The resulting package of models also allows for system modeling of interconnected units, which allows you to find the “bottleneck” of the CTS.

Originality and novelty of the research: Due to the use of available fuzzy information and data of a different nature in the conditions of uncertainty and fuzziness of the initial information, the proposed approach allows developing a package of models of interrelated CTS units. At the same time, due to the synergistic effect and the emergence property, the proposed system method makes it possible to construct

more adequate and efficient models of the studied CTS. The models and code developed in this case study can be exported to other systems, and applied in the development of models of various technological units for oil refining, petrochemistry, and other industries.

VI. CONCLUSION

As a result of studying the problems of developing mathematical models of complex CTS, consisting of interconnected aggregates characterized by the fuzziness of some part of the initial information, a systematic approach to their solution is proposed. In the developed method for developing a package of models of interconnected CTS technological units under uncertainty, based on various available information, it is proposed to jointly use formal and informal methods of system analysis.

The proposed systematic approach allows, due to the synergy and emergence of the system of methods, to develop adequate and effective models under conditions of uncertainty using the available information of a different nature, including fuzzy information.

The importance and novelty of the proposed method lies in the application of a systematic approach to the development of a package of models of interconnected CTS units based on available information of a different nature, which makes it possible to create a package of adequate models of interconnected units and systematically model and optimize CTS.

The practical significance of the research results is that the developed system method for developing a package of models of interconnected CTS units under conditions of uncertainty can be successfully applied in the development of mathematical models of various technological units of oil refining, petrochemistry and other industries.

In accordance with the objectives of the study, the following results were obtained:

1. A method for developing a package of models of interconnected CTS units under uncertainty using various available information has been rewritten. The proposed method makes it possible to determine and develop effective types of models for each CTS unit in conditions of scarcity and fuzziness of the initial information and combine them into a single package of models for system modeling of complex objects.

2. Based on the proposed method, a package of models was developed and applied to a case study of interconnected reactors and a reforming furnace of the LG-35–11/300–95 Atyrau refinery based on the available statistical and fuzzy information. The scheme of combining the models of the main units of the reforming unit of the LG-35–11/300–95 unit into a single package of models is given.

3. To determine the optimal operating mode of the reformer unit, a system was created for computer simulation and optimization of the operating modes of the reformer unit of the LG-35–11/300–95 Atyrau refinery catalytic reformer. A comparative analysis of the obtained results of computer simulation and optimization with the results of other

well-known deterministic models and real data is carried out. The results of the comparison show the improvements using the developed models, taking into account fuzzy information, and the effectiveness of the proposed approach to solving problems of uncertainty.

In the future, we shall introduce advanced fuzzy intelligent theories and technologies (such as fuzzy clustering and fuzzy learning as well as analysis of neuro-fuzzy approaches for model identification [38], [39], [40], [41]) to our proposed models, which help to further enhance the practical effect.

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Abbreviations

Chemical-technological system – CTS
 Hydrogen - containing gas – HCG
 Leningrad-Germany – LG
 decision-maker – DM

Notations

Catalytic reforming unit with a capacity of 300000 tons/year of produced gasoline octane number 95 - LG-35–11/300–95
 Hydrotreating unit catalyst of LG unit - UOP - S-12T
 Reforming unit catalyst of LG unit - R–56
 Connected to each other through the reforming reactor furnaces - R-2, R-3, R-4, 4a
 Reforming furnace - F-1
 Reforming separators - S-7, S-9
 Fuzzy subsets – \tilde{A}_i, \tilde{B}_j
 Universal sets – X, Y
 Input, operating parameters of reactors – $\tilde{x}_i, i = \overline{1, n}$
 Output parameters of reactors – $\tilde{y}_j, j = \overline{1, m}$
 Input and output linguistic variables of reactors – $\tilde{x}_i, i = \overline{1, n}, \tilde{y}_j, j = \overline{1, m}$
 Term set – $T(X, Y)$
 Membership functions of fuzzy parameters of an object – $\mu_{A_i}(\tilde{x}_i), \mu_{B_j}(\tilde{y}_j)$.
 Parameters describing the level of fuzziness, which are determined when identifying the membership function – $Q_{B_j}^t$
 Coefficients that determine the domain of definition in the membership function of fuzzy parameters and allow changing the shape of the membership function graph – $N_{B_j}^t$
 Term number – t

Fuzzy mappings between \tilde{x}_i and $-\tilde{y}_j R_{ij}$
 compositional inference rules $\tilde{B}_j = \tilde{A}_i \circ R_{ij}$
 The calculated values of the output parameters $-y_j^M$
 Experimental (real) values of the output parameters $-y_j^E$
 Permissible deviation $-R_D$
 Output parameters, volumes of catalyzate from reactors P -2,
 P -3, P-4, $4a - y_1^{R_2}, y_1^{R_3}, y_1^{R_{4,4a}}$
 Dry gas and hydrogen-containing gas output $-y_j, j = 2, 3$
 Octane number of gasoline \tilde{y}_4
 Fractional composition of gasoline: 10% and 50% distillation
 $-\tilde{y}_5, \tilde{y}_6$
 The flow rate of the supplied raw material into the reactor $-x_1$
 Space velocity in reforming reactors $-x_2$
 Temperature in reforming reactors $-x_3$
 Reforming reactor pressure $-x_4$
 Hydrogen/feed ratio $-x_5$

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