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Methods for Developing Models in a Fuzzy Environment of Reactor and Hydrotreating Furnace of a Catalytic Reforming Unit

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Abstract: Methods for the development of fuzzy and linguistic models of technological objects, which are characterized by the fuzzy output parameters and linguistic values of the input and output parameters of the object are proposed. The hydrotreating unit of the catalytic reforming unit was investigated and described. On the basis of experimental and statistical data and fuzzy information from experts and using the proposed methods, mathematical models of a hydrotreating reactor and a hydrotreating furnace were developed. To determine the volume of production from the outlet of the reactor and furnace, nonlinear regression models were built, and fuzzy models were developed in the form of fuzzy regression equations to determine the quality indicators of the hydrotreating unit—the hydrogenated product. To identify the structure of the models, the ideas of sequential inclusion regressors are used, and for parametric identification, a modified method of least squares is used, adapted to work in a fuzzy environment. To determine the optimal temperature of the hydrotreating process on the basis of expert information and logical rules of conditional conclusions, rule bases are built. The constructed rule bases for determining the optimal temperature of the hydrotreating process depending on the thermal stability of the feedstock and the pressure in the hydrotreating furnace are implemented using the Fuzzy Logic Toolbox application of the MatLab package. Comparison results of data obtained with the known models, developed models and real, experimental data from the hydrotreating unit of the reforming unit are presented and the effectiveness of the proposed approach to modeling is shown.

Keywords: catalytic reforming; hydrotreating reactor; hydrotreating furnaces; fuzzy models; linguistic models; hydrogenate; hydrogen-containing gas

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1. Introduction

At present, the market of oil products of the Republic of Kazakhstan, as in other states, dictates the intensive development of the processes of deep oil refining and the production of high-quality and environmentally friendly motor fuels [1,2]. In this regard, there are problems of optimizing the operating modes of technological objects of deep oil refining according to economic and environmental criteria in the presence of various restrictions arising in production. Increasing the productivity of deep oil refining technological facilities and the quality of products is possible through optimal control of the operating modes of technological facilities for the production of high-quality fuels based on modeling methods and multi-criteria optimization [3].

The process of formalizing and solving problems of developing mathematical models, optimization problems in the presence of conflicting criteria, i.e., decision-making and management tasks for many technological objects of oil refining production, are complicated by the multi-criteria and fuzzy initial information [4–6]. Under these conditions, a more effective approach for solving these problems is the use of search methods of multicriteria (vector) optimization [7,8] and the mathematical apparatus of the theory of fuzzy [6,8–10], as well as the creation of a knowledge base and intellectualized decision support systems for the optimal management of technological objects and processes [8,11–15]. Thus, the development of mathematical support for intellectualized decision support systems for the optimal management of oil refining facilities in a fuzzy environment based on the knowledge and experience of experts are currently very important and urgent tasks of science and oil refining.

Currently, all refineries use catalytic cracking and catalytic reforming process units for the production of high-quality gasoline, which uses various catalysts and includes various blocks and interconnected process units [3,16,17].

In this work, the objects of modeling are the main hydrotreating units of the catalytic reforming unit of the LG-35-11/300-95 type, operating at the Atyrau refinery (AOR) since 1971 [18]. The design capacity of this unit was 300 thousand tons per year. As a result of modernization carried out at the Atyrau refinery, the capacity has now been increased to 450 thousand tons per year. The LG unit carries out the process of catalytic reforming of straight-run gasoline from the primary oil refining unit, which is the most important technological process of modern oil refining and petrochemistry. The catalytic reforming unit LG-35-11/300-95 uses the catalysts UOP—S-12T (in the hydrotreating unit) and UOP—R-56 (in the reforming unit).

In the investigated hydrotreating block of the catalytic reforming unit LG-35-11/300-95 of the Atyrau refinery for which the model is being built, an aluminum-cobalt-molybdenum catalyst of the S–12T type, developed by the American company UOP, is used. The main composition of this catalyst: aluminum oxide, which is a carrier of 65–75%; molybdenum trioxide 13–23%; amorphous silicon dioxide 5–10%, as well as a small amount of cobalt oxide 2–5%. The developed models take into account the nature of the specific catalyst UOP S—12T of the reactor of the hydrotreating unit of the reforming unit of the Atyrau refinery.

Catalytic reforming is a process of catalytic aromatization, i.e., an increase in the content of arenes as a result of the formation of aromatic hydrocarbons. This process, like the process of catalytic isomerization of light alkanes, belongs to the hydrocatalytic processes of reforming petroleum feedstock. The catalytic reforming unit is used for the production of high-octane motor gasoline, aromatic hydrocarbons (feedstock for petrochemical synthesis) and hydrogen-containing gas (HCG) (technical hydrogen), and is used in the hydrogenation processes of oil refining. Such catalytic reforming units are available at almost all domestic and foreign refineries [19–21].

Thus, the object of study in this work is the hydrotreating unit of the catalytic reforming unit LG-35-11/300-95 of the Atyrau refinery.

The aim of the study was to develop methods for constructing models of technological objects in conditions of a deficit and indistinctness of the initial information, which are the hydrotreating unit of the catalytic reforming unit using the available information of a different nature. In addition, the goal is to develop mathematical models of the main units of the hydrotreating unit of the catalytic reforming unit.

To ensure the achievement of the set goal, the following main tasks are solved in the work:

- to develop methods for the development of mathematical models of technological objects, which are characterized by the fuzziness of initial information;
- to develop mathematical models of the R-1 hydrotreating reactor in conditions of deficit and indistinctness of initial information;
- to construct models of the F-101 hydrotreating furnace based on experimental and statistical information.

2. Materials and Methods

2.1. Brief Description of the Hydrotreating Unit of the Catalytic Reforming Cracking Unit LG-35-11/300-95

The unit for catalytic reforming cracking LG-35-11/300-95 consists of 4 blocks, the main of which is a hydrotreating unit and a reforming unit, which in turn have many interconnected technological units. At the same time, the hydrotreating unit is designed to purify straight-run gasoline coming from the primary oil refining unit from organic compounds of sulfur, oxygen and nitrogen, and in the reforming unit, the process of converting naphthenes and paraffin into aromatic hydrocarbons takes place.

In the hydrotreating unit, the process of hydrotreating straight-run gasoline from the primary oil refining unit takes place. At the same time, the quality of straight-run gasoline is improved due to the removal of sulfur, as well as other harmful compounds and impurities from their composition, which worsen the operational characteristics of technological equipment and metal units [22,23]. Thus, the hydrotreating process can reduce corrosion of metal equipment and pollution of the environment and atmosphere. Therefore, the study and improvement of the processes of hydrotreating oil refining on the basis of scientifically grounded methods, for example, methods of mathematical modeling and optimization, is an urgent task of science and practice of oil refining.

A brief description of the process flow diagram of the hydrotreating unit of the catalytic reforming unit of the Atyrau refinery shown in Figure 1, is given.

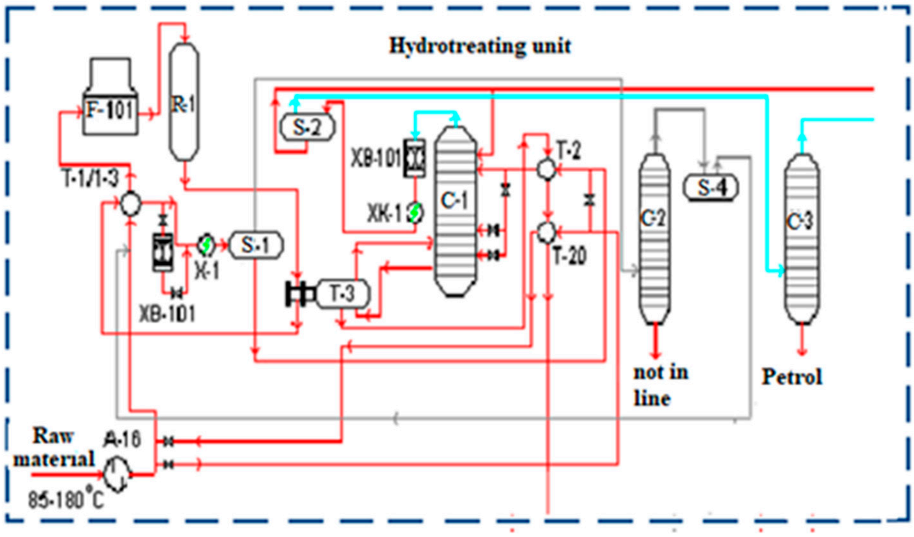


Figure 1. Technological scheme of hydrotreating unit at the catalytic reforming unit of the Atyrau refinery.

Raw materials from the tank farm are fed by the A16 pump for mixing together with the HCG. The mixture of raw materials and HCG is fed to 3 heat exchangers T-1/1-3 connected in series, here, due to the counterflow of carbonated raw materials from the R-1 reactor and the T-3 reboiler, it is heated to a temperature of 260 °C, then it enters the F-101 hydrotreating furnace. From the F-101 furnace, a mixture of feedstock and gas with a temperature of 300–343 °C is fed to the hydrotreating reactor R-1, where the feedstock hydrotreating reaction takes place with the participation of catalyst S-12, i.e., the raw material is preliminarily hydrotreated from sulfur, nitrogen and oxygen-containing compounds. The heat of the mixture of unstable hydrogenate, circulating gas from the outlet of the reactor and the heat of reaction of gases with a temperature of 340–420 °C is used to heat the mixture of raw materials and gas, first in the heat exchanger T-3 of the stripping column C-1, then in the heat exchangers T-1/1-3 [18].

In gaseous form, the products after cooling in refrigerators XB-101 and X-1 to a temperature of 35 °C are fed to the separator S-1. There HCG is separated from the liquid and for cleaning it from hydrogen it enters the absorber C-2. The gas from the outlet of this absorber passes through the separator S-4, where it is divided into two streams:

(1) Circulating gas, which, after being compressed in the compressors, is fed back to the feedstock hydrotreating system;
(2) Excessive HCG from the unit outlet.

The liquid phase of the separator S-1, passing through the heat exchanger T-2, is heated to a temperature of 150 °C and fed to the 7, 9, 23 trays of the stripping column C-1. From the stripping column C-1, from the hydrogenate at a temperature of up to 270 °C and a pressure of up to 15 atm, sulfuric hydrogen and water are stripped, and light hydrocarbons are removed from the top of the column C-1.

After the stripping column C-1, the total composition of sulfur compounds in the hydrogenation product according to the standard should not exceed 0.0005% by weight. Gases in the state of steam from the top of the stripping column C-1 come out with a temperature of 135 °C, then they pass through the chiller-condensers XB-101 and XK-1 and with a temperature of 35–40 °C enter the separator S-2. From this separator S-2, the liquid phase is returned to the stripper C-1. The settled water in the S-2 separator is discharged into the sewer. Hydrocarbon gas from the S-2 separator for hydrogen sulfide removal enters absorber C-3, and hydrocarbon gas from the top of absorber C-3 is fed to the fractionating absorber C-6 of the reformer or the refinery's fuel network.

Thus, in the process of hydrotreating, a chemical transformation of a substance occurs under the influence of hydrogen gas with high pressure and high temperature. In the process of hydrotreating, sulfur compounds are reduced in the composition of petroleum products, fuels, a saturation of additional unsaturated hydrocarbons occurs, the composition of tar, oxygenated compounds decreases, as well as hydrocracking of hydrocarbon molecules.

Improving refinery hydrotreating processes using modeling methods allows [24]:

- to carry out hydrotreating processes in the optimal mode, which maximizes the productivity of the facility and the yield of target products;
- to improve quality indicators of manufactured products.

This paper proposes an effective approach to the development of mathematical models and modeling of technological objects on the example of units of the hydrotreating block of the Atyrau refinery. A number of research works are known on methods of mathematical modeling and optimization of technological objects and oil refining processes, including the process of hydrotreating, for example [25,26]. However, in practice, production situations can often arise associated with a shortage and indistinctness of initial information, problems of modeling and optimization of their operating modes, the formulation and solution of which using traditional methods do not provide adequate solutions. Such objects include the hydrotreating unit of the LG unit at the Atyrau refinery, the main units of which operate under conditions of uncertainty associated with randomness and with indistinctness of initial information [27]. In this regard, it will be necessary to develop mathematical models of the main hydrotreating unit the Atyrau refinery on the basis of a systematic approach, i.e., using available information of various nature.

2.2. Development of Mathematical Models of Technological Objects Functioning in Conditions of Indistinctness of Initial Information

To develop methods for constructing models of technological objects, which are characterized by the fuzzy initial information, we use the methodology for modeling complex objects in conditions of uncertainty and a hybrid approach to the development of mathematical models, proposed by us elsewhere [27,28].

Of the various approaches to developing models based on fuzzy information, three can be distinguished:

(1) an approach based on the idea of regression analysis, taking into account the fuzziness of some part of the initial information;

(2) an approach based on the use of logical rules for conditional inference, used in the conditions of fuzzy input and output parameters of the object;
(3) combined approaches.

We turn to the study and description of the first approach based on the use of regression analysis taking into account fuzzy information. Using this approach, the structure of the models is identified in the form of regression models with fuzzy coefficients. Fuzzy models built on the basis of this approach are successfully used in modeling and control of a number of chemical–technological systems of oil refining [3,4,27] and can be used to model objects in other industries.

In this approach, the values of the input parameters $x_i,\ i = \overline{1,n}$ are quantitatively measurable, and the values of the output parameters of the object $\widetilde{y}_j^M,\ j = \overline{1,m}$ are immeasurable, they can be evaluated by a specialist, a decision-maker (DM) unclearly based on their experience, knowledge and intuition.

Under these conditions, the mathematical relationship between input and output parameters, i.e., the model is obtained in the form of fuzzy regression equations:

$$\widetilde{y}_j^M = \widetilde{f}_j^M(x_1, \ldots, x_n) \tag{1}$$

where ~—fuzzy operator.

Suppose that as a result of observing the operation of the object and the experiments carried out, k values of the input parameters $x_i\left(x_{i1},\ i = \overline{1,n},\ 1 = \overline{1,k}\right)$ were obtained, and the corresponding fuzzy values of the output parameters $\widetilde{y}_j^M\left(\widetilde{y}_{j1}^M,\ j = \overline{1,m},\ 1 = \overline{1,k}\right)$ were estimated by experts.

Then, to build fuzzy models of this object, it is necessary to carry out the following two stages of solving the identification problem.

Stage 1. Choose the structure of the function (structural identification):

$$\widetilde{y}_j^M = \widetilde{f}_j^M(x_1, \ldots, x_n,\ \widetilde{\alpha}_0, \ldots, \widetilde{\alpha}_n),\ j = \overline{1,\ k} \tag{2}$$

which corresponds to Equation (1).

At this stage, the qualitative analysis of the object is of decisive importance, as a result of which the main parameters affecting the functioning of the object, their interrelationships, the influence of these parameters on the optimization criteria are revealed. To determine the structure of the model, you can use a fuzzy analog of the method of sequential inclusion of regressors [28].

Stage 2. Determine the estimates of the parameters of the selected function (2), for example, the values of fuzzy coefficients $\widetilde{\alpha}_0, \ldots, \widetilde{\alpha}_n$, i.e., the problem of parametric identification is being solved. For such an assessment, you can use the criterion of minimizing the deviation of the fuzzy values of the output parameter $\widetilde{y}_j^M$ obtained by the model from its sample fuzzy values obtained on the basis of expert judgment y_j^e:

$$\widetilde{R}_j = \min \sum_{I=1}^{k} \left(\widetilde{y}_{j1}^e - \widetilde{y}_{j1}^M\right)^2 = \min \sum_{I=1}^{k} \left(\widetilde{y}_{j1}^E - \widetilde{f}_{j1}^M(x_{1I}, \ldots, x_{n1},\ \widetilde{\alpha}_{01}, \ldots, \widetilde{\alpha}_{n1})\right)^2 \tag{3}$$

Note that when calculating criterion (3), operations are performed on fuzzy sets and numbers [4,6,9]. At this stage, the main questions are the choice of a method for estimating unknown parameters that ensure the adequacy of the model.

In the general case, the fuzzy models obtained on the basis of this approach have the form:

$$\widetilde{y}_j^M = \widetilde{\alpha}_{oj} + \sum_{i=1}^{n} \widetilde{\alpha}_{ij} x_{ij} + \sum_{i=1}^{n} \sum_{k=i}^{n} \widetilde{\alpha}_{ikj} x_{ij} + \ldots,\ j = \overline{1,m} \tag{4}$$

Based on the set of level α ($\alpha \in [0,1],\ A_\alpha = \{x : x \in X,\ \mu_A(x) \geq \alpha\}$), the problem of estimating the fuzzy coefficients of the model can be reduced to the classical problems of estimating the parameters of multiple regression equations using the idea of the least squares method.

As a result of this approach, we obtain the values of the estimated coefficients of various levels $\alpha_q,\ q = \overline{1, L} - \alpha_{ij}^{\alpha q}$.

To obtain the coefficients $\widetilde{\alpha}_{ij}$, the obtained values $\alpha_{ij}^{\alpha q}$ are combined:

$\widetilde{\alpha}_{ij} = \underset{\alpha \in [0.5 \div 1]}{U} \alpha_{ij}^{\alpha}$ or $\mu_{\widetilde{\alpha}_{ij}}(\alpha_{ij}) = \sup_{\alpha \in [0.1 \div 1]} \min\left\{\alpha_q,\ \mu_{\alpha_{ij}}^{\alpha_q}(\alpha_{ij})\right\}$.

The second approach is based on the use of logical rules for conditional inference. This approach to modeling in a fuzzy environment is based on the use of logical rules for conditional inference, which in general can be written:

$$IF\ \widetilde{x}_1 \in \widetilde{A}_1(\widetilde{x}_2 \in \widetilde{A}_2(, \ldots, (\widetilde{x}_n \in \widetilde{A}_n), \ldots,)\ THEN\ \widetilde{y}_j^M \in \widetilde{B}_j,\ j = \overline{1, m} \quad (5)$$

where $\widetilde{x}_i(i = \overline{1, n}),\ \widetilde{y}_j^M$—respectively, the input and output linguistic variables of the object, $\widetilde{A}_i,\ \widetilde{B}_j$—are the fuzzy subset characterizing $\widetilde{x}_i,\ \widetilde{y}_j^M$.

The advantage of this approach is the possibility of using it when modeling objects for which the collection of statistical, quantitative information is very difficult or impossible. In this case, the obtained models are the result of a survey of experts, decision-makers, operating, as a rule, with information of a fuzzy nature. Such information, in the conditions of the competence of specialists, allows the obtained models to take into account not formalized internal interconnections of the parameters of the object.

Based on the two approaches described above, we propose the following methods for constructing models, taking into account the fuzzy initial information.

2.3. A Method for Constructing Fuzzy Models Using Fuzzy Initial Information with Clear Input and Fuzzy Output Parameters of the Object

Present and briefly describe the main stages of the Fuzzy Modeling (FM) method.

1. Select the input (mode—control) $x_i \in X_i,\ i = \overline{1, n}$ and output $\widetilde{y}_j \in Y_j,\ j = \overline{1, m}$ parameters of the object necessary for building the model. In this case, the parameters that are informative and affect the output parameters are selected as input parameters, and those fuzzy parameters that assess the quality of the object's operation are selected as the output parameters;

2. To collect and process data on parameters $x_i \in X_i,\ i = \overline{1, n}$ and expert information, which allows determining the term-set of fuzzy parameters $T(X, Y)$, describing the state and output of the object;

3. Determine the structure of fuzzy equations $\widetilde{y}_j = \widetilde{f}_j(x_1, \ldots, x_n, \widetilde{a}_0, \widetilde{a}_1, \ldots, \widetilde{a}_n)$, $j = \overline{1, m}$, i.e., solve the problem of structural identification. To identify the structure of the models, we can recommend applying the method of sequential inclusion of regressors [28].

4. Construct the membership function of the fuzzy parameters of the object. Based on practical experience, when constructing such functions, it is recommended to apply the following structure with adjustable coefficients:

$$\mu_{B_j}^p(\widetilde{y}_j) = \exp(Q_{B_j}^p \left| (y_j - y_{md_j})^{N_{B_j}^p} \right|) \quad (6)$$

where $\mu_{B_j}^p(\widetilde{y}_j)$—are the membership functions of fuzzy output parameters $\widetilde{y}_j$ belonging to a fuzzy set $\widetilde{B}_j$; p—quantum number; $Q_{B_j}^p$—coefficient, which is determined when identifying the membership function and characterizing the degree of fuzziness; $N_{B_j}^p$—coefficient that changes the domains of definition of terms and the shape of the graph of the membership function of fuzzy parameters; $y_{md_j}^p$—is the fuzzy variable that most closely matches a given term (in the quantum p) for this quantity $\mu_{B_j}^p(y_{mdi}) = \max_j \mu_{B_j}^p(y_j)$. At this point, you can select the appropriate type of membership function and build them using the Fuzzy Logic Toolbox application [29].

5. Identify fuzzy parameters of the function model $(\widetilde{a}_0, \widetilde{a}_1, \ldots, \widetilde{a}_n)$, i.e., solve the problem of parametric identification of fuzzy regression coefficients. The identification of the parameters of fuzzy models can be carried out using a modification of the least squares method for working in a fuzzy environment based on a set of level α from fuzzy set theories, which allows for the transforming of a fuzzy problem into a system of clear problems at different levels.

6. Check the conformity of the model to real data, i.e., the adequacy of the constructed model. In this case, the following condition can be used as an adequacy criterion:

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

where y_j^M—calculated (model), and y_j^E—experimental (real) values of the object's output parameters, R_D—permissible deviation.

If the adequacy condition is met, then the model is recommended for modeling and determining the optimal operating modes of the object. Otherwise, the reason for the inadequacy of the model is determined and the transition is processed to the corresponding points of the described methodology. In this case, the reason for the inadequacy of the model can be: not including some parameters in the model that significantly affect the process; incorrect structural and/or parametric identification of the model, etc.

2.4. A Method for Constructing Linguistic Models with Fuzzy Values of the Input and Output Parameters of the Object

We present and briefly describe the main stages of the method for the development of linguistic models (LM).

This method implements the above described second approach to developing models based on fuzzy information and is based on the use of linguistic variables that describe the input and output parameters of the object. Some points of this method (1, 2 and 6) are similar to the corresponding points of the FM method, but it is necessary to take into account the fuzziness of the input parameters—$\widetilde{x}_i,\ i = \overline{1,m}$.

1. Select the input $\widetilde{x}_i \in X,\ i = \overline{1,n}$ and output $\widetilde{y}_j \in Y,\ j = \overline{1,m}$ parameters of the object that are necessary for building the model, which are linguistic variables ($X,\ Y$—universal sets);

2. On the basis of expert assessments, evaluate the values of the parameters $\widetilde{x}_i,\ \widetilde{y}_j$ and determine the term-set $T(X,Y)$.

3. Construct membership functions of fuzzy parameters—$\mu_{\widetilde{A}_i}(\widetilde{x}_i),\ \mu_{\widetilde{B}_j}(\widetilde{y}_j)$ $\widetilde{A}_i,\ \widetilde{B}_j$—fuzzy subsets $\widetilde{A}_i \subset X,\ \widetilde{B}_j \subset Y$). At this point, Equation (6) can be used as the structure of the membership function, as well as in the FM method.

4. Build a linguistic model of the object and formalize fuzzy mappings that determine the relationship between the parameters $\widetilde{x}_i$ and $\widetilde{y}_j$—R_{ij}. For the convenience of using fuzzy mapping in the calculation, you should construct a matrix of connections between input and output parameters with membership functions:

$$\mu_{R_{ij}}(\widetilde{x}_i, \widetilde{y}_j) = \min[\mu_{A_i}(\widetilde{x}_i), \mu_{B_{ji}}(\widetilde{y}_j), i = \overline{1,n},\ j = \overline{1,m}].$$

5. Determine the fuzzy values of the object's output parameters and select their numerical values from the fuzzy set of solutions. Then, a linguistic model is built, with a general structure as in (5), i.e.,

$$IF\ \widetilde{x}_1 \in \widetilde{A}_1(\widetilde{x}_2 \in \widetilde{A}_2(, \ldots, (\widetilde{x}_n \in \widetilde{A}_n), \ldots,)\ THEN\ \widetilde{y}_j^M \in \widetilde{B}_j,\ j = \overline{1,m}$$

6. Check the conditions for the adequacy of the model. The adequacy of the model can be checked both in the corresponding, i.e., 6-point of the FM method. If the model is inadequate, find out the reason and return to the appropriate point to refine the model.

3. Results

3.1. Building Models of the Reactor and Hydrotreating Furnace of the Catalytic Reforming Unit Using Experimental-Statistical and Fuzzy Information

As a result of the research and processing of data results, it was established that to determine the volume of production output, i.e., y_1 hydrogenated product from the outlet of the hydrotreating reactor of the R-1 unit, on the basis of experimental and statistical data, it is possible to build a statistical model that, using a nonlinear regression equation, makes it possible to estimate the values y_1 (m^3/h) from the input and operating parameters x_i, $i = \overline{1,5}$. Input and operating parameters are: x_1—the volume of raw materials, straight-run gasoline (45–80 m^3/h); x_2—pressure in the reactor R-1 (20–35 kg/cm^2); x_3—temperature in the reactor R-1 (300–343 °C); x_4—volumetric feed rate (0.5–5 h^{-1}); x_5—circulating hydrogen-containing gases (HCG)—hydrogen/hydrocarbon ratio (200–500 nm^3). The intervals in which the input and operating parameters change are indicated in brackets.

After structural (based on the method of sequential inclusion of regressors) and parametric (using the least squares method based on the REGRESS software package) identification, a mathematical model that allows us to determine the volume of hydrogenate from the outlet of the reactor R-1, depending on $x_i,\ i = \overline{1,5}$, is obtained in the form:

$$\begin{aligned} y_1 &= 7.00 + 0.233x_1 + 0.130x_2 + 0.011x_3 + 2.333x_4 - 0.0175x_5 \\ &+0.0031x_1^2 + 0.0048x_2^2 + 0.00003x_3^2 + 0.7778x_4^2 - 0.00004x_5^2 \\ &+0.0017x_1x_2 + 0.00015x_1x_3 + 0.03111x_1x_4 + 0.00023x_1x_5 \\ &+0.08642x_2x_4 - 0.00065x_2x_5 + 0.00730x_3x_4 \end{aligned}$$

A graph of the dependence of the hydrogenated product output on the temperature in the reactor x_3 is plotted at fixed values of the remaining input, operating parameters: x_1, x_2, x_4 and x_5 (Figure 2).

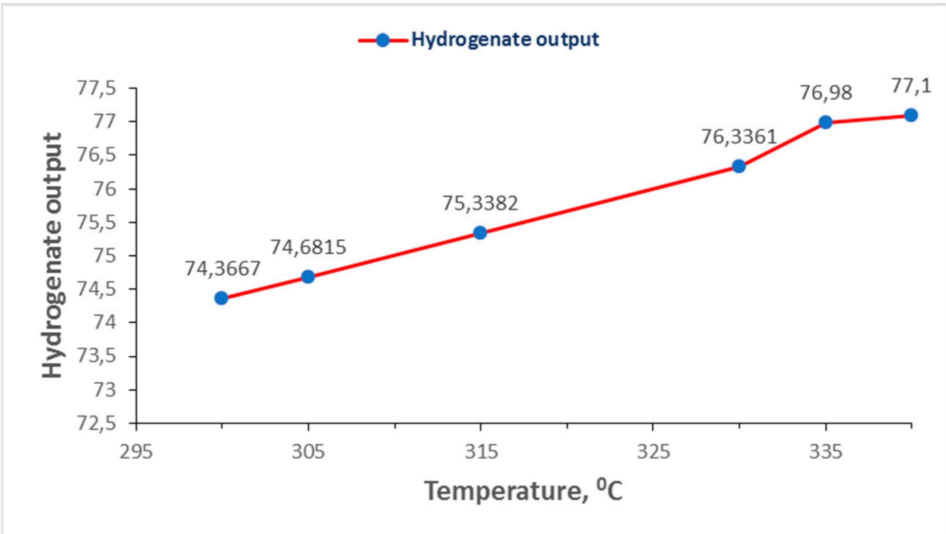


Figure 2. Dependency graph $y_1 = f_1(x_3)$ for fixed x_1, x_2, x_4 and x_5 (x_1—volume of raw materials, 80 m^3/h, x_2—pressure in R-1, 30 kg/cm^2, x_4—volumetric velocity, 3 h^{-1}, x_5—HCG circulation, 400 nm^3).

In the process of developing mathematical models describing the qualitative indicators of the produced hydrogenation (the content of unsaturated hydrocarbons, sulfur, water-soluble acids and alkali in the hydrogenation product) at the Atyrau refinery, problems of uncertainty related to the lack and unclearness of the initial information arose. Therefore, to develop models for assessing the quality of hydrogenated products, a systematic approach was applied using methods of expert assessments and theories of fuzzy sets based on the methods proposed in Section 2 for constructing mathematical models under conditions of fuzzy initial information.

For this purpose, with the involvement of experts from the number of process operators, the head of the installation and researchers of the subject area, an expert assessment of the influence of input and operating parameters on the quality of hydrogenated product was carried out. As a result of processing experimental–statistical and expert information using the fuzzy modeling method described in Section 3.1, the following structure of fuzzy models was identified, describing the product quality of the R-1 hydrotreating reactor in the form of fuzzy multiple regression equations:

$$\widetilde{y}_j = a_{0j}x_{ij} + \sum_{i=1}^{5} a_{ij}x_{ij} + \sum_{i=1}^{5}\sum_{k=i}^{5} a_{ijk}x_{ij}x_{kj},\ j = \overline{2,4} \quad (7)$$

where $\widetilde{y}_2$ is the unsaturated hydrocarbons in the product, i.e., hydrogenated products, which are characterized by indistinctness (should be no more, i.e., $\widetilde{\leq}1\%$); $\widetilde{y}_3$—sulfur in the hydrogenated product ($\widetilde{\leq}0.00005\%$); $\widetilde{y}_4$—water-soluble acids and alkalis in the hydrogenated product ($\widetilde{\cong}0\%$); The admissible fuzzy values of the hydrogenated product quality indicators are indicated in brackets; $x_i,\ i = \overline{1,5}$—input, operating parameters of the hydrotreating reactor, i.e., respectively, the volume of raw materials, pressure, temperature, space velocity and circulation of HCG; $\widetilde{a}_{0j}, \widetilde{a}_{ij}, \widetilde{a}_{ikj}, i = \overline{1,5}$—parameters, fuzzy regression coefficients subject to regression identification.

To identify unknown parameters (regression coefficients) of the model (7): $\widetilde{a}_{ij}$ ($i = \overline{0,5}$, $j = \overline{2,5}$) and $\widetilde{a}_{ikj}$ ($i,k = \overline{1,5}$, $j = \overline{2,5}$), the membership functions of fuzzy sets describing the qualities of the hydrogenate are divided into the following sets of level α: α = 0.5; 0.85; 1. Since in our case the membership function has a bell-shaped form, the values of fuzzy parameters at five points α = 0.5; 0.85 (left); 1; 0.85; 0.5 (right). The values of the input, mode $x_{ij},\ i,j = \overline{1,5}$ and output $\widetilde{y}_2, \widetilde{y}_3, \widetilde{y}_4$ parameters for each selected α level are observed.

Thus, we obtained models describing the quality of the product from the outlet of the R-1 reactor in the form of multiple regression for each α level. Since the obtained equations have the form of regression equations, the problem of identifying their unknown coefficients $\alpha_{ij}^{\alpha_q}, i = \overline{0,5},\ j = \overline{2,4},\ \ q = \overline{1,3}$ can be solved using known methods of parametric identification, for example, using the least squares method. In this work, to identify the regression coefficients, the REGRESS program package was used, which, based on modified least squares methods, allows one to determine the regression coefficients of linear and nonlinear regression models with any number of input parameters $x_i, i = \overline{1,n}$.

Thus, after parametric identification, mathematical models describing the influence of input, operating parameters $x_i,\ i = \overline{1,5}$ on the quality of the hydrogenated product, i.e., on the content of unsaturated hydrocarbons ($\widetilde{y}_2$), sulfur ($\widetilde{y}_3$) and water-soluble acids and alkalis ($\widetilde{y}_4$) for each α level have the form:

$$\begin{aligned}
y_2 = {} & \left(\tfrac{0.5}{0.05} + \tfrac{0.85}{0.07} + \tfrac{1}{0.08} + \tfrac{0.85}{0.09} + \tfrac{0.5}{0.095}\right) - \left(\tfrac{0.5}{0.00215} + \tfrac{0.85}{0.0029} + \tfrac{1}{0.00324} + \tfrac{0.85}{0.00375} + \tfrac{0.5}{0.00425}\right)x_1 \\
& + \left(\tfrac{0.5}{0.00591} + \tfrac{0.85}{0.00592} + \tfrac{1}{0.00593} + \tfrac{0.85}{0.00594} + \tfrac{0.5}{0.00595}\right)x_2 + \left(\tfrac{0.5}{0.0002} + \tfrac{0.85}{0.0005} + \tfrac{1}{0.0007} + \tfrac{0.85}{0.00095} + \tfrac{0.5}{0.0013}\right)x_3 \\
& + \left(\tfrac{0.5}{0.03125} + \tfrac{0.85}{0.04333} + \tfrac{1}{0.05333} + \tfrac{0.85}{0.06333} + \tfrac{0.5}{0.007333}\right)x_4 + \left(\tfrac{0.5}{0.0004} + \tfrac{0.85}{0.0005} + \tfrac{1}{0.0006} + \tfrac{0.85}{0.0007} + \tfrac{0.5}{0.0008}\right)x_5 \\
& - \left(\tfrac{0.5}{0.00002} + \tfrac{0.85}{0.00003} + \tfrac{1}{0.00004} + \tfrac{0.85}{0.00005} + \tfrac{0.5}{0.00007}\right)x_1^2 + \left(\tfrac{0.5}{0.00021} + \tfrac{0.85}{0.00022} + \tfrac{1}{0.00023} + \tfrac{0.85}{0.00024} + \tfrac{0.5}{0.00025}\right)x_2^2 \\
& + \left(\tfrac{0.5}{0.00012} + \tfrac{0.85}{0.00018} + \tfrac{1}{0.00023} + \tfrac{0.85}{0.00028} + \tfrac{0.5}{0.00033}\right)x_3^2 - \left(\tfrac{0.5}{0.01675} + \tfrac{0.85}{0.01727} + \tfrac{1}{0.01777} + \tfrac{0.85}{0.01713} + \tfrac{0.5}{0.01818}\right)x_4^2 \\
& + \left(\tfrac{0.5}{0.000008} + \tfrac{0.85}{0.000014} + \tfrac{1}{0.00002} + \tfrac{0.85}{0.00003} + \tfrac{0.5}{0.00005}\right)x_5^2 - \left(\tfrac{0.5}{0.0003} + \tfrac{0.85}{0.00035} + \tfrac{1}{0.0004} + \tfrac{0.85}{0.00045} + \tfrac{0.5}{0.0005}\right)x_1x_2 \\
& + \left(\tfrac{0.5}{0.000024} + \tfrac{0.85}{0.00003} + \tfrac{1}{0.000033} + \tfrac{0.85}{0.00004} + \tfrac{0.5}{0.000047}\right)x_1x_3 - \left(\tfrac{0.5}{0.00068} + \tfrac{0.85}{0.0007} + \tfrac{1}{0.00073} + \tfrac{0.85}{0.00075} + \tfrac{0.5}{0.00077}\right)x_1x_4 \\
& + \left(\tfrac{0.5}{0.000012} + \tfrac{0.85}{0.000019} + \tfrac{1}{0.000027} + \tfrac{0.85}{0.000035} + \tfrac{0.5}{0.000043}\right)x_1x_5 - \left(\tfrac{0.5}{0.00083} + \tfrac{0.85}{0.0009} + \tfrac{1}{0.00098} + \tfrac{0.85}{0.0001} + \tfrac{0.5}{0.0015}\right)x_2x_4 \\
& + \left(\tfrac{0.5}{0.000005} + \tfrac{0.85}{0.000006} + \tfrac{1}{0.000007} + \tfrac{0.85}{0.000008} + \tfrac{0.5}{0.000009}\right)x_2x_5 - \left(\tfrac{0.5}{0.0001} + \tfrac{0.85}{0.00015} + \tfrac{1}{0.00012} + \tfrac{0.85}{0.00015} + \tfrac{0.5}{0.00018}\right)x_3x_5;
\end{aligned}$$

$$
\begin{aligned}
y_3 = &\left(\frac{0.5}{0.002}+\frac{0.85}{0.003}+\frac{1}{0.004}+\frac{0.85}{0.005}+\frac{0.5}{0.006}\right)-\left(\frac{0.5}{0.00014}+\frac{0.85}{0.00015}+\frac{1}{0.00016}+\frac{0.85}{0.00017}+\frac{0.5}{0.00018}\right)x_1\\
&+\left(\frac{0.5}{0.00027}+\frac{0.85}{0.00028}+\frac{1}{0.00029}+\frac{0.85}{0.0003}+\frac{0.5}{0.00031}\right)x_2+\left(\frac{0.5}{0.00002}+\frac{0.85}{0.00003}+\frac{1}{0.00004}+\frac{0.85}{0.000045}+\frac{0.5}{0.0005}\right)x_3\\
&+\left(\frac{0.5}{0.00044}+\frac{0.85}{0.0005}+\frac{1}{0.00053}+\frac{0.85}{0.00054}+\frac{0.5}{0.00055}\right)x_4+\left(\frac{0.5}{0.000002}+\frac{0.85}{0.0000025}+\frac{1}{0.000003}+\frac{0.85}{0.0000035}+\frac{0.5}{0.000004}\right)x_5\\
&-\left(\frac{0.5}{0.000001}+\frac{0.85}{0.0000015}+\frac{1}{0.000002}+\frac{0.85}{0.0000025}+\frac{0.5}{0.000003}\right)x_1^2+\left(\frac{0.5}{0.00001}+\frac{0.85}{0.000015}+\frac{1}{0.00002}+\frac{0.85}{0.000025}+\frac{0.5}{0.00003}\right)x_2^2\\
&+\left(\frac{0.5}{0.00015}+\frac{0.85}{0.00017}+\frac{1}{0.00018}+\frac{0.85}{0.00019}+\frac{0.5}{0.0002}\right)x_4^2+\left(\frac{0.5}{0.00002}+\frac{0.85}{0.00003}+\frac{1}{0.00004}+\frac{0.85}{0.00005}+\frac{0.5}{0.00006}\right)x_1x_2\\
&+\left(\frac{0.5}{0.000001}+\frac{0.85}{0.000009}+\frac{1}{0.00001}+\frac{0.85}{0.00002}+\frac{0.5}{0.00003}\right)x_1x_3-\left(\frac{0.5}{0.00007}+\frac{0.85}{0.00013}+\frac{1}{0.00018}+\frac{0.85}{0.00023}+\frac{0.5}{0.00030}\right)x_1x_4\\
&+\left(\frac{0.5}{0.00001}+\frac{0.85}{0.00009}+\frac{1}{0.00010}+\frac{0.85}{0.00020}+\frac{0.5}{0.00030}\right)x_2x_3-\left(\frac{0.5}{0.00038}+\frac{0.85}{0.00044}+\frac{1}{0.00049}+\frac{0.85}{0.00054}+\frac{0.5}{0.00064}\right)x_2x_4\\
&+\left(\frac{0.5}{0.000002}+\frac{0.85}{0.000003}+\frac{1}{0.000004}+\frac{0.85}{0.000005}+\frac{0.5}{0.000006}\right)x_3x_4;
\end{aligned}
$$

$$
\begin{aligned}
y_4 = &\left(\frac{0.5}{0.00023}+\frac{0.85}{0.00024}+\frac{1}{0.00025}+\frac{0.85}{0.00026}+\frac{0.5}{0.00027}\right)-\left(\frac{0.5}{0.001}+\frac{0.85}{0.0015}+\frac{1}{0.002}+\frac{0.85}{0.0025}+\frac{0.5}{0.003}\right)x_1\\
&+\left(\frac{0.5}{0.00024}+\frac{0.85}{0.00032}+\frac{1}{0.00037}+\frac{0.85}{0.00042}+\frac{0.5}{0.005}\right)x_2-\left(\frac{0.5}{0.00003}+\frac{0.85}{0.00004}+\frac{1}{0.00005}+\frac{0.85}{0.00006}+\frac{0.5}{0.00007}\right)x_3\\
&+\left(\frac{0.5}{0.00659}+\frac{0.85}{0.00664}+\frac{1}{0.00667}+\frac{0.85}{0.00670}+\frac{0.5}{0.00675}\right)x_4+\left(\frac{0.5}{0.000002}+\frac{0.85}{0.000003}+\frac{1}{0.000004}+\frac{0.85}{0.000005}+\frac{0.5}{0.000006}\right)x_5\\
&-\left(\frac{0.5}{0.000001}+\frac{0.85}{0.000005}+\frac{1}{0.00001}+\frac{0.85}{0.000015}+\frac{0.5}{0.000020}\right)x_2^2+\left(\frac{0.5}{0.000207}+\frac{0.85}{0.000215}+\frac{1}{0.000222}+\frac{0.85}{0.000230}+\frac{0.5}{0.000330}\right)x_4^2\\
&+\left(\frac{0.5}{0.000001}+\frac{0.85}{0.000005}+\frac{1}{0.00001}+\frac{0.85}{0.000015}+\frac{0.5}{0.000020}\right)x_1x_2-\left(\frac{0.5}{0.000005}+\frac{0.85}{0.00001}+\frac{1}{0.00002}+\frac{0.85}{0.00003}+\frac{0.5}{0.00004}\right)x_1x_4\\
&+\left(\frac{0.5}{0.000004}+\frac{0.85}{0.000005}+\frac{1}{0.000006}+\frac{0.85}{0.000007}+\frac{0.5}{0.000008}\right)x_2x_4-\left(\frac{0.5}{0.000001}+\frac{0.85}{0.000005}+\frac{1}{0.000001}+\frac{0.85}{0.0000015}+\frac{0.5}{0.00002}\right)x_3x_4\\
&+\left(\frac{0.5}{0.0000001}+\frac{0.85}{0.0000005}+\frac{1}{0.0000010}+\frac{0.85}{0.0000015}+\frac{0.5}{0.0000020}\right)x_4x_5.
\end{aligned}
$$

The identified values of the coefficients $a_{ij}^{\alpha_q}$, $i=\overline{0,5};\ j=\overline{2,4};\ \ q=\overline{1,3}$ are combined using the following expression of the theory of fuzzy sets [6,9]:

$$a_{ij}=\bigvee_{\alpha\in[0.5,1]} a_{ij}^{\alpha_q} \text{ or } \mu\,\widetilde{a}_{ij}(a_{ij})=SUP\min_{\alpha\in[0.5,1]}\left\{\alpha,\mu\, a_{ij}^{\alpha}(a_{ij})\right\}, \text{ where } a_{ij}^{\alpha_q}=\left\{a_i\middle|\mu\,\widetilde{a}_{ij}(a_{ij})\right\}$$

In the obtained models, regressors that have no effect on the quality of the hydrogenated product, i.e., on $\widetilde{y}_2$, $\widetilde{y}_3$ and $\widetilde{y}_4$ or very little influence are set to zero, i.e., not shown.

Mathematical models of the F-101 hydrotreating furnace of the hydrotreating unit.

The cylindrical hydrotreating furnace F-101 is designed for heating the hydrotreating product, i.e., gadrogenizate to the temperature required by the regulation. Based on the results of research and analysis, the following main parameters were identified that affect the operation of the F-101 furnace and the hydrotreating process:

x_1—consumption, volume of raw materials at the entrance of the F-101 furnace, in the range of $60 \div 80\ \mathrm{m}^3/\mathrm{h}$;

x_2—temperature at the inlet of the F-101 furnace, within the range of $170 \div 190\ ^\circ\mathrm{C}$;

x_3—pressure in the F-101 furnace, in the range of $40 \div 43\ \mathrm{kg/cm}^2$.

As a result of the analysis of the collected data and the study of the operating modes of the hydrotreating furnace for the development of its model, an experimental–statistical method was chosen. The optimal operating mode of the furnace can be selected based on a mathematical model describing the influence of input variables on output parameters, i.e., allowing to obtain information about the thermal operation of the furnace. The mathematical description, which is the basis of the mathematical model, must determine the parameters of the thermal operation of the furnace [30,31].

The main disadvantage of the methods for calculating furnaces used so far is that in these methods only integral indicators of the heat exchange process are determined, they do not determine the possibility of heating the furnace tubes. Recently, modeling methods based on theoretical studies were proposed, which make it possible to determine local heat transfer parameters, for example, the zonal method. In mathematical terms, the meaning of the zonal calculation method: replacement of integral–differential equations describing the process of heat transfer, with a limited system of algebraic equations approximating them. By solving the obtained algebraic equations, the energy characteristics of heat transfer are determined, i.e., temperature and flows of local zones. For this purpose, the research furnaces are divided into a limited number of zones with the same radiation properties. This approach in calculating the furnace can provide sufficient accuracy; to increase the accuracy, it is necessary to increase the number of zones. However, this method is rather complicated and the collection of the necessary information for its application in practice is also difficult.

To simulate the operation of industrial furnaces in an interactive mode and to quickly obtain the necessary information and results, simple models are required. For this reason, the analytical method of N.I. Belokon based on the joint solution of the heat transfer equation and heat balance [32] can be used.

Regression models were identified to calculate the output parameters of the F-101 hydrotreating furnace based on statistical and experimental data. In this case, the distribution law of random measurements ε_j is taken close to the normal law, i.e., $M[\varepsilon_j] = 0$, $D[\varepsilon_j] = G^2 = const, j = \overline{1,m}$.

Thus, the structure of the model that estimates the yield of the hydrotreating furnace: y_1—the volume of the mixture of feed and gas and y_2—the temperature of the outlet flow from the furnace, are identified in the form of the following nonlinear regression equations:

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

In the model (8), the following designations are adopted: $a_{ij}, i = \overline{0,3},\ j = 1,2$ are parameters of the model that must be identified, for their assessment, one can use the well-known least squares method; x_1, x_2, x_3—operating parameters of the F-101 furnace, respectively: the volume of raw materials (x_1); furnace inlet temperature (x_2) and pressure in the F-101 furnace (x_3).

Results of identification of regression coefficients of the model (8) using processed statistical data and using the REGRESS program:

$$\begin{aligned} y_1 = 3.7500 + 0.2922x_1 + 0.0208x_2 - 0.0893x_3 + 0.0025_1^2 + 0.0001x_2^2 + 0.0021x_3^2 \\ +0.0011x_1x_2 + 0.0023x_1x_3 + 0.0045x_2x_3; \end{aligned}$$

$$\begin{aligned} y_2 = 17.0000 - 0.2208x_1 + 0.7555x_2 + 0.4047x_3 - 0.0028_1^2 + 0.0016x_2^2 - 0.0096x_3^2 \\ +0.0037x_1x_2 + 0.0157x_1x_3 + 0.0045x_2x_3. \end{aligned}$$

In order to determine the optimal temperature of the hydrotreating process on the basis of expert information and a logical rule of conditional conclusions and a rule base, a linguistic model was built using the method proposed in Section 2.3. The resulting linguistic model implements the logical dependence:

IF thermal stability of raw materials is low AND pressure is below average,
THEN process temperature is low;
IF thermal stability of raw materials is average AND pressure is average,
THEN process temperature is average;
IF thermal stability of raw materials is high AND pressure is above average,
THEN process temperature is high.

Formation of a rule base for fuzzy inference systems, which is a set of rules for fuzzy products, in which conditions and conclusions are formulated in terms of fuzzy statements. In our problem, the input parameters (variables), the values of which are set outside the model of the fuzzy inference system, are: $\tilde{x}_1$—"quality of raw materials" and $\tilde{x}_3$—"pressure", and the output variable, the value of which is formed inside the model, is $\tilde{y}_2$—the temperature of the hydrotreating process.

For an abbreviated notation of the rules, we use the designations presented in Table 1. Universal sets (universes) of the given fuzzy parameters necessary for constructing the membership function are given in Table 2.

Table 1. Values of fuzzy parameters for forming the rule base.

Fuzzy Parameter Values	Designation
low stability of raw materials, process temperature	LW
below average stability of raw materials, process temperature	BA
average stability of raw materials, process temperature	AG
above average stability of raw materials, process temperature	AA
high stability of raw materials, process temperature	HG
low pressure	LP
pressure below average	PBA
medium pressure	MP
pressure above average	PAA
high pressure	HP

Table 2. Universums for fuzzy parameters $\widetilde{x}_1$, $\widetilde{x}_3$ and $\widetilde{y}_2$.

Fuzzy Parameter	Level of Values of Fuzzy Parameters				
	LW, LP low	BA, PBA lower average	AG, MP average	AA, PAA higher average	HG, HP high
$\widetilde{x}_1$quality, sustainability of raw materials	180–19	175–185	165–175	160–170	155–165
$\widetilde{x}_3$pressure of the hydrotreating furnace	37–39	38–40	39–41	40–42	41–45
$\widetilde{y}_2$hydrotreating process temperature	270–330	320–340	330–370	360–380	370–430

Tables 1 and 2 show the 5th level of values of fuzzy parameters (LW, LP—Low; BA, PBA—below average; AG, MP—average; AA, PAA—above average; HG, HP—High), i.e., values of linguistic variables.

Fuzzification procedures and other procedures for the fuzzy inference algorithm are implemented in MatLab using the Fuzzy Logic Toolbox package. Figure 3 shows the editor window with the set parameters of the fuzzy inference system.

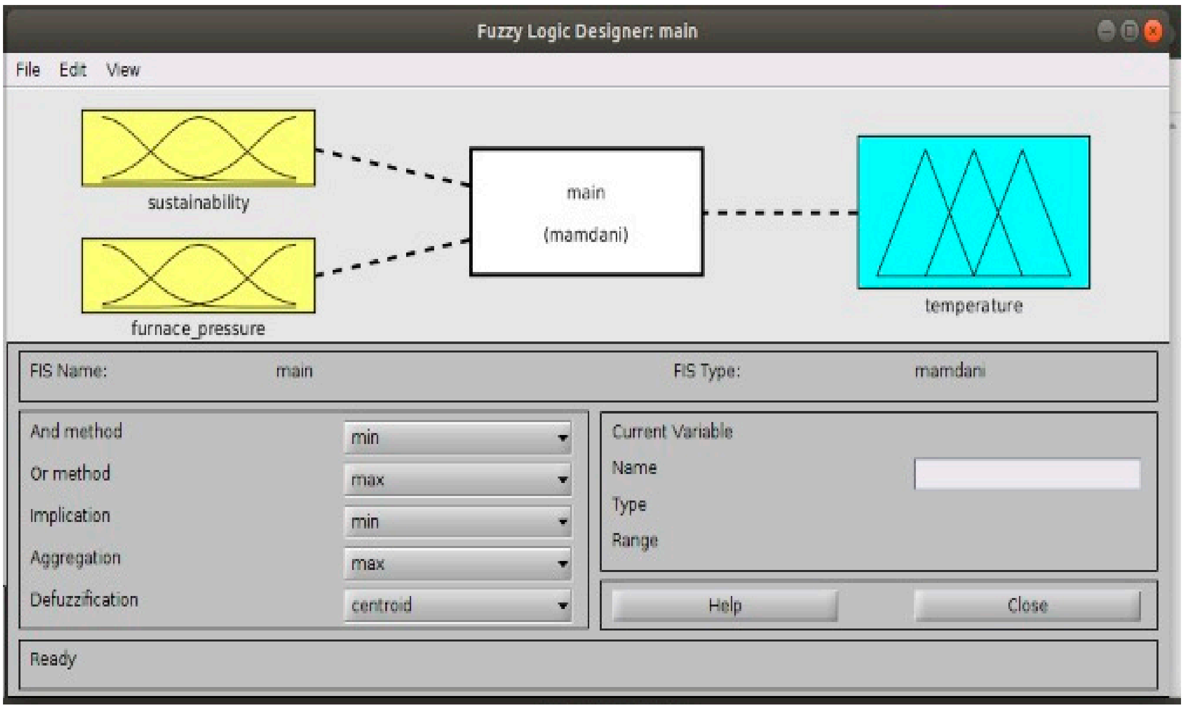
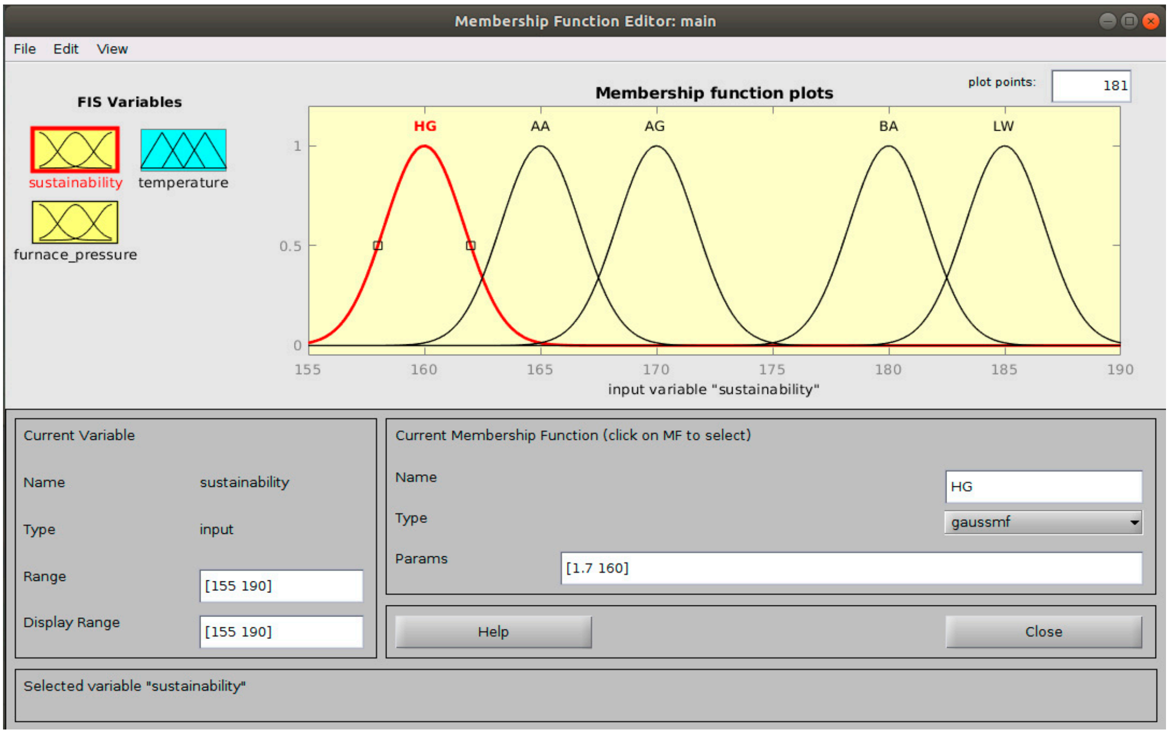


Figure 3. FIS-Editor window for the problem being solved.

Figure 4a–c shows the Gausto-type membership functions for two fuzzy input parameters and an output parameter, constructed using this package.

(**a**)



(**b**)

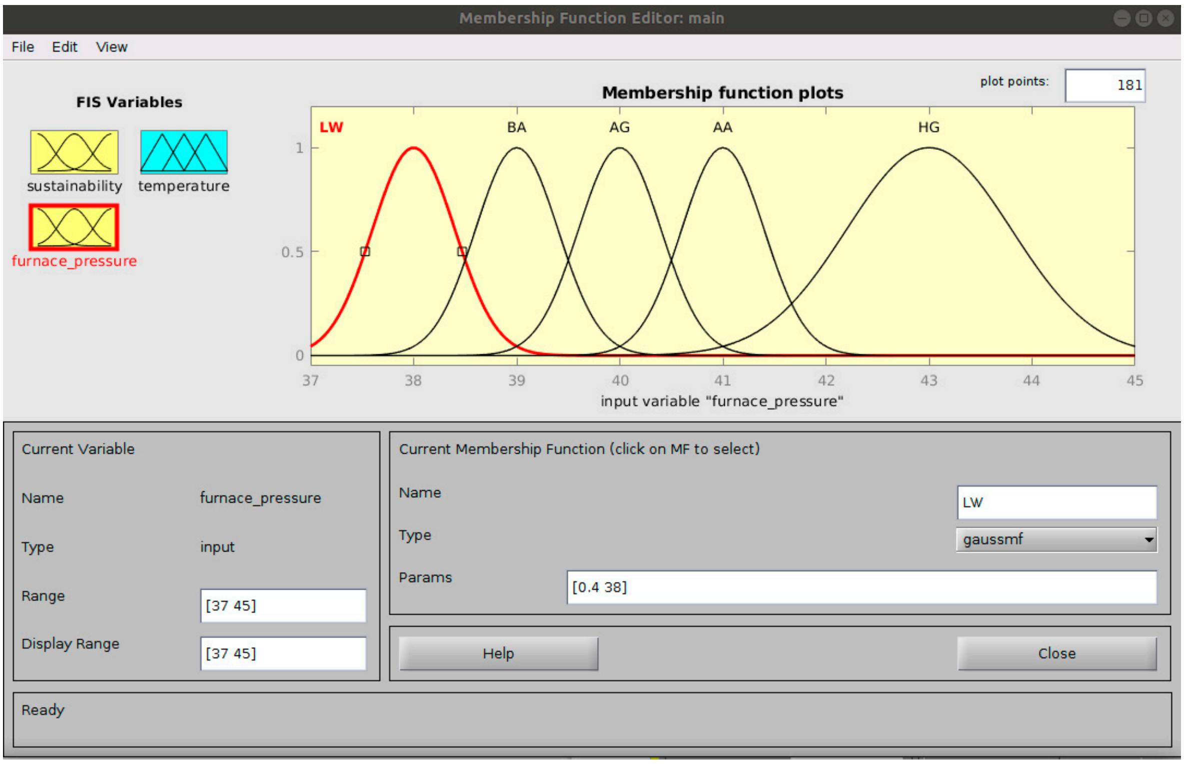


Figure 4. *Cont.*

(c)

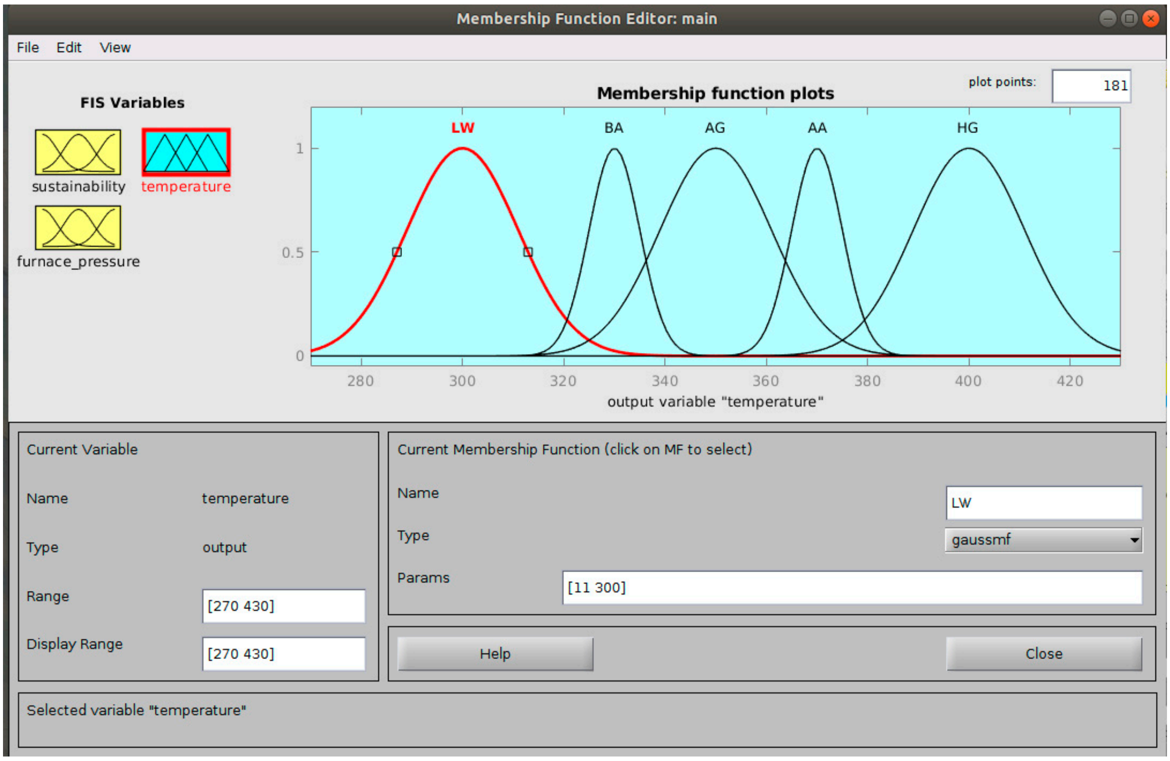


Figure 4. Membership functions of fuzzy input parameters (**a**) sustainability, (**b**) furnace_pressure and fuzzy output parameter, (**c**) temperature of the hydrotreating process.

The developed rules of fuzzy productions for the fuzzy inference system, i.e., linguistic models that allow us to determine the optimal temperature of the hydrotreating process are presented in the form of the following rules of fuzzy products:

Rule 1: IF «$\tilde{x}_1$ is LG» and «$\tilde{x}_3$ is LP» THEN «$\tilde{y}_2$ is LW» F_1;
Rule 2: IF «$\tilde{x}_1$ is LG» and «$\tilde{x}_3$ is PBA» THEN «$\tilde{y}_2$ is LW» F_2;
Rule 3: IF «$\tilde{x}_1$ is LG» and «$\tilde{x}_3$ is MP» THEN «$\tilde{y}_2$ is LW» F_3;
Rule 4: IF «$\tilde{x}_1$ is LG» and «$\tilde{x}_3$ is PAA» THEN «$\tilde{y}_2$ is BA» F_4;
Rule 5: IF «$\tilde{x}_1$ is LG» and «$\tilde{x}_3$ is HP» THEN «$\tilde{y}_2$ is BA» F_5;
Rule 6: IF «$\tilde{x}_1$ is BA» and «$\tilde{x}_3$ is LP» THEN «$\tilde{y}_2$ is BA» F_6;
Rule 7: IF «$\tilde{x}_1$ is BA» and «$\tilde{x}_3$ is PBA» THEN «$\tilde{y}_2$ is AG» F_7;
Rule 8: IF «$\tilde{x}_1$ is BA» and «$\tilde{x}_3$ is MP» THEN «$\tilde{y}_2$ is AG» F_8;
Rule 9: IF «$\tilde{x}_1$ is BA» and «$\tilde{x}_3$ is PAA» THEN «$\tilde{y}_2$ is AG» F_9;
Rule 10: IF «$\tilde{x}_1$ is BA» and «$\tilde{x}_3$ is HP» THEN «$\tilde{y}_2$ is BA» F_{10};
Rule 11: IF «$\tilde{x}_1$ is AG» and «$\tilde{x}_3$ is LP» THEN «$\tilde{y}_2$ is BA» F_{11};
Rule 12: IF «$\tilde{x}_1$ is AG» and «$\tilde{x}_3$ is PBA» THEN «$\tilde{y}_2$ is AG» F_{12};
Rule 13: IF «$\tilde{x}_1$ is AG» and «$\tilde{x}_3$ is MP» THEN «$\tilde{y}_2$ is AG» F_{13};
Rule 14: IF «$\tilde{x}_1$ is AG» and «$\tilde{x}_3$ is PAA» THEN «$\tilde{y}_2$ is AG» F_{14};
Rule 15: IF «$\tilde{x}_1$ is AG» and «$\tilde{x}_3$ is HP» THEN «$\tilde{y}_2$ is PAA» F_{15};
Rule 16: IF «$\tilde{x}_1$ is AA» and «$\tilde{x}_3$ is LP» THEN «$\tilde{y}_2$ is PAA» F_{16};
Rule 17: IF «$\tilde{x}_1$ is AA» and «$\tilde{x}_3$ is PBA» THEN «$\tilde{y}_2$ is PAA» F_{17};
Rule 18: IF «$\tilde{x}_1$ is AA» and «$\tilde{x}_3$ is MP» THEN «$\tilde{y}_2$ is PAA» F_{18};
Rule 19: IF «$\tilde{x}_1$ is AA» and «$\tilde{x}_3$ is PAA» THEN «$\tilde{y}_2$ is AA» F_{19};
Rule 20: IF «$\tilde{x}_1$ is AA» and «$\tilde{x}_3$ is HP» THEN «$\tilde{y}_2$ is AA» F_{20};
Rule 21: IF «$\tilde{x}_1$ is HG» and «$\tilde{x}_3$ is LP» THEN «$\tilde{y}_2$ is AA» F_{21};
Rule 22: IF «$\tilde{x}_1$ is HG» and «$\tilde{x}_3$ is PBA» THEN «$\tilde{y}_2$ is AA» F_{22};
Rule 23: IF «$\tilde{x}_1$ is HG» and «$\tilde{x}_3$ is MP» THEN «$\tilde{y}_2$ is HG» F_{23};
Rule 24: IF «$\tilde{x}_1$ is HG» and «$\tilde{x}_3$ is PAA» THEN «$\tilde{y}_2$ is HG» F_{24};

Rule 25: IF «$\widetilde{x}_1$ is HG» and «$\widetilde{x}_3$ is HP» THEN «$\widetilde{y}_2$ is HG» F_{25}.

Here $F_1, \ldots, F_{25}$—are weighting factors reflecting the degree of confidence in the truth of the subconclusions. These coefficients take values in the range from zero to one.

The given rule base, a fuzzy knowledge base, is implemented using Fuzzy Logic Toolbox and a fragment of the base is shown in Figure 5. The obtained results of visualization of fuzzy inference in RuleViewer are shown in Figure 6.

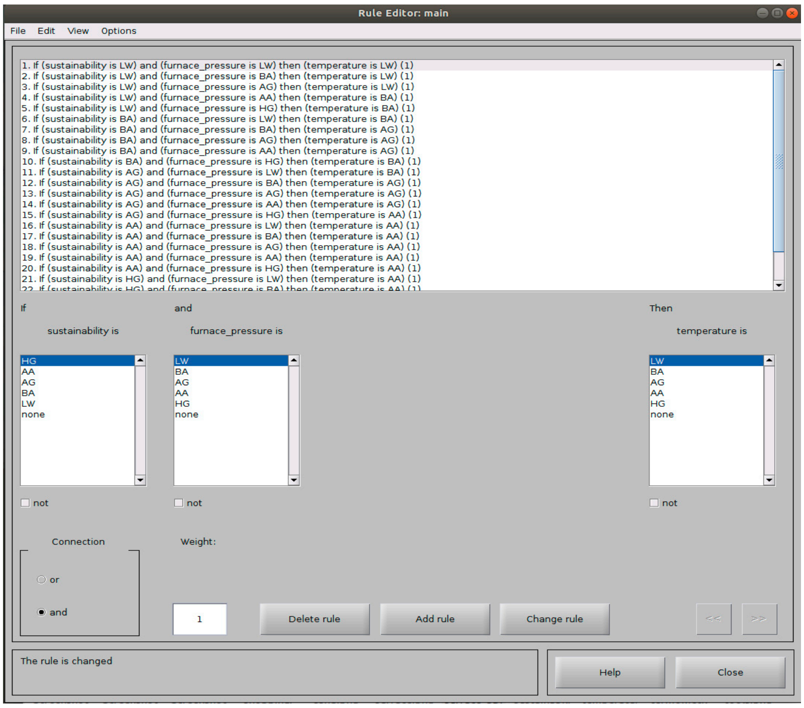


Figure 5. Fuzzy knowledge base for input and output parameters.

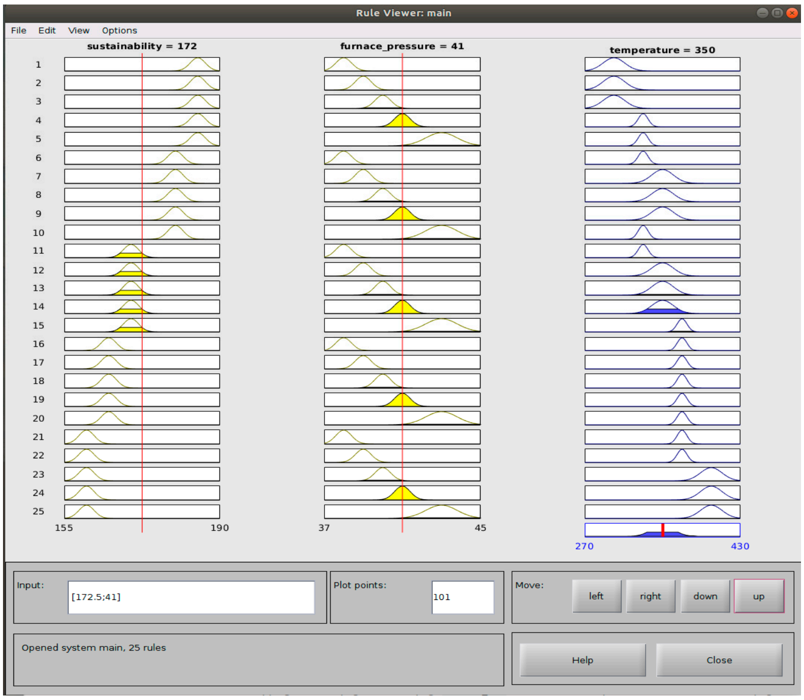


Figure 6. Visualization fuzzy inference in RuleViewer.

The Input field contains the values of the input variables for which inference is performed. The "inputs–output" surface corresponding to the synthesized fuzzy system is shown in Figure 7.

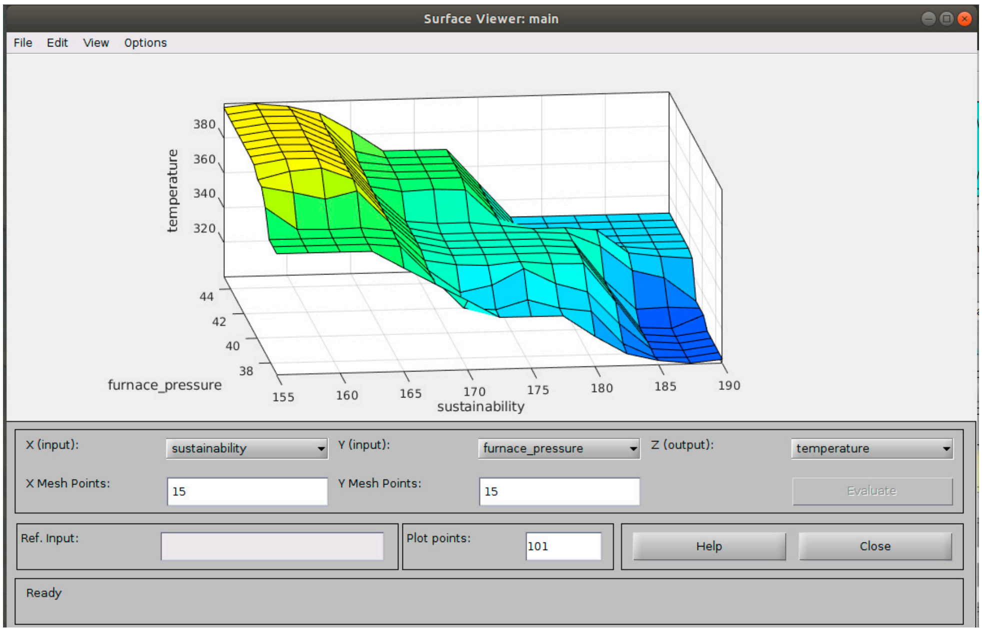


Figure 7. Inputs–output surface in the SurfaceViewer window.

3.2. Discussion of Results

The methods proposed in the work for the development of mathematical models of technological objects functioning in conditions of indistinctness of the initial information allow us to build fuzzy models with clear input and fuzzy output parameters of the object (FM method) and linguistic models with fuzzy values of the input and output parameters of the object (LM method). The method for constructing fuzzy models is based on the use of methods of sequential inclusion of regressors (for structural identification of the model) and a modified least squares method using a set of level α (for identification of model parameters). The method of constructing a linguistic model is based on the use of logical rules for conditional inference and linguistic variables that describe the input and output parameters of the object.

To determine the volume of hydrogenate, i.e., of the target product from the outlet of the hydrotreating reactor R-1 using the methods of sequential inclusion of regressors and least squares on the basis of the experimental statistical data package and the REGRESS software package, a statistical model was built that makes it possible to determine the volume of hydrogenate from the outlet of the reactor depending on the input, operating parameters x_i, $i = \overline{1,5}$.

Since the initial information for assessing the quality of the produced hydrogenated product is characterized by indistinctness, a systematic approach using the methods of expert assessments and theories of fuzzy sets was applied to construct models for assessing the quality of the hydrogenated product. An expert assessment of the influence of the input and operating parameters on the quality parameters of the hydrogenated product was carried out. Then, processing the collected data and expert information using the fuzzy modeling method proposed in Section 3.1, the structure of fuzzy models was identified to describe the product quality of the hydrotreating reactor R-1 in the form of fuzzy multiple regression Equation (7).

The main disadvantage of the methods used in practice for calculating furnaces is that they determine only the integral indicators of the heat transfer process, and allow the possibility of heating the local tubes of the furnace. To eliminate this drawback, it is proposed to apply the zonal method, which is based on replacing integral–differential equations that describe the process of heat transfer by a system of algebraic equations. The zonal method of calculating the furnace can provide sufficient accuracy; to increase the accuracy, it is necessary to increase the number of zones. However, this method is rather complicated and the collection of the necessary information for its application in practice is also difficult. Therefore, to simulate the operation of the F-101 hydrotreating furnace, it is proposed to use an analytical method based on the joint solution of the heat transfer and heat balance equation to quickly obtain the necessary information and results. Statistical models were built that make it possible to determine the output of the hydrotreating furnace: the volume of the mixture of raw materials and gas and the temperature of the outlet flow from the furnace, in the form of nonlinear regression Equation (8). To determine the optimal temperature of the hydrotreating process, based on expert information and a logical rule of conditional conclusions and a rule base, a linguistic model was built that estimates the optimal temperature depending on the quality of raw materials and furnace pressure.

Based on the simulation of the operation of the furnace and the hydrotreating reactor of the reactor and the analysis of their results, it is possible to select the optimal operating mode that provides the effective values of the optimization criteria, for example, maximizing the hydrogenated product yield from the R-1 reactor while ensuring the required quality indicators. Comparison of the results of modeling and selection of the effective operating mode of the hydrotreating unit based on the known and constructed models and real experimental data from the hydrotreating unit of the Atyrau refinery is shown in Table 3.

Table 3. Results of comparison of data obtained with known models, developed models and real, experimental data from the hydrotreating unit of the LG-35-11/300-95 unit of the Atyrau refinery.

Output and Input Parameters	Known Models [33]	Taking Into Account the Fuzzy Information of the Model	Real, Experimental Data
hydrogenate output from reactor R-1, m^3/h	76	77.1	77
unsaturated hydrocarbons in hydrogenate, $\tilde{y}_2$, %	-	$\tilde{\leq}0.97$	$\tilde{\leq}(0.98)^{P}$
sulfur in the hydrogenated product, $\tilde{y}_3$, %	-	$\tilde{\leq}0.00005$	$\tilde{\leq}(0.00005)^{P}$
water-soluble acids and alkalis in the hydrogenated product, $\tilde{y}_4$, %	-	$\tilde{=}0$	$(\tilde{=}0)^{P}$
the volume of raw materials at the entrance R-1, x_1, m^3/h;	83	80	80
pressure in R-1, x_2, kg/cm;	30	30	30
temperature in R-1, x_3, °C	345	340	340
Volumetric velocity, x_4, h^{-1}	3	3	3
HCG circulation, x_5, nm^3.	420	400	400

Note: means that the corresponding parameters are not determined by this method, $(\cdot)^{P}$—means that these data are determined with the participation of people in the laboratory of the plant.

The analysis of the data obtained and given in Table 3 allows us to conclude that the simulation results using the developed models, taking into account fuzzy information, are superior to the known deterministic approaches, since the simulation results coincide more accurately with the real (experimental–production) data. In addition, using the proposed approach, product quality indicators are determined, which are described indistinctly ($\tilde{y}_2$, $\tilde{y}_3$, $\tilde{y}_4$), which cannot be determined by traditional modeling methods.

The graphical results on the visualization of fuzzy inference and the "inputs–output" surface, built using the Fuzzy Logic Toolbox application, testify to the adequacy and effectiveness of the proposed method for solving the problem since the graphs obtained correspond to the results of the expert assessment.

4. Conclusions

In this work, methods were developed for constructing models of technological objects in conditions of a deficit and indistinctness of initial information, which are the main components of the hydrotreating unit of a catalytic reforming unit, using the available information of an experimental–statistical and fuzzy nature. Methods for constructing fuzzy models for objects with fuzzy output parameters and constructing linguistic models with fuzzy input and output parameters of the object are proposed. Using the proposed methods, fuzzy models were built for assessing the quality of products (hydrogenate) from the outlet of the hydrotreating reactor and linguistic models for determining the optimal hydrotreating process depending on the thermal stability of the feedstock and the pressure in the hydrotreating furnace.

Mathematical models of the R-1 hydrotreating reactor were developed on the basis of experimental–statistical and fuzzy information.

Mathematical models of the F-101 hydrotreating furnace were built using the available information of an experimental and statistical nature.

The rules of fuzzy productions for the fuzzy inference system, i.e., linguistic models that allow for the determining of the optimal temperature of the hydrotreating process depending on the quality of the feedstock and the pressure in the hydrotreating furnace.

To solve the problems of deficiency and fuzziness of initial information in the construction of mathematical models, it is proposed to use the available information of a different nature, including fuzzy information. Mathematical models of the hydrotreating unit are developed on the basis of experimental statistical data and fuzzy information from experts. Mathematical models for determining the volume of products from the output of the aggregates are identified in the form of statistical models of the regression type, and the models evaluating the indistinctly described qualitative indicators of the produced product: the content of unsaturated hydrocarbons—$\widetilde{y}_2$; sulphur—$\widetilde{y}_3$ and water-soluble acids and alkalis—$\widetilde{y}_4$, in the form of fuzzy equations. The structural identification of the developed models was carried out on the basis of the method of sequential inclusion of regressors, and parametric identification was carried out using a modified least squares method using the REGRESS software package.

A graph of the dependence of the hydrogenated product yield on the temperature in the hydrotreating reactor R-1 with fixed values of the remaining operating parameters was plotted. In conditions of indistinctness of both input and output parameters, i.e., when the input and output of the hydrotreating reactor are described by linguistic variables, it is proposed to build linguistic models on the basis of logical rules of the conventional form. This approach was implemented when constructing a linguistic model describing the dependence of the optimal temperature of the hydrotreating process on the thermal stability of the feedstock and on the pressure in the hydrotreating furnace.

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