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Development of Mathematical Models and Modelling of Chemical Technological Systems using Fuzzy-Output Systems

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Abstract: The paper proposes a systematic approach to the development of structured mathematical model and modelling of Chemical-Technological Systems (CTSs) of refinery under fuzzy conditions. Idea and novelty of the proposed method are based on the study of each unit of chemical-technological systems, and based on obtained results, the model of separate element of chemical-technological systems unit is designed. At the next stage, separately-developed models are combined into a single system to fully model the process. The developed method has been successfully implemented during the construction of models system of the basic reforming units of catalytic reforming at Atyrau oil refinery. Comparison of the known results and modelling results based on the proposed method demonstrates the effective realization for constructing a system of models for main units of sulfur production in Atyrau oil refinery.

Keywords: systematic approach, mathematical models, modeling, Chemical-Technological Systems (CTSs) refinery, reforming unit, the theory of fuzzy sets, accessory function, Decision-Maker (DM), linguistic models.

1 Introduction

The actual objectives of any production are known as intensification of production, improvement of quality and efficiency of technological production processes. Promising and effective methods for formulating these problems are to increase control efficiency of production objects through the use of scientific methods of system analysis, development and decision-making on the basis of a mathematical models constructed with the use of a systematic approach [**?**, 1 - 4] Currently, there are series of works devoted to the method of mathematical modeling and control of refinery technological objects [**?**, 3-7] However, there is a class of objects of oil refining, different production situations and their control tasks. Their formalization and decision cannot be obtained in the traditional ways and it does not give significant results. These objects and tasks include CTS, operating in conditions of uncertainty associated with randomness and fuzzy initial information fuzziness and also problems of formalization and solution of the simulation problem, and also considering the optimization of operating modes for various production situations. In addition to the fuzziness of initial information the solution of these problems complicate the complexity and multi-criteria of control objects [**?**, 8, 9]

Due to the complexity or inability to measure a number of parameters and indicators, many of the technological and production processes are difficult to quantify and describe what makes it difficult to use deterministic methods of mathematics and probabilistic approaches for modeling and optimizing their operating modes. This led to the emergence of new methods of formalization and considered problems solving that rely on fuzzy information from the Decision - Maker (DM) person , specialists and experts in the form of judgments on the functioning of the object and taking into account their preferences in the solutions process selection [**?**, 2, 10]

The research task of the paper is to solve the problems of modelling and tasks of multi-criteria optimization, which appear during the control of production objects in conditions of uncertainty and fuzziness of initial information. Moreover, it requires the methodology

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development of CTS mathematical models in conditions of uncertainty and fuzziness of initial information, the development and further development of the formalization methods and simulation solutions, optimization in fuzzy environment, the algorithms and programs processing for implementing these techniques using modern computers.

Oil processing is a set of physical, chemical and physical processes at refinery, including crude-oil treatment processes for primary deep processing of oil and petroleum products [?, 11, 12] Various technological processes of refining take place in specially-designed units. In the production conditions the final products are usually obtained in a complex of technological units (installation, CTS), which includes different interconnected units, such as oven, reactors, distillation columns, heat exchangers and others.

Effective control questions of technological processes of oil refining and its optimization according to economic and environmental criteria on the basis of mathematical models using computer systems have become topical in recent years. In this regard, active research is aimed to solve them [?, 10, 13 - 15]

The mathematical model is a mathematical description system with reflected features of the processes occurring in the modeling object (CTS Technology), which by means of an algorithm allows to predict the behavior of an object when you change inputs and control parameters. Formally, the mathematical description is a set of connections linking the various parameters of the object, the process is in a single system of relations [?, 16, 17] In the application of the idea of a systematic approach among these relations can be expressions that reflect the general physical laws (e.g, the laws of mass and energy), the equations describing the "elementary" processes (e.g, interactions, chemical and physical conversion). Moreover the mathematical description also includes a variety of empirical and semi-empirical relationships between different object parameters, whose theoretical form is unknown or too complicated, and with indistinct connections and expression, based on the knowledge and experience of specialists- experts in the form of logical rules of conditional output [?, 17, 18]

It is known that for modeling of complex objects, CTS under uncertainty caused due to the stochastic nature of the process, the method of the theory of probabilities and mathematical statistics is used [?, 19, 20] Often, however, the uncertainty can be caused due to the nature of the initial fuzzy information. Under these uncertainty conditions, the axioms of probability theory are not always satisfied, i.e., the use of probabilistic methods is not justified. In addition, even if the possibility of describing processes and systems by probabilistic methods exist, due to the shortage of initial information and due to the complexity and economic expediency of reliable statistical information gathering, it is necessary to describe and to build not statistics, such as fuzzy models of real objects and processes. In this regard, one of the most promising approaches is the use of methods of fuzzy set theory [?, 2, 18, 21, 22]

For qualitative analysis of real technological objects, CTS approaches are needed, for which high accuracy and rigor of the mathematical formalism is not something absolutely necessary. The problem of uncertainty because of the lack of clarity of the initial information in the study and simulation of complex technological objects can be solved by applying fuzzy mathematics apparatus. Thus, there is a need to develop a systematic method of mathematical models and simulation of complex objects of CTS functioning in the conditions of uncertainty of various kinds. The purpose of this paper is to develop this method of simulation model development and CTS (for example, processing facilities of oil refining), which allows you to build a system of mathematical models of CTS of oil-refining production under condition of uncertainty and probabilistic fuzzy character on the basis of the initial information of various kinds.

2 Mathematical models of CTS units based on a systematic approach under fuzzy conditions.

CTS, i.e. refinery process units are composed of several interlinked units. Therefore, to conduct research into the process in the rational regime, one must have structural model, i.e., mathematical models of the aggregates work out on the basis of a systematic approach. These models should make it possible to predict the impact of aggregates parameters on the processes occurring in them, intermediate and final products and on the work object as a whole. For the mathematical description of links of parameters of CTS the various types of information are used:

- Theoretical ideas about the nature and character of the process occurring in the system;
- Basic statistical data that characterizes the functioning of studied CTS;
- Data obtained in the result of the expert assessment, including fuzzy information, while qualitatively describing the state of the object.

The main approaches to build mathematical models of CTS and processes are theoretical, experimental and statistical approaches; an approach is based on the use of methods of fuzzy set theory, and combined approach.

Consider the main types of mathematical models, obtained on the basis of represented approaches used in the study and control of CTS.

Deterministic models of CTS, of technological refining units are developed on the basis of theoretical ideas about the structure of the described system and laws of functioning of its individual components and sub-systems, i.e. these models are based on a theoretical approach, using equations describing every essential processes for the real object. Construction of technological units models by the theoretical approach is possible mainly for the simple processes. For more complicated unites, or when there is a set of interconnected units to receive their deterministic models is practically impossible. It is connected with the fact that in these cases there are no or limited theoretical information about characterized processes of modeled object. Obtained model may be too cumbersome, complex and its information services (search, identification of factor-coefficients model) is very time-consuming so that the development of such a model is inexpedient. However, the methodological value of this approach is important in order to assess the state of the object by means of equations that take into account the common fundamental laws of nature. And these laws tend to reflect and control processes and phenomena in nature and technology.

In industrial environments, when simultaneously a large number of parameters affect the CTS state, random effects play an important role. To describe CTS, one takes a look at any object, a process which is characterized by random fluctuations, for example caused by physical variability of some factors $x_i + x_i(\tau)$ or external random effects. Because of this, during equal average values of the input features $x(\tau)$ in moments τ_1 and τ_2 output parameters $y(\tau)$ are supposed to change. Therefore for such stochastic (probabilistic) processes, where one cannot neglect random oscillations $\Delta x_i(\tau)$ of relative $x_i(\tau)$ and random external influences $\xi_i(\tau)$, it is necessary to characterize the system, taking into account the statistical law of distribution of instantaneous values $y(\tau)$ relative to the average value $yav(\tau)$ by the equation:

$$y(\tau) = y_{\text{cp}}(\tau) + \Delta y(\tau) = f(y_{\text{cp}}) + \xi(\Delta x,\ \xi) \qquad (1)$$

Models such as (1), reflecting the random nature of the object parameters and factors are called stochastic [20, 23]. By decreasing the value of the parameters ξ and Δx the equation (1) is continuously close to the structure of the equation $y = f(x)$, which describes the deterministic system. That is, the stochastic models are more broad class models and include deterministic model as a limiting special case, where output variables y are uniquely determined by the input variable x.

One of the difficulties appears due to the fact that the initial information that can be gathered for the modelling and optimization of the object may be incomplete and fuzzy, i.e. uncertain because of the uncertainty of the initial information. This difficulty comes from the fact that the majority of complex objects is usually difficult to quantify. Special facilities for collecting and processing statistical data of real CTS in industrial conditions are not sufficient, they do not have the necessary quality. To simulate such objects the traditional approaches (determinate experimental statistics), discussed above, are inexpedient because they do not give significant results.

One of the promising approaches to solve these problems is the use and formalization of a priori information about distinction of functioning of the system. This approach considerably improves the efficiency of mathematical modeling and control of complex, quantitatively hardly-described CTS refinery. Qualitative information refer to knowledge or expert judgment of specialists about the object. The effective formalization of qualitative information can be done based on methods of fuzzy set theory, mathematical apparatus which are described in works [**?**, 2, 10, 18, 24]

Consider the technological object for which mathematical model construction is complicated by two reasons. On the one hand, it is difficult to built models by a priori uncertainty of high values, lack of process data, on the other hand, it is sophisticated due to fact that the input and output variables have a fuzzy nature. However, the human operator is able to manage it, based on a model of a qualitative nature, formed in his mind during the training and monitoring of the object functioning. One can obtain formalized model of such object, without the aid of complex mathematical structures. One can express its essence in terms of fuzzy natural language. The simplest model of this type would be the expression "If on the system input $\tilde{E}_i$, at the output we get $\tilde{C}_j$", where $\tilde{E}_i$ and $\tilde{C}_j$ are some terms from the term set $T(X,Y)$. Next, having constructed a function of belonging to fuzzy parameters and processing the qualitative information we can obtain the model of this object used in the optimization and control.

Thus, the use of the mathematical apparatus of fuzzy sets theory makes it possible to build simpler and more efficient models and algorithms to optimize the control of CTS in the face of uncertainty (fuzziness), where the use of traditional approaches is impractical or impossible.

Along with the effective application of the theory of fuzzy sets, one should overcome some of its limitations: the relative difficulty of obtaining and organizing primary-term high-quality information, the need for additional validation of information, increase of the objectivity of the collected subjective data, and the difficulty of the choice of decision rules to be submitted in the form of conditional sentences for the synthesis of control algorithm. In addition, the applied and theoretical aspects of this theory have some difficulties associated with the interpretation of the content of membership functions and methods of construction.

Using different methods of constructing mathematical models of complex objects based on the methodology of the theory of fuzzy sets and expert assessment we can offer following systematic approach to the development of mathematical models and modeling work of CTS refinery on the basis of data of various types (theoretical, statistical, fuzzy ones). The developed method of constructing mathematical models of CTS in the conditions of uncertainty and on the basis of information of different nature there are following main steps:

1. Research and analysis of CTS which consists of interconnected units. Collection of accessible information and its processing. Determination of simulation purposes;

2. Determination of the evaluation criteria and the comparison and selection of models, which is possible to build for a system of elements with the goal of modeling;

3. In the selected criteria to conduct an expert assessment of the possible models of each element of CTS and according to the sum of the values of the criteria to determine the best type of model of each element (unit);

3.1 If the theoretical information to describe the work of a single element of the system is sufficient and the sum of the evaluation criteria is a deterministic model of efficiency term, then for this element on the basis of the analytical methods the deterministic models are built;

3.2 If the statistics to describe the work of a single element of CTS is sufficiently accurate or collection of such data is possible, as well as on the amount of assessment criteria, the statistical model is effective, the statistical model of this item are constructed on the base of experimental and statistical methods;

3.3 If the theoretical and statistical data to describe the work of the individual elements is insufficient, collection of such impractical data, and the collection of fuzzy information describing the operation of the element of CTS (unit) and its processes is possible, as well as the sum of the evaluation criteria and selection of fuzzy model is effective, then for the object based on the methods of fuzzy sets theory the fuzzy models are build (for this go to step 4);

3.4 If the theoretical, statistics and fuzzy expert information to describe the work of a single element of CTS are insufficient, the collection of such data, then for this object based on the information gathered combined with various nature (theoretical, statistical, fuzzy) the combined (hybrid) model are constructed. For a description of the various parameters of a particular unit, depending on the information go to steps 3.1-3.3, or 4;

4. Determination and selection of required fuzzy inputs to build a model $\tilde{E}_i \in \tilde{A}_i, i = \overline{1,n}$ and outputs parameters $\tilde{y}_j \in \tilde{B}_j j = \overline{1,m}$ $.\tilde{}_i \in X$, $\tilde{B}_j \in Y$- Fuzzy subset, X, Y - universal set. The input parameters can be precise (deterministic) i.e. $x_i \in X_i, i = \overline{1,n}$;

5. If $x_i \in X_i$, i.e. the input parameters of the complex are determinate, then one hast to determine the structure of fuzzy equations of multiple regression$\tilde{y}_j = f_j(x_1, ..., x_n, \ \tilde{a}_0, \ \tilde{a}_1, ..., \tilde{a}_n), j = \overline{1,m}$ (solution of the structural identification problem);

6. On the basis of expert judgments methods to collect information to describe the object of research and determination of the term-fuzzy sets parameters $T(\tilde{X}_i, \tilde{Y}_j)$;

7. Construction of the fuzzy membership function parameters$\mu_{A_i}(\tilde{x}_i)$, $\mu_{B_1}(\tilde{y}_j)$;

8. If the input and output parameters of the object are fuzzy, then formalize fuzzy mapping R_{ij}, which define the links between $\tilde{E}_i$and $\tilde{y}_j$. Specifically, a linguistic model should be built and transition to step 10 should be made;

9. If the condition of step 5 is made, then evaluate the value of fuzzy factors $(\tilde{a}_0, \tilde{a}_1, ..., \tilde{a}_n)$identified in step 5 models $\tilde{y}_j$ (decision parametric identification problem), go to step 11;

10. If the conditions of step 8 is realized, the composite based on the rules of inference (fuzzy inference system) to hold the definition of fuzzy values of object parameters, the determination of their numerical values from the set of fuzzy solution;

11. Check the condition of the adequacy of the model. If the adequacy of the condition is satisfied, it is to recommend the developed model for the study and determination of optimum work regime CTS. Otherwise, find the cause of the inadequacy and return to the corresponding conductive-points to address the issue to ensure the adequacy of the model.

Let us give explanations of steps offered in the aforementioned method of constructing mathematical models of CTS with the uncertainty of various kinds.

In *step 1* a systematic study of the modeling of the object, i.e., technological CTS refinery units are conducted, the system structure, elements and processes that occur in them are studied. The collected theory information, statistics, empirical and semi-empirical dependence, as well as expert information and its processing are done. At this point, the goal of modelling is determined. The collected and processed information is used to build a mathematical model.

In step 2 taking into account the simulation goal in the previous step, the criteria for evaluation and mutual comparison of models, which may be built for each element of CTS are determined. As such criteria, we can determine: the collection possibility, i.e., availability of the necessary information to build a mathematical model of the appropriate type; the amount of costs required to build the model (cost, the difficulty of developing a model); the accuracy of the model; the applicability of these models for other purposes (e.g for multi-criteria optimization, facility control under uncertainty); the possibility of combining a model of this type in a single package for the purpose of system simulation modes of CTS as whole.

In step 3, according to selected criteria for model evaluation, we perform the expert assessment of possible model types of each CTS unit. Based on assessment results (for example, by summation of points given by experts during the assessment), we determine for each unit of the system the efficient type of mathematical model. Completion and registration of the results of this item is convenient to do in the form of table (see. Table 1, shown below). Sub-steps 3.1 and 3.2 of step 3 are implemented on the base of known methods for developing deterministic-mining and statistical models. Step 3.3 is implemented on the basis of methods in building fuzzy models application of the methodology of the theory of fuzzy sets and expert methods of estimation.

In carrying out substep 3.4 the combined information of different nature is used (theoretical, statistical, fuzzy) and combinated model is built.

In step 4, depending on the required accuracy of the developed models linguistic, fuzzy parameters (variables) are chosen, which describe the quality of the simulation object. For convenience, fuzzy-described range change of parameters given in the form of segments, indicating the minimum ($x^{\min}$, $y^{\min}$) and max ($x^{\max}$, $y^{\max}$) values. These segments, depending on the judgment of professional experts are divided into several sampling intervals (quanta):

$$x_j^{\min} = x_j^1 < x_j^2 < ... < x_j^n = x_j^{\max},$$

$$y_j^{\min} = y_j^1 < y_j^2 < ... < y_i^n = y_j^{\max}$$

To determine the structure of fuzzy equations of multiple regression (step 5), one can use the approach of fuzzy regression analysis. At this stage the qualitative analysis of the object is important, as a result that the main parameters identifies affecting the performance of their relationship and the method chosen to identify the structure of the model. In general, the fuzzy models are built in the form of fuzzy multiple regression equations.

To construct the term set describing the state of the object (step 6) each quantum selections are verbally characterized by corresponding fuzzy terms. For example, if we suppose that $\tilde{y}j$ - oil products quality (such as gasoline), then it can be described by terms:

$\tilde{y}j$ = {very low, low, medium, high, very high}.

Accepted term set is a collection of values of linguistic variables describing the work of the tested object. Each sampling interval (quantum) obtained in the fourth step, is characterized by a certain term. This term corresponds to the fuzzy set, which is described by the membership function at the appropriate level of its graduation.

In step 7, we construct membership function of fuzzy parameters. Therefore, this step is one of the main stages in the modeling of CTS using methods of fuzzy set theory. The main method of recovery of the analytical form of this function is a graphical plot of the curve degree of affiliation of a parameter corresponding to fuzzy set. On the basis of the resulting graph, one can choose this kind of function that best approximates it. After that, the parameters of the selected function are identified.

Based on the experience of modeling of technological objects of refinery in fuzzy environment, we propose the following structure for a function:

$$\mu_{B_j}^p(\tilde{y}_j) = \exp(Q_{B_j}^p \left| (y_j - y_{md\,j})^{N_{B_j}^p} \right|) \qquad (2)$$

where $\mu_{B_j}^p(\tilde{y}_j)$– the function parameters $\tilde{y}_j$of fuzzy sets $\tilde{B}_j$, characterize the values of output parameters; p – quantum number; $Q_{B_j}^p$–the option that is in the identification of the membership functions determining the level of fuzziness; $N_{B_j}^p$– coefficients to change the domain of the terms and form of the graph of fuzzy parameters; $y_{md\,j}^p$ – fuzzy variable, the most relevant to this term (in quantum p), for which $\mu_{B_j}^p(y_{mdi}) = \max_j \mu_{B_j}^p(y_j)$.

In step 8, for the construction of the object of the linguistic model of conditional logic inference rules can be used. The linguistic model of the object is based on the results of the processing of expert information. For convenience, it can be arranged in a table, where the different values of the input parameters $\tilde{E}_i$ and the corresponding values of these options, the output parameters are indicated$\tilde{y}_j$. The table must be filled with the selected step 4 term-set. On the basis of the model obtained in this way, fuzzy mapping R_{ij}determining the connection between fuzzy input$\tilde{E}_i$ and output parameters$\tilde{y}_j$ is formalized.

Fuzzy mapping for quantum p can be determined as follows: $R_{ij}^p = A_i^p \circ B_j^p$. For ease of fuzzy mapping, we use R_{ij} in the calculations, where it is necessary to build a matrix in fuzzy relations $\mu_{R_{ij}}(\tilde{x}_i,\, \tilde{y}_j)$ - for example, in the general case, for quantum:

$$\mu_{R_{ij}}^p(\tilde{x}_i,\, \tilde{y}_j) = \min[\mu_{A_i}^p(\tilde{x}_i),\, \mu_{B_i}^p(\tilde{y}_j),\, i = \overline{1,n},\, j = \overline{1,m}].$$

To determine the estimates of the parameters of the function selected in step 5 in 9-step, one can use the criterion of minimizing the deviation of the fuzzy values of the output parameter$\tilde{y}_j^<$ obtained by the model from its sample of fuzzy values obtained on the basis of expert estimation$\tilde{y}_j^M$, i.e. .:. $R_j = \min \sum_{l=1}^{L} (\tilde{y}_{jl}^< - y_{jl}^M)^2$

At this stage, the main issue is the choice of the method of estimation of unknown parameters, providing the necessary properties of the object. This fuzzy models have the form of multiple regression equation [2, 25]:

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

Step 10 of the proposed method of constructing mathematical models of technological objects in conditions of uncertainty is the use of composite inference rules:. $B_j = A_i \circ R_{ij}$

With this rule, one can carry out the calculation of the output variables, e.g, the measures based on the maximin product:

$$\mu_{B_i}^p(\tilde{y}_j^*) = \max_{x_i \in X_i} \{\min[\mu_{A_i}^p(\tilde{x}_i^*),\, \mu_{R_{ij}}^p((\tilde{x}_i^*,\, \tilde{y}_j)]\}. \qquad (3)$$

Suppose $\tilde{E}_i^*$– measured (estimated by experts) values of the input variables, then the desired set, which holds the current measured values of the input variables, is defined as a set for which the measured values are the highest (maximum) degree of adjunct: $\mu_{A_i}(\tilde{x}_i^*) = \max(\mu_{A_i}(\tilde{x}_i))$. The predicted values of the output variables (fuzzy values) are determined as the corresponding membership functions $\mu_{B_i}^p(\tilde{y}_j^*)$ (4). Specific numerical values of the output parameters y_j^c of the fuzzy set of solutions are determined from the following relationship:

$$y_j^c = \arg\max_{\tilde{y}_j^*} \mu_{B_i}^p(\tilde{y}_j^*)$$

i.e. the values of the input parameters, for which the maximum function are selected.

The objective of the final stage of the method (step 11) is to check compliance of the model object. The model is considered to be adequate to modeled object, if it is found with the help of a computer. Object characteristics coincide with a given degree of accuracy, actual data are obtained experimentally at the object.

As a general rule, as an adequate criterion, which is a measure of compliance with model object, one uses the value of the calculated error (model) $y^<$ and the real (experimental) – y^M data: $R = \left|y^< - C^M\right|$. In addition, an acceptable error level value is selected – R. The model is considered to be adequate if $R = \left|y^< - C^M\right| \leq R$.

In the case that the mathematical model is inadequate, the sources of inadequacy are determined and the model is improved. The possible reasons for poor model adequacy can be the following factors: an underestimation of the importance of some significant variable and the underestimation of its model, incorrect or incomplete structure of fuzzy equations, error with parametric identification, etc. When the reason is identified and the problem is fixed, then it is necessary to return to the appropriate step of the algorithm for the model refinement.

3 Results of the aforementioned studies and discussion.

We concretize results of the mentioned studies and implement them in practice in the development of the system of mathematical models of the main aggregates of the Installation of Sulfur Production (ISP) of the Atyrau refinery. In step 3 of the proposed method the separate procedure is implemented [31]. According to the first results of research on each unit and on the basis of the collected information and the selection criteria its model is built. On purpose of simulating the operation of ISP system, designed models are combined into a single system. The proposed approach has been successfully implemented in the construction of a system of models of main aggregates of the Atyrau refinery installation of sulfur production.

ISP is a complex CTS, consisting of interconnected units, which simultaneously affects a large number of different parameters. The main unit of the installation are of the reactor (F-001, R-001, R-002, R-003), condenser (E-001, E-002, E-004), the oven (F-002), separators (D-001, D-004) and pumps (B-001, B-002).

These installation units (elements CTS) are interrelated and changes of regime parameters of one of them lead to a change of other parameters that influence the process of production of sulfur. In this regard, for the optimization and the sulfur production process control in the rational mode, one must have related mathematical models of the main installation units, compiled on the basis of a systematic approach, taking into account the effect of technological parameters on every unit on intermediate and final products and installation work as whole.

Models of each unit in the system can be built using a variety of approaches and methods discussed above, i.e., one can get a set of models for each of unit of processing installation, such as statistics, fuzzy or combined. These various models of ISP units can be integrated into a system of models. In order to optimize and control the plant, it is necessary to analyze the advantages and disadvantage of each model, which is possible to build and develop criteria for the selection of models for cost price ISP, on purpose, accuracy, etc., as well as to determine the principles of the developed models in the system.

For this purpose, we have analyzed the possible types of mathematical models of main aggregates installation sulfur production. The results are obtained from the following steps: analysis of processes and units of Atyrau refinery, the experimental data, expert assessment and analysis of approaches to modeling such or similar units [16, 26, 27]. Based on the results, estimation of possible types of models of each unit of the installation is carried out. The result of this analysis (model estimation) is designed on a table 1. To estimate the (ranking) types of models a five-point scale is used.

As the main criteria for comparing different types of models on which they are evaluated, we can highlight: availability of necessary information for the construction of the appropriate type of mathematical model; price of (difficulty) model development; the accuracy of the model; the applicability of these models to the destination (for system simulation, the optimization and control under uncertainty) and the possibility of combining a model of this type in a single package for the purpose of system simulation modes of set as whole.

Table 1 shows the estimation for each type of basic installation model of sulfur production unit based on the processing results of the analysis. On the basis of the information provided in the above table, one can make the choice of the unit models type of sulfur production unit according to given criteria.

Research results of installation system of sulfur production unit operating at the Atyrau Refinery, a possible set of models shows that because of the complexity of the units, the difficulties of studying the processes occurring in them and the inability to obtain reliable data of construction of deterministic models for

Table 1: Analysis and assessment of models of sulfur production unit elements at Atyrau Oil Refinery

Basic units SPI	**Criterion**	**Types of models**			
		Deterministic	**statistical**	**Fuzzy**	**Combined**
Reactors (F-001, R-001, R-002, R-003)	The availability of the necessary information	2.5	4.5	4.5	5.0
	The cost of developing	1.0	4.0	3.5	3.0
	Accuracy	4.5	3.0	2.5	4.0
	Applicability for purpose	3.5	4.0	3.5	5.0
	The possibility of combining into a package	4.0	3.5	3.5	3.5
	Adequacy	3.0	3.5	3.5	4.0
	The amount of assessment	**18.5**	**22.5**	**21.5**	**24.5**
Capacitors (boilers)(Å-001,Å-002,Å-004)	The availability of the necessary information	3.5	4.0	4.5	4.0
	The cost of developing	1.5	4.0	4.0	3.0
	Accuracy	4.5	3.5	3.5	3.5
	Applicability for purpose	4.0	4.0	4.0	4.5
	The possibility of combining into a package	4.5	4.0	4.0	4.0
	Adequacy	3.5	3.5	3.5	3.5
	The amount of assessment	**21.5**	**23.0**	**23.5**	**22.5**
Oven (F-002)	The availability of the necessary information	4.0	5.0	4.5	4.0
	The cost of developing	3.0	5.0	4.0	4.0
	Accuracy	4.5	4.5	3.5	4.0
	Applicability for purpose	4.0	4.0	4.0	4.0
	The possibility of combining into a package	4.0	4.5	4.0	5.0
	Adequacy	4.0	4.5	4.5	5.0
	The amount of assessment	**23.5**	**27.5**	**24.5**	**25.0**
Separators (D-001, D-004)	The availability of the necessary information	4.5	5.0	4.0	4.5
	The cost of developing	3.0	5.0	4.0	2.5
	Accuracy	4.5	4.5	2.0	4.0
	Applicability for purpose	4.0	4.5	4.5	4.5
	The possibility of combining into a package	3.5	4.0	3.5	4.0
	Adequacy	4.0	4.0	3.5	4.0
	The amount of assessment	**23.5**	**27.0**	**21.5**	**23.5**
Pumps (B-001, B-002)	The availability of the necessary information	4.5	4.0	4.0	4.5
	The cost of developing	5.0	4.5	4.0	4.0
	Accuracy	5.0	4.0	4.0	4.5
	Applicability for purpose	4.5	4.5	4.0	4.5
	The possibility of combining into a package	4.5	4.0	4.0	4.0
	Adequacy	4.5	4.0	4.0	4.5
	The amount of assessment	**28.0**	**25.0**	**24.0**	**26.0**

Note: The rating (ranking) on the scale (1-5) where 1 is the lowest score; 5 is the highest rating. Estimates may not be clear, i.e, fuzzy numbers.

the reactors is practically impossible or economically impractical. According to the results of evaluation the fuzzy models for sulfur production have received high scores, but the most effective kind of model for the reactor by the sum of evaluation criteria is the combination model.

For pumps of models built from deterministic models according estimation criteria of comparison is higher than the other, i.e., for them it is advisable to develop a deterministic model.

According to the results of the study it can be concluded that the condenser because of uncertainty of the initial information, it is necessary to build a fuzzy model. For separators and for the oven the best is to build statistical models.

In a functioning ISP at Atyrau Refinery the collection of reliable statistical data to build models of reactors and condenser- boilers is complicated by a lack of special industrial devices and low reliability of available funds.

In this regard, as a more effective means of supplementing the missing data on the basis of qualitative information (knowledge of specialists), the methods of expert estimates [28, 29], and the methods of constructing models - methods based on fuzzy sets and capabilities theories and combined methods are selected [18, 21, 30-33].

In practice, for the construction of models with the lack of information it is necessary to use available information of any nature. Models of production units, obtained on a base of such data are called combined. They can be obtained by using various combinations of the available data. However, the construction of combined models may not be appropriate due to the fact that we need a phase of the organization, carrying out research and experiments of various kinds, as well as pre-processing of the collected data.

During the development of models of technological units, which are parts of complexes of technological units, often the approach of decomposition is used, in which models of separate units (elements) are constructed separately, and they often do not take into account the issue of further combining of the obtained models in a single complex. This particular solution of the problem does not give the desired effect and the final positive result. Simulation and optimization of a single technological complex unit in the full sense is impossible, because the work of this unit is connected with the work of the other units of the complex.

Therefore, to fully solve the problem of modeling and control of complex technological units, we need to create a coherent system of object model based on the relationship between the units, i.e., outputs of one models may be the other, but the inputs and outputs of these models can be input of the other and previous models. With the use of such models complex we can carry out systematic simulation of technological complex. As a result, system simulation of technological complex is possible to identify ”bottlenecks” of the object, the solution of that increases the power and productivity of technological complex.

Combining the individual units models in system is made in accordance with the flow of the process in the processing facility. At the same outputs of one model are inputs of another. For example, ISP output parameters of thermoset model F-001 and boiler E-001 are the input parameters of the model E-004 condenser, output model of this unit are the input parameters of the model of the reactor R-001. In turn, the results of the reactor R-001 modeling are the initial data to simulate condenser E-002 and the parallel-connected reactor R-002, R-003, and part of the output condenser parameters E-002 model are input parameters for reactors R -002 and R-003 models.

Thus, simplicity of integration of different models into a single system can be the main criteria for the choice of aggregates models types due to tis mutual consistency of output and input variables between linked models. Nevertheless, one still should consider accuracy and efficiency of their application in computer system simulation and optimization.

For a system simulation of technological complex in the dialog mode, you must have simple mathematical model of the basic units, as the cost of computer time for modeling should be minimized, because any optimization algorithm repeatedly refers to the routine simulation, and the response time of the system for recommendations issuing for control also needs to be small. Therefore, when building models of complex industrial facilities such as sulfur production installing, and other refining settings, the most suitable approach is the following. In this paper, we propose a new approach, according to which, at first, the model of unit is constructed based on the results of studies of each unit and the data collected. Then these models are combined in order to describe the whole process in a single models system.

Mathematical models of the F-001 thermal reactor and the Claus reactor R-001. We turn to the development of mathematical models of reactors ISP at Atyrau refinery. The basis of mathematic thermal reactor model F-001, and Claus reactor R-001 are the statistics, expert information processed by methods of fuzzy set theory.

For example, treatment of experimentally-statistical and expert data, and applying the idea of the method of successive inclusion of covariates, with use of method of mathematical models of technology based on information of various kinds, the following plural-term equations structure, high-quality regression and conditional inference, as a model of studied reactor is received:

$$y_1 = a_0 + \sum_{i=1}^{4} a_i x_i + \sum_{i=1}^{4} \sum_{k=i}^{4} a_{ik} x_i x_k, \quad (4)$$

$$y_2 = a_0 + \sum_{i=5}^{7} a_i x_i + \sum_{i=5}^{7} \sum_{k=i}^{7} a_{ik} x_i x_k, \quad (5)$$

$$\tilde{y}_j = \tilde{a}_{0j} + \sum_{i=5}^{7} \tilde{a}_{ij} x_{ij} + \sum_{i=5}^{7} \sum_{k=i}^{7} \tilde{a}_{ikj} x_{ij} x_{kj}, \; j = \overline{3,4} \quad (6)$$

where $y1$ and $y2$ are the sulfur output from the thermal reactor and the Claus reactor respectively; quality data of the sulfur, respectively, the mass fraction of sulfur (depending on the grade at least from 99.20 to 99.98%), mass fraction of water production (up from 1.0 to 0.2% depending on the variety); $x1$ is loading, row material consumption of thermal reactor F–001 (26–28 t/h) entering; $x2$ is thermal reactor F-001 (1000 – 1413 îÑ) temperature; $x3$ is thermal reactor outlet temperature (180-350 îÑ); $x4$ is combustion air flow at F–001 thermal reactor (200–700 nm/m3); $x5$ is feed to the Claus reactor R–001 (6-8 t/h); $x6$ is inlet temperature of reactor R–001 (180-290 îÑ); $x7$ is R–001 reactor outlet temperature (300-345 îÑ); a_{0j}, a_{ij}, a_{ikj} and$\tilde{a}_{0j}$, $\tilde{a}_{ij}$, $\tilde{a}_{ikj}$, $i,k = \overline{1,7}$ are identified conventional and fuzzy regression coefficients, respectively: the constant term; taking into account the influence of linear (xij), square and mutually influence (xij, xkj), on the output parameters of the reactor.

As it is clear, the models describing the output ISP products have the form of multiple regression, respectively identified by experimentally-statistical methods and the model evaluating the quality of sulfur have the form of fuzzy multiple regression equations and they are obtained on the basis of information quality from experts. Identification of regression coefficients in the models (4) - (6)is carried out by well-known parametric identification methods, based on the method of least squares with REGRESS software package (A.G. Kuznetsov, Orazbayev B.B.).

The results of the parametric identification of models that determine the dependence of the sulfur output from the reactors are of the form (7) - (8):

$$y_1 = f_1(x_1,x_2,x_3,x_4) = 0.686792x_1 + 0.012480x_2 - 0.052000x_3 - 0.026000x_4 + 0.025917x_1^2 - 0.000208x_3^2 - 0.0000520x_4^2 + 0.000471x_1x_2 - 0.000589x_1x_4 + 0.0000250x_2x_4 - 0.000104x_3x_4 \quad (7)$$

$$y_2 = f_2(x_5,x_6,x_7) = 0.671233x_5 + 0.017143x_6 - 0.012923x_7 + 0.078814x_5^2 + 0.000058x_6^2 - 0.00003x_7^2 - 0.001566x_5,x_6 - 0.000590x_5,x_7 + 0.000035x_6,x_7 \quad (8)$$

Fig. 1 shows the dependence graph of the sulfur output from the thermal reactor F-001 with temperature of the reactor.

To identify the unknown fuzzy coefficients$\tilde{a}_{0j}$, $\tilde{a}_{ij}(i=\overline{5,7})$ and $\tilde{a}_{ikj}(i,k=\overline{5,7},\ \ j=\overline{3,4})$ in equations (6) the fuzzy sets, describing the quality of production indicators, are divided into the following level sets of α = 0,5; 0.75; 1. In accordance to the chosen level the values of input $\tilde{o}ij$ and output $\tilde{y}_3$, $\tilde{y}_4$parameters at every level $a_q(q=\overline{1,3})$*are* observed.

For each level αq models of quality indicators of sulfur (6), can be represented as a multiple regression equation system, then the problem of identification of coefficients $a_{ij}^{aq}(i=\overline{5,7}),\ j=\overline{3,4},\ q=\overline{1,3})$,is reduced to the classical problems of estimating the parameters of multiple regression. To solve the latter problem the known algorithms or standard multiple regression program can be used. We have used REGRESS package.

The resulting values of the model coefficients $a_{ij}^{aq}(i=\overline{5,7}),\ j=\overline{3,4},\ q=\overline{1,3})$ (6) are unified with use of the following equation

$$\tilde{a}_{ij} = \bigvee_{\alpha\in[0.5,1]} \text{ or } \mu\tilde{a}_{ij}(a_{ij}) = \underset{\alpha\in[0.5,1]}{SUP} \min\{\alpha,\ \mu\alpha_{ij}^{\alpha}(a_{ij})\}$$

when $a_{ij}^{aq} = \{a_i \,|\, \mu\tilde{a}_{ij}(a_{ij}) \geq \alpha\}$. Thus, mathematical models describing the fuzzy dependence of the quality indicators of sulfur, for example, the mass fraction of sulfur from the input parameters x_i, $i=\overline{1,3}$ (x_1-temperature of thermal reactor F–001 (1000–1413°Ñ); x_2-combustion air flow in the thermal reactor F–001 (200-700 nm/m^3); x_3 - temperature of the reactor R–001 (280-300°Ñ)) are as follows; are as follows;

$$\begin{aligned}
y_3 = f_3(x_1,x_2,x_3) &= (0.5/0.037008 + 0.75/0.037020 + \\
&+1/0.037033 + 0.75/0.037045 + 0.5/0.037057)x_1 + \\
&+(0.5/0.076885 + 0.75/0.076900 + 1/0.076915 + \\
&+0.75/0.076930 + 0.5/0.076945)x_2 - (0.5/0.16943 + \\
&+0.75/0.169455 + 1/0.169475 + 0.75/0.169495 + \\
&+0.5/0.169520)x_3 + (0.5/0.00001 + 0.75/0.00002 + \\
&+1/0.000027 + 0.75/0.000034 + 0.5/0.000044)x_1^2 \\
&+(0.5/0.000093 + 0.75/0.000108 + 1/0.000118 + \\
&+0.75/0.000132 + 0.5/0.000143)x_2^2 - \\
&-(0.5/0.000007 + 0.75/0.000057 + 1/0.000574 + \\
&+0.75/0.000157 + 0.5/0.000207)x_3^2 + \\
&+(0.5/0.000050 + 0.75/0.000070 + 1/0.000080 + \\
&+0.75/0.000090 + 0.5/0.000110)x_1x_2 - \\
&-0.5/0.000045+0.75/0.000065+1/0.000075+ \\
&+0.75/0.000085+0.5/0.000105)x_1x_3- \\
&-(0.5/0.00017+0.75/0.0002+1/0.00021+ \\
&+0.75/0.00022+0.5/0.00024)x_2x_3
\end{aligned}$$

We have investigated the influence of other regime parameters on output parameters, including multi-dimensional space.

Study and construction of linguistic models to determine the quality of the obtained sulfur. To assess the quality of the resulting sulfur, that is based on logical rules of conditional output and a knowledge base the linguistic models are built describing the dependence of sulfur quality (grade) of the mass fraction of sulfur, ash mass fraction, mass fraction of organic substances and the mass fraction of water. These models realize linguistic dependence as a production base of knowledge [?]:

If $M_S \tilde{\geq} 99,98\% \wedge M_Z \tilde{\leq} 0,02\% \wedge M_{OB} \tilde{\leq} 0,01\% \wedge M_B \tilde{\leq} 0,2\%$, *Then* Q_S – “high”, *Else*

If $M_S \tilde{\geq} 99,95\% \wedge M_Z \tilde{\leq} 0,03\% \wedge M_{OB} \tilde{\leq} 0,03\% \wedge M_B \tilde{\leq} 0,2\%$, *Then* Q_S – “above average”, *Else*

If $M_S \tilde{\geq} 99,90\% \wedge M_Z \tilde{\leq} 0,05\% \wedge M_{OB} \tilde{\leq} 0,06\% \wedge M_B \tilde{\leq} 0,2\%$, *Then* Q_S – “average”, *Else*

If $M_S \tilde{\geq} 99,50\% \wedge M_Z \tilde{\leq} 0,02\% \wedge M_{OB} \tilde{\leq} 0,25\% \wedge M_B \tilde{\leq} 0,2\%$, *Then* Q_S – “below average”, *Else*

If $M_S \tilde{\geq} 99,20\% \wedge M_Z \tilde{\leq} 0,40\% \wedge M_{OB} \tilde{\leq} 0,50\% \wedge M_B \tilde{\leq} 1,0\%$, *Then* Q_S – “low”.

In the above given linguistic model of quality assessment of sulfur, the following adopted are M_S - mass fraction of sulfur; M_Z - mass fraction of ash; M_{OB} - mass fraction of organic substances; M_B - the mass fraction of the water; - Fuzzy restriction ”no more”; Q_S –sulfur quality.

In the production ”high quality” refers to a sulfur grade 9998; ”Above average” - 9995; ”Average” - 9990; ”Below average” - 9950; ”Low” - 9920.

As seen from the linguistic model of sulfur quality, it mainly depends on the sulfur composition. According to this practice in violation of other requirements (mass ash fraction, organic substances and water), the sulfur quality is determined by the value of the first criterion requirements. That is why knowledge base is supplemented by other terms and conclusions, such as:

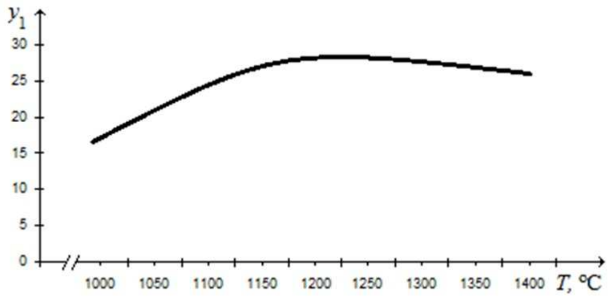

Fig. 1: Fig. 1. Dependence graph of the sulfur output from thermal reactor temperature $y_1 = f_1(x_2), x_1, x_3, x_4)$– constants. x_1 – the raw material input of 26.5 t/h; x_3 – outlet temperature F–001, 250 °C; x_4 – air flow of combustion at thermal reactor F–001, 500 nm/m^3.

If $M_S \tilde{\geq} 99,98\% \wedge M_Z \tilde{\leq} 0,03\% \wedge M_{OB} \tilde{\leq} 0,03\% \wedge M_B \tilde{\leq} 0,2\%$, *so* Q_S – "above average",

If $M_S \tilde{\geq} 99,95\% \wedge M_Z \tilde{\leq} 0,04\% \wedge M_{OB} \tilde{\leq} 0,05\% \wedge M_B \tilde{\leq} 0,5\%$, *so* Q_S – "average",

If $M_S \tilde{\geq} 99,90\% \wedge M_Z \tilde{\leq} 0,25\% \wedge M_{OB} \tilde{\leq} 0,30\% \wedge M_B \tilde{\leq} 0,3\%$, *so* Q_S – "below average",

If $M_S \tilde{\geq} 99,50\% \wedge M_Z \tilde{\leq} 0,35\% \wedge M_{OB} \tilde{\leq} 0,50\% \wedge M_B \tilde{\leq} 0,5\%$, *so* Q_S – "low", etc.

Thus, in violation of the requirements for a mass fraction of ash, organic substances and water, quality grade of sulfur is usually determined by one grade below.

These linguistic models as a production base of knowledge allow to formalize and describe the quality and grade of the resulting sulfur. The functions of fuzzy parameters and indicators of the sulfur quality can be built on the basis of a priory and expert information. For example, the membership function of fuzzy parameters, describing "the high quality" of sulfur has the following types:

$$\mu_A^S(x) = \begin{cases} 1, \; if \; E \geq 99.98 \\ 12.5 \cdot E - 1248.75, \; if \; 99.90 \leq E < 99.98 \\ 0, \; if \; E < 99.90 \end{cases};$$

$$\mu_A^Z(x) = \begin{cases} 1, \; if \; 0 \leq E \leq 0.020 \\ 33.33 \cdot E - 0.66, \; if \; 0.020 < E \leq 0.050 \\ 0, \; if \; E > 0.050 \end{cases};$$

$$\mu_A^{OB}(x) = \begin{cases} 1, \; if \; 0 \leq E \leq 0.010 \\ 20 \cdot E - 0.2, \; if \; 0.010 < E \leq 0.060 \\ 0, \; if \; E > 0.060 \end{cases};$$

$$\mu_A^B(x) = \begin{cases} 1, \; if \; 0 \leq E \leq 0.20 \\ 20 \cdot E - 4, \; if \; 0.20 < E \leq 0..25 \\ 0, \; if \; E > 0.25 \end{cases}$$

where $\mu_A^{OB}(x), \mu_A^S(x), \mu_A^Z(x), \mu_A^B(x)$ are the membership functions, describing fuzzy indicators of sulfur composition, ash, organic substances and water. According to these formula it is easy to build graphics functions of described membership function

Table 2: Comparison results of the of the proposed models and experimental ISP Atyrau refinery data

Defined parameters	**The simulation results**	**test data**
The target output - sulfur, t/h	26.0	25.3
Sulfur content,%	99.98	(99.96)^l
Ash content,%	0.018	(0.02)^l
Mass fraction of organic substances,%	0.01	(0.01)^ё
Water content,%	0.15	(0.18)^ё

The results of simulation work of thermal reactor production at ISP of Atyrau refinery on the basis of the above-identified models are compared with experimental production data. The main results of the comparison are shown in tabular form (see. Table 2).

Note: The input and operating parameters of the process are taken about the same, () l means that they are received by the laboratory.

The tabulated data show simulation results of sufficient accuracy which coincide with the actual experimental data. On the base of obtained models we can determine the quality parameters of products in uncertain medium that is not detected by conventional modeling methods.

4 Conclusions

The originality and novelty of the results of the work lie in the fact that the proposed method of mathematical modeling of CTS under condition of uncertainty makes it possible, on the basis of different character information to build the adequate models of complicated facilities, consisting of a plurality of interconnected units. For the purpose of implementation and practical application of this approach, possible models for basic units of ISP Astyrau refinery are analyzed and evaluated. The mathematical models for system of reactors of sulfur production installation is developed.

Thus, a systematic approach to the development of a mathematical modeling set of interconnected technological units CTS is justified, which allows to solve basic problems of mathematical models construction and system simulation of work regime of the units processing facility under the fuzzy initial information. The proposed complex model development method differs from other approaches by using available information of various kinds, including fuzzy information. Different models of the studied objects are built, which are then combined into single-system models. This approach is implemented in the construction of the model system, of the main ISP units at Atyrau refinery. On the basis of this study the structure and parameters of mathematical models of thermal reactor F-001 and Claus reactor R-001 ISP are identified. To evaluate the quality indicators of sulfur, the linguistic models and membership functions are built, describing the fuzzy quality indicators. The comparison of the simulation results of the thermal reactor work of ISP Atyrau refinery with the experimental and industrial plant data is given. The results of the simulation with high accuracy coincide with the real (experimental) data; and on the base of obtained models we can determine the quality of products, in fuzzy environment, which is not defined by traditional modeling methods.

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