

Study and Design of Mathematical Models for Chemical-Technological Systems under Conditions of Uncertainty Based on the System Analysis

Kenzhebaeva T.S., Orazbayev B.B., Abitova G.A.

Department of System Analyses and Control
L.N. Gumilyov Eurasian National University
Astana, 010000, Kazakhstan
togzhan_kenzhebaeva@mail.ru, batyr_o@mail.ru, gulya.abitova@gmail.com

Orazbayeva K.N.

Department of Management
Kazakh University of Economy, Finance and International Trade
Astana, 010000, Kazakhstan
kulman_o@mail.ru

Spichak Y.V.

Department of Electroenergy and Automation of the Technical Systems
Karaganda State Industrial University
Temirtau, 101400, Kazakhstan
nolaseren@mail.ru

Abstract

The paper proposes a new approach to designing of a structured mathematical model for chemical-technological systems (further - CTS) of refinery in uncertainty. These uncertainties are depending from randomness and a fuzziness of the input data for a various types of information. Idea and novelty of the proposed method lies in the fact that at first the results of studies of each CTS unit based on the gathered information and the adopted criteria for evaluating the model of separate element is constructed. Then to simulate the whole process the developed models are combined into a single system. The designed method has been successfully implemented during the design of models of units of catalytic reforming at Atyrau oil refinery. Analyses and comparison of the known results and simulation results of the proposed method, and the experimental data from Atyrau refinery have shown the effectiveness and advantage of proposed modeling approach to interrelated technological units complex.

Keywords

Mathematical models, technological systems, the theory of fuzzy sets, accessory function, the decision-maker

1. Introduction

The vital problems of any production are intensification of production, improving of the quality and efficiency of technological and production processes. One of the most promising and effective way to solve these problems is an increased production facilities control efficiency through the use of scientific methods of system analysis, development and decision-making on the basis of mathematical models constructed with the use of a systematic approach [1 - 3]. Currently, there are series of works devoted to the method of mathematical modeling and control of refinery technological objects [1, 3, 5]. However there is a class of objects of oil refining, different production situations and their control tasks. Their formalization and decision can be not obtained in the traditional ways; 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, 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 [6, 7].

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 to 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 person (further - DM), 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, 8].

The successful solution of the problems of modeling and tasks of multi-criteria optimization arising in the control of production facilities under uncertainty and fuzziness of initial information, requires the mathematical methodology development of CTS models in these conditions, 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. These issues are the subject of this research work.

For conducting the process in the desired mode in the complex technological machines, one must install the relationship law between the input and output parameters of individual units that can be not done without special tools and mathematical apparatus. An effective solution to this problem and control of real CTS is possible with the help of computer systems based on mathematical models and algorithms taking into account the nature and structure of the technological object, processes types occurring in them, and also types of regimes.

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 works are aimed to solve them [9 - 11].

Questions developing a system of interconnected models and systematic CTS simulation, what is the installation of oil refining, optimization methods of work mode in a multi-criteria and uncertainty caused by the lack of clarity of initial information is one of the little-studied and is not completely solved problem in research. In this context, the development of effective methods of mathematical simulation CTS of refinery in the real conditions, which are often characterized as uncertainty are actual scientific and practical task of the petroleum industry.

The mathematical model is a mathematical description system, 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 in a single system of relations [12, 13]. 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, which theoretical form is unknown or too complicated, and indistinct connections and expression, based on the knowledge and experience of specialists- experts in the form of logical rules of conditional output [4, 6 - 9, 11, 13].

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 [11, 14, 15]. 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, due to the shortage, 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, 6, 8, 13, 16].

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 need to develop a systematic method of mathematical models and simulation of complex objects 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. A Proposed New Approach to Design of Mathematical Models for CTS under Uncertainty of Different Nature

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 worked 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 characterize the functioning of studied CTS;
- Data obtained in the result of the expert assessment, including fuzzy information, the qualitatively describing the state of the object.

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

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). 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 points:

1. Research and analysis of CTS, consisting of interconnected units, the collection of accessible information and its processing, the determination of simulation purposes;

2. Determination of the evaluation criteria, 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 combining of 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 paragraphs 3.1-3.3, or 4;

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

5. If $x_i \in X_i$, the input parameters of the complex deterministic (clear), so the determination of the structure of fuzzy equations of multiple regression $\tilde{y}_j = f_j(x_1, \dots, x_n, \tilde{a}_0, \tilde{a}_1, \dots, \tilde{a}_n), j = \overline{1, m}$ (identification of the structural solution of the 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 $\mu_{A_i}(\tilde{x}_i), \mu_{B_j}(\tilde{y}_j)$;

8. If the input and output parameters of the object are not clear, then formalize fuzzy display R_{ij} , define the links between \tilde{x}_i and \tilde{y}_j , i.e., linguistic model is built and transition to step 10 is made;

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

10. If the conditions of paragraph 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 items offered above method of constructing mathematical models of CTS with the uncertainty of various kinds.

In paragraph 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 is done. At this point, the goal of modelling is determined. The collected and processed information is used to build a mathematical model.

In paragraph 2 taking into account the simulation goal in the previous paragraph, 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 management 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 a whole.

In paragraph 3 according to selected model evaluation criteria the expert estimation of possible models types of each CTS unit is made based on an estimation of results (for example, by summation of set ranks – point i.e. the evaluation of experts). For each unit of the system the type of mathematical model is determined, which is item-efficient for every unit. Completion and registration of the results of this item is convenient to do in the form of table (Table 1). Sub-paragraphs 3.1 and 3.2 of paragraph 3 are implemented on the base of known methods for developing deterministic-mining and statistical models. Paragraph 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 subparagraph 3.4 the combined information of different nature is used (theoretical, statistical, fuzzy) and combined model is built.

In paragraph 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 change range 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):

$$x_j^{\min} = x_j^1 < x_j^2 < \dots < x_j^n = x_j^{\max}, \quad y_j^{\min} = y_j^1 < y_j^2 < \dots < y_j^n = y_j^{\max}$$

To determine the structure of fuzzy equations of multiple regression (paragraph 5), you can use the approach of fuzzy regression analysis. At this stage the qualitative analysis of the object is important, as a result of which 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 (item 6) each quantum selections verbally characterized by corresponding fuzzy terms. For example, if \tilde{y}_j - oil products quality (such as gasoline), then it can be described by terms:

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

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 4th paragraph, 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.

7 - *The point* where the constructed fuzzy function parameters, are 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, you 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:

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

where $\mu_{B_j}^p(\tilde{y}_j)$ – the function parameters \tilde{y}_j of fuzzy sets \tilde{B}_j , characterized the values of output parameters; p – quantum number; $Q_{B_j}^p$ – the option that is in the identification of the membership functions and 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_{mdi} – 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 *paragraph 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 verbally (clearly) the different values of the input parameters \tilde{x}_i and the corresponding values of these options, the output parameters are indicated \tilde{y}_j . The table must be filled with the selected *paragraph 4* term-set. On the basis of the model obtained in this way fuzzy mapping R_{ij} determining the connection between fuzzy input \tilde{x}_i and output parameters \tilde{y}_j are 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 use R_{ij} in the calculations 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:

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

To determine the estimates of the parameters of the function selected in *paragraph 5* in *9-paragraph*, you can use the criterion of minimizing the deviation of the fuzzy values of the output parameter \tilde{y}_j^m obtained by the model from its sample of fuzzy values obtained on the basis of expert estimation \tilde{y}_j^g , i.e. ... $R_j = \min \sum_{i=1}^L (\tilde{y}_j^m - y_j^g)^2$.

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]:

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

Paragraph 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, you can carry out the calculation of the output variables, e.g, the measures based on the maximin product:

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

Let \tilde{x}_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 $\mu_{B_j}^p(\tilde{y}_j^*)$ (3).

Specific numerical values of the output parameters y_j^c of the fuzzy set of solutions are determined from the following relationship:

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

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

The objective of the final stage of the method (*paragraph 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, the actual data obtained experimentally at the object.

As a general rule, as an adequate criterion, which is a measure of compliance with model object, use the value of the calculated error (model) y^m and the real (experimental) – y^o data: $R = |y^m - y^o|$. In addition, an acceptable error level value is selected – $R_{\text{д}}$. The model is considered to be adequate if $R = |y^m - y^o| \leq R_{\text{д}}$.

In the case of the mathematical model inadequacy is finalized, the sources of inadequacy are determined. This may be 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. Then you return to the appropriate step of the algorithm for the model refinement.

3. The results of the practical application of the proposed method and discussion

We concretize results above mentioned studies and implement them in practice in the development of the system of mathematical models of the main aggregates of the processes of sulfur production (PSP) of the Atyrau refinery. In paragraph 3 of the proposed method the separate procedure is implemented [18]: 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 ISP.

PSP is a complex CTS, consisting of interconnected units, which simultaneously affects a large number of different parameters. The main unit of the installation is of the reactor (F-001, R-001, R-002, and R-003), condenser (E-001, E-002, and 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 leads 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, you 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 a whole.

Models of each unit in the system can be built using a variety of approaches and methods discussed above. So, you can get a set of models for each of unit of processing installation, such as statistics, fuzzy or combines. To combine these various models of PSP units in a system of models, on the basis of which the system modeling is carried out. 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, develop criteria for the selection of models for cost price STI, 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. On the basis of the results of research specific process and PSP units of Atyrau Refinery, of the experimental data, expert demand and analysis of approaches to modeling such or similar units [19, 20] the 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 the table 1.

For pumps of models building of 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.

Table 1. Analysis and assessment of technological models types of the ISP of Atyrau 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 (E-001, E-002, E-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.

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 [21, 22], and the methods of constructing models - methods based on fuzzy sets and capabilities theories and combined methods are selected [4, 8, 11, 12, 14, 16, 23 - 25].

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 be not 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 part of complexes of technological units, often approach of decomposition is used, in which models of separate units (elements) are constructed separately, and 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 solve fully the problem of modeling and control of complex technological units, you need to create a coherent system of object model based on the relationship between the units, i.e., outputs of one model may be other, but the inputs and outputs of these models can be input of other and previous models. With the use of such models complex you 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 will increase the power and productivity of technological complex.

Combining the individual unit's models in system is made in accordance with the flow of the process in the processing facility. At the same outputs of one model (calculation results) are inputs of another. For example, PSP 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, the main criteria for the choice of aggregates models types, except requiring accuracy and efficiency of their application in computer system simulation and optimization applies ease of their integration into the system, i.e., mutual consistency of output and input variables, linked models.

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, what are sulfur production installing, and other refining settings as the most suitable approach. In this paper we propose a new approach, according to which first the results of studies of each unit and on the basis of the data collected model of unit is based. Then these models in order to describe the whole process in a single models system are combined.

3.1 Mathematical models of the F-001 thermal reactor and the Claus reactor R-001

We turn to the development of mathematical models of reactors PSP 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:

$$y_1 = a_0 + \sum_{i=1}^4 a_i x_i + \sum_{i=1}^4 \sum_{k=i}^4 a_{ik} x_i x_k, \quad (3),$$

$$y_2 = a_0 + \sum_{i=5}^7 a_i x_i + \sum_{i=5}^7 \sum_{k=i}^7 a_{ik} x_i x_k, \quad (4),$$

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

Where:

y_1, y_2 - 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);

x_1 - loading, raw material consumption of thermal reactor F-001 (26–28 t/h) entering;

x_2 - thermal reactor F-001 (1000 – 1413 °C) temperature;

x_3 - thermal reactor outlet temperature (180-350 °C);

x_4 - the combustion air flow at F-001 thermal reactor (200–700 nm/m³);

x_5 - feed to the Claus reactor R-001 (6-8 t/h);

x_6 - inlet temperature of reactor R-001 (180-290 °C);

x_7 - R-001 reactor outlet temperature (300-345 °C); a_{0j}, a_{ij}, a_{ikj} and $\tilde{a}_{0j}, \tilde{a}_{ij}, \tilde{a}_{ikj}, i, k = \overline{1,7}$ - identified conventional and fuzzy regression coefficients, respectively: the constant term; taking into account the influence of linear (x_{ij}), square and mutually influence (x_{ij}, x_{kj}), on the output parameters of the reactor.

As you can see, the models describing the output ISP products have the form of multiple regressions, respectively identified by experimentally-statistical methods and the model evaluating the quality of sulfur have the form of fuzzy multiple regression equations and obtained on the basis of information quality from experts.

Identification of regression coefficients in the models (3) - (5) is carried out by well-known parametric identification methods, based on the method of least squares with REGRESS software package.

The results of the parametric identification of models that determine the dependence of the sulfur output from the reactors are of the form (6) - (7):

$$y_1 = f_1(x_1, x_2, x_3, x_4) = 0.686792x_1 + 0.012480x_2 - 0.052000x_3 - 0.026000x_4 + 0.025917x_1^2 - 0.000208x_3^2 - 0.0000520x_4^2 + 0.000471x_1x_2 - 0.000589x_1x_4 + 0.0000250x_2x_4 - 0.000104x_3x_4 \quad (6)$$

$$y_2 = f_2(x_5, x_6, x_7) = 0.671233x_5 + 0.017143x_6 - 0.012923x_7 + 0.078814x_5^2 + 0.000058x_6^2 - 0.00003x_7^2 - 0.001566x_5x_6 - 0.000590x_5x_7 + 0.000035x_6x_7 \quad (7)$$

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 (5) the fuzzy sets, describing the quality of production indicators, are divided into the following level sets of $\alpha = 0.5; 0.75$;

1. In accordance to the chosen level the values of input x_{ij} and output \tilde{y}_3, \tilde{y}_4 parameters at every level $\alpha_q (q = \overline{1,3})$ are observed.

For each level α_q models of quality indicators of sulfur (5), can be represented as a multiple regression equation system, then the problem of identification of coefficients $a_{ij}^{\alpha q} (i = \overline{5,7}, j = \overline{3,4}, q = \overline{1,3})$, 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 used REGRESS package.

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

$$\tilde{a}_{ij} = \bigvee_{\alpha \in [0.5, 1]} \mu \tilde{a}_{ij}(a_{ij}) = SUP \min \{ \alpha, \mu \alpha_{ij}^{\alpha}(a_{ij}) \} \quad \text{when} \quad a_{ij}^{\alpha q} = \{ a_i \mid \mu \tilde{a}_{ij}(a_{ij}) \geq \alpha \}$$

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 °C); x_2 - combustion air flow in the thermal reactor F-001 (200-700 nm/m³); x_3 - temperature of the reactor R-001 (280-300 °C)) are as follows;

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

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

3.2 Study and construction of linguistic models to determine the quality of the obtained sulfur

To assess the quality of the resulting sulfur-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 [25]:

$$\begin{aligned} & \text{If } M_s \gtrsim 99,98\% \wedge M_z \lesssim 0,02\% \wedge M_{OB} \lesssim 0,01\% \wedge M_B \lesssim 0,2\% , \text{ Then } Q_s - \text{“high”}, \text{ Else} \\ & \text{If } M_s \gtrsim 99,95\% \wedge M_z \lesssim 0,03\% \wedge M_{OB} \lesssim 0,03\% \wedge M_B \lesssim 0,2\% , \text{ Then } Q_s - \text{“above average”}, \text{ Else} \\ & \text{If } M_s \gtrsim 99,90\% \wedge M_z \lesssim 0,05\% \wedge M_{OB} \lesssim 0,06\% \wedge M_B \lesssim 0,2\% , \text{ Then } Q_s - \text{“average”}, \text{ Else} \\ & \text{If } M_s \gtrsim 99,50\% \wedge M_z \lesssim 0,02\% \wedge M_{OB} \lesssim 0,25\% \wedge M_B \lesssim 0,2\% , \text{ Then } Q_s - \text{“below average”}, \text{ Else} \\ & \text{If } M_s \gtrsim 99,20\% \wedge M_z \lesssim 0,40\% \wedge M_{OB} \lesssim 0,50\% \wedge M_B \lesssim 1,0\% , \text{ Then } Q_s - \text{“low”}. \end{aligned}$$

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, 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:

$$\begin{aligned} & \text{If } M_s \gtrsim 99,98\% \wedge M_z \lesssim 0,03\% \wedge M_{OB} \lesssim 0,03\% \wedge M_B \lesssim 0,2\% , \text{ so } Q_s - \text{“above average”}, \\ & \text{If } M_s \gtrsim 99,95\% \wedge M_z \lesssim 0,04\% \wedge M_{OB} \lesssim 0,05\% \wedge M_B \lesssim 0,5\% , \text{ so } Q_s - \text{“average”}, \\ & \text{If } M_s \gtrsim 99,90\% \wedge M_z \lesssim 0,25\% \wedge M_{OB} \lesssim 0,30\% \wedge M_B \lesssim 0,3\% , \text{ so } Q_s - \text{“below average”}, \\ & \text{If } M_s \gtrsim 99,50\% \wedge M_z \lesssim 0,35\% \wedge M_{OB} \lesssim 0,50\% \wedge M_B \lesssim 0,5\% , \text{ so } Q_s - \text{“low”}, \text{ etc.} \end{aligned}$$

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 formalizing and describing 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 priori and expert information. For example, the membership function of fuzzy parameters, describing "high quality" of sulfur has the following types:

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

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

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

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

Where:

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

3.3 Comparison and reliability evaluation of the simulation results

The results of simulation work of thermal reactor production at PSP 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 (Table 2).

Table 2. Comparison analysis of the results of the of the proposed models and experimental results of processes of sulfur production at Atyrau Refinery Plant

Defined parameters	The simulation results	The Experimental data
The target output - sulfur, t/h	26.0	25.3
Sulfur content, %	99.98	(99.96) ¹
Ash content, %	0.018	(0.02) ¹
Mass fraction of organic substances, %	0.01	(0.01) ¹
Water content, %	0.15	(0.18) ¹

Note: The input and operating parameters of the process are taken about the same, ()¹ 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 lies in the fact that the proposed method of mathematical modeling of CTS under condition of uncertainty, make 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 PSP at Atyrau Refinery are analyzed and evaluated. The mathematical models system of reactors of ISP is developed.

Thus, systematic approach to the development of a mathematical model set of interconnected technological units CTS is justified, which allows to solve basic problems of mathematical models constructing 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 a single-system models.

This approach is implemented in the construction of the model system, of the main SPI 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 PSP 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 PSP at 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 can determine the quality of products, in fuzzy environment, which is not defined by traditional modeling methods.

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Biography

Batyr Orazbayev is Doctor of Technical Sciences, Professor and Member of the International Association of Artificial Intelligence Systems. His scientific research interest areas: mathematical modeling and management of complex objects; formalization and development of methods for solving decision-making problems in a fuzzy environment. Dr. Orazbayev was headed the universities department at various universities of Kazakhstan. Previous positions are follow: Dean, Vice-Rector for scientific work, First Vice-Rector, acting Rector of the Atyrau Institute of Oil and Gas. Currently, he is a Professor of the Department of System Analysis and Control at the Eurasian National University. He takes an active part in conducting fundamental and applied research. Batyr Orazbayev has opened a new scientific direction in formalizing and solving production problems in a fuzzy environment. He is the author of more than 400 scientific and educational works. A special his contribution to science is that a new class of problems has been formalized - multicriteria problems of fuzzy mathematical programming and for the first time a set of methods for their solution has been developed that allows to effectively solving the problems of planning and managing production under different production situations. Under his leadership, 3 doctoral and 11 candidate dissertations were successfully defended.

Gulnara Abitova holds Master's degree in Cybernetics of Technological Processes from Moscow State University of Steel and Alloys at Moscow (Russian Federation), PhD degree in Automation of Metallurgy Production from National Academic Research Institute of Metallurgy and Enrichment of the Ministry of Education and Science at Almaty (Kazakhstan). She has been an invited to the Computer and Electrical Engineering Department in State University of New York (NY, USA) as a Researcher. Dr. Abitova is Professor in the Department of System Analyses and Control at L.N. Gumilyov Eurasian National University (Kazakhstan) and Founded President of IEOM Society in Kazakhstan. Dr. Abitova was awarded the International Grant from the President of Republic of Kazakhstan – Scholarship for the study abroad at the USA (2011-2012) and the prestigious Diploma from the Administration of President of the Republic of Kazakhstan (OCSE, December 2010). She has been an invited speaker at the International conferences (IEEE, SPIE, CSDM and ICUMT) and published more than 40 research articles in the reputed international proceedings at the USA, Canada, France, Turkey, Malaysia, Bulgaria, and Hungary. She served as the Session and Track Chair in the IEOM conferences and as a Distinguished Speaker of the Global Education Engineering Forum at IEOM (2014-2017).

Kulman Orazbayeva is the Doctor of Technical Sciences, Professor. Her areas of scientific research are marketing, management, mathematical modeling, organization and management of production, as as objects and processes of the petrochemical industry. She graduated from the Atyrau Institute of Oil and Gas and was qualified as an engineer-economist, masters in Economics and Management and full-time postgraduate study in the field of Mathematical Modeling, Numerical Methods and Programs. At the Atyrau Institute of Oil and Gas, she held the positions of economist, laboratory assistant, teacher, senior lecturer, and associate professor, professor of the departments «Accounting and Audit and Information Systems". She conducts research work on increasing the efficiency of technological complexes for oil refining and petro chemistry on the basis of economic and mathematical methods. The results of the research are published in international journals from the Thomson Reuter's database and Scopus, in the central scientific journals and editions of the Republic of Kazakhstan and Russia. In the process of Orazbaeva's research, several scientific projects have been completed. On the basis of the research and results obtained, Orazbayeva K.N. fulfilled and successfully defended her doctoral thesis on "Improving the efficiency of oil refining and petrochemical complexes based on mathematical methods". The results of the research are introduced into production at Atyrau Oil Refinery and are used in practice and in the training process (at the Research Institute of KazNIGRI and the Atyrau Institute of Oil and Gas).

Togzhan Kenzhebaeva is Master of Technical Sciences and PhD Student in Automation and Control of the Department of System Analyses and Control at L.N.Gumilyov Eurasian National University. She has a master's degree in Automation and Control of Karaganda State Technical University (Kazakhstan). Kenzhebaeva is Lecturer of the Department of Power Engineering and Automation of Technical Systems at the Karaganda State Industrial University (Kazakhstan).

Spichak E.V. has the qualification "Telecommunications and Communications Engineer", as well as a Master of Engineering degree in Design of the Karaganda State Industrial University (Kazakhstan). She is senior lecturer of the Department "Power engineering and automation of technical systems" of Karaganda State Industrial University (Kazakhstan).