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Systematic Approach to the Elaboration of a Structured Model of a Sulfur Production Unit under Uncertainty

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Abstract. The paper proposes a systematic approach to the elaboration of a structured mathematical model and modeling of chemical and technological systems under uncertainty exemplified by a sulfur production unit. The novelty of the suggested method lies in the choice of a suitable model type for each element of the system based on the systematic analysis, development of the selected model type and their merger into a unified system of models. The method was successfully implemented to construct a system of models for major units of the catalytic reforming plant at the Atyrau Oil Refinery (Republic of Kazakhstan). The study compares existing results, modeling results based on the suggested method and experimental results obtained using an LG-setup of the Atyrau Oil Refinery. The deliverables demonstrate high efficacy and excellence of the approach to the modeling of interconnected equipment (chemical and technological systems).

1. Introduction.

Urgent tasks for any manufacturing enterprise are effective management of the plant, improving quality and efficacy of technological and production processes, increasing output and characteristics of the product. One of the promising methods for solving these tasks is enhanced proficiency in managing production facilities based on scientifically justified methods of systematic analysis, elaborating and making decisions resting upon mathematical models built using the systematic approach [1–4].

The subject of the study is successful solution of modeling problems and multicriteria optimization problems occurring in the process of management of production facilities under uncertain and fuzzy initial information, which requires elaborating a methodology for constructing mathematical models of chemical and technological systems in such conditions.

The optimal technological regime requires establishing relations between input and output parameters of separate units, i.e. developing mathematical models of objects. These are impossible without special means and mathematical apparatus, therefore, a lot of research works towards their solution have been undertaken [6–9].

The goal of the present work is to develop structured system of models for the chemical and technological system under uncertainty of its probabilistic and fuzzy nature on the basis of various initial information.

The construction algorithm of the mathematical models of the chemical and technological system under uncertainty based on various information is depicted in Figure 1.

The construction of mathematical models for different production technologies often suffers from insufficient information, i.e. demands organizing expert assessments [1–3]. Therefore, the expert assessments—in this case—are a method for organizing the work with experts and processing their opinions expressed in quantities and qualities to gather initial information. This will be used to develop the mathematical models of the subject under study and prepare information for decision makers [4].

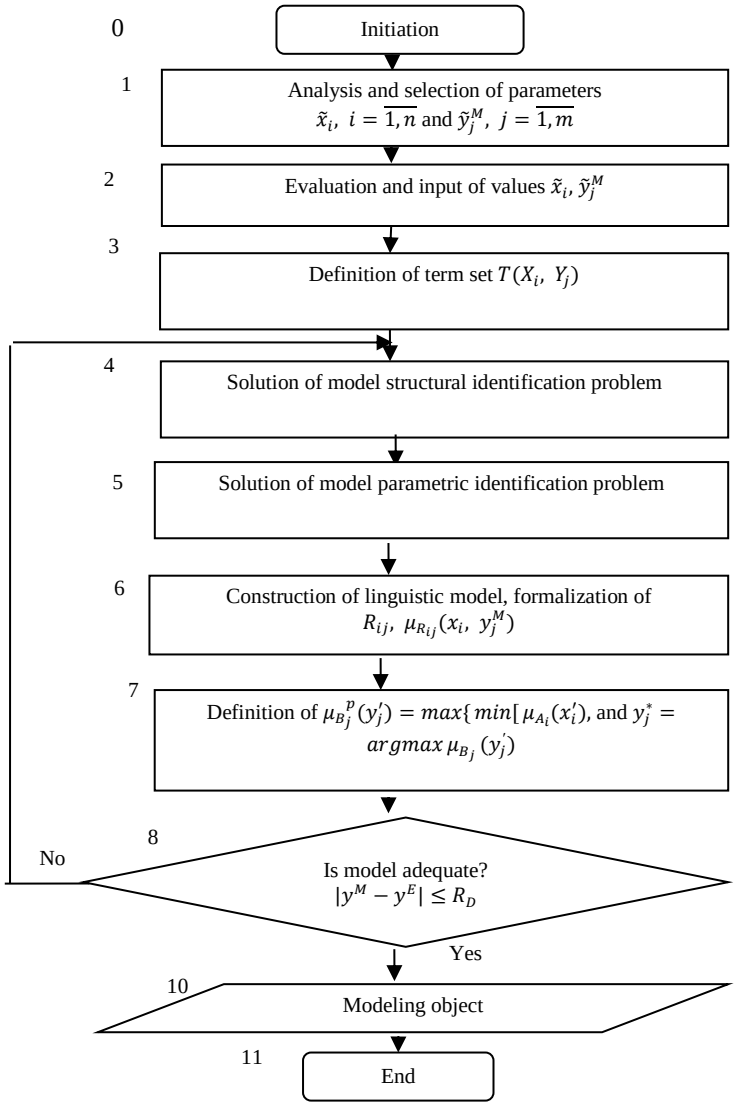

Figure 1. Flow chart of mathematical model construction for a chemical and technological system under uncertainty based on various information:

$\tilde{x}_i, \tilde{y}_j$ fuzzy input and output parameters; $T(X_i,\ Y_j)$ are term sets of fuzzy parameters*; X,Y* are universal subsets; R_{ij} are fuzzy mappings that relate fuzzy input $\tilde{x}_i$ and output $\tilde{y}_j$ parameters; $\mu_{R_{ij}}(\tilde{x}_i,\ \tilde{y}_j)$ is fuzzy matrix; $\mu_{B_j}^{p}(\tilde{y}_j)$ is the membership function of parameters $\tilde{y}_j$ in fuzzy set $\tilde{B}_j$ characterizing the output values; p is quantum number; y_j^c are specific numerical output values; R_D is admissible discrepancy level.

Let us consider the main results of expert assessments that were to collect necessary information for the development of mathematical models of sulfur production units at the Atyrau Oil Refinery.

The expert survey included researchers, decision makers (product engineers), senior operators and operators maintaining the unit. The experts were technical engineer of the unit, four senior operators that maintain the unit and work in shifts, two instrumentation and control engineers, sulfur production unit supervisor and two researchers studying sulfur production management problems. In total, ten experts were involved into the survey. The expert assessment was performed using the Delphi method [4, 5].

We composed a questionnaire with a list of input and operational parameters of the main sulfur production units and asked the experts to assess their effect on the process, i.e. the amount and quality of the product (sulfur, in particular). The assessment results after the fourth round, i.e. adjustment of the list, are presented in Table 1.

Evidently, the experts have arranged the parameters using scores and mainly used numbers: more 1s and 2s, and less 3s and 4s.

Table 1. Survey results after fourth stage of expert assessment

No.	Parameter	Rank	Interval (min-max)	At the moment
1.	Pressure in boilers 33-E-002 ref.33-PI-011	2	3.0–6 kg/m	4.5 kg/m
2.	Pressure in boilers 33-E-002 ref.33-PI-012	2	2.0–3.5 kg/m	2.5 kg/m
3.	Output from 33-E-002 ref.33-TI-039	3	130–210 °C	150–200 °C
4.	Output from 33-E-002 ref.33-TI-040	4	130–210 °C	150–200 °C
5.	Output from 33-E-002 ref.33-TI-041	4	130–210 °C	150–200 °C
6.	Air consumption in 33-T-001 ref.33-FI-022A	1	0–150 Nm^3/h	70 Nm^3/h
7.	Temperature in 33-T-001 ref.33-TI-042	2	120–145 °C	125–130 °C
8.	Temperature in 33-T-001 ref.33-TI-043	2	120–145 °C	125–130 °C
9.	Temperature in 33-T-001 ref.33-TI-044	2	120–145 °C	125–130 °C
10.	Temperature in 33-T-001 ref.33-TI-045	2	120–145 °C	125–130 °C
11.	Input into 33-D-004 and 33-F-002 ref.33-TI-041	1	0–210 °C	130 °C
12.	Furnace gas 33-F-002 ref.33-TI-047	3	0–100 °C	60 °C
13.	Air combustion in furnace 33-F-002 ref.33-FI-030	2	0–700 Nm^3/h	300 Nm^3/h
14.	Temperature at reactor input 33-R-001 ref.33-TI-021	1	0–410 °C	290 °C
15.	Catalyst temperature 33-R-001 ref.33-TI-23	1	200–360 °C	300 °C
16.	Catalyst temperature 33-R-001 ref.33-TI-024	1	200–360 °C	300 °C
17.	Catalyst temperature 33-R-001 ref.33-TI-025	1	200–360 °C	300 °C
18.	Catalyst at reactor output 33-R-001 ref.33-TI-026	1	300–735 °C	345 °C
19.	Combustion air consumption 33-F-001 ref.33- FI-07	1	400–1220 Nm^3/h	500 Nm^3/h
20.	Combustion air consumption 33-F-001 ref.33- FI-08	1	400–500 Nm^3/h	200 Nm^3/h
21.	Furnace output temperature 33-E-001 ref.33-TI-013	1	150–300 °C	250 °C
22.	Furnace output temperature 33-E-001 ref.33-TI-050	1	300–760 °C	645 °C

The experts were proposed a five-point scale, and 5s were used almost never. They are excluded from the table as having almost no effect on the process.

Therefore, the expert assessment has defined the most important parameters that affect sulfur production process, i.e. input and output parameters necessary for elaborating the models. Thus, after the fourth stage of the expert assessment, the input and operating parameters affecting the sulfur production process were ranked. At the second stage of the assessment, the results of the first stage were used to estimate the interrelation between chosen input and output parameters of sulfur production unit.

2. Results and Discussion

Below, we summarize the results of the studies above and use them for developing the system of mathematical models of the main constituents of the sulfur production unit at the Atyrau Oil Refinery.

The unit is a complex chemical and technological system consisting of interconnected elements that simultaneously affect a lot of different parameters. The main elements of the unit are reactor (F-001, R-001, R-002, R-003), condenser (E-001, E-002, E-004), furnace (F-002), separators (D-001, D-004) and pumps (B-001, B-002).

The results of investigated specific processes and elements of the unit, experimental data, expert assessment and analysis of approaches to modeling of similar units [8, 9, 10] were used to estimate possible types of models for each element of the unit. The result of the analysis (model estimation) is given in Table 2. To estimate the model types, a five-point scale was used.

Table 2 shows the estimations for each type of basic model of sulfur production unit resting upon the analysis results. The information provided in the table above can be used to choose the type of sulfur production unit model according to a given criteria.

The study of the operating elements of the sulfur production unit at Atyrau Oil Refinery show that due to the complexity of the equipment and processes in them and impossibility of obtaining adequate data, the construction of deterministic models for the reactors is virtually impossible or not economically feasible. According to the assessment, the statistic and fuzzy models of these sulfur production unit elements received relatively high scores. However, the most effective reactor models—in terms of total score—are combined models.

Therefore, to construct the models for complex industrial facilities, namely the sulfur production units and other oil refining installations, this paper proposes a new approach based on the study of each unit operation and consequent construction of a model on the basis of the data collected. Then, these models are combined to describe the whole process by a single system of models.

3. Comparison of simulation results and reliability evaluation

The simulation of thermal production reactor of sulfur production unit at the Atyrau Oil Refinery based on the proposed models was compared with experimental production data. The main results of the comparison are shown in Table 2.

Table 2. Results of proposed models v. experimental data of sulfur production unit at Atyrau Oil Refinery

Defined parameters	Modeling results	Experimental data
Sulfur yield [t/h]	26.0	25.3
Mass fraction of sulfur [%]	99.98	$(99.96)^{lab}$
Mass fraction of ash [%]	0.018	$(0.02)^{lab}$
Mass fraction of organic substances [%]	0.01	$(0.01)^{lab}$
Mass fraction of water [%]	0.15	$(0.18)^{lab}$

Note: input and operation parameter of the process taken are similar; $()^{lab}$ means laboratory data.

The data in the table demonstrates that the modeling results fairly well comply with real (experimental) data. The models can be used to determine qualitative indicators of the product in fuzzy conditions that cannot be determined by usual modeling methods.

Table 3. Analysis and assessment of models of sulfur production unit elements at Atyrau Oil Refinery

Main elements	Criterion	Model types			
		Deterministic	Statistical	Fuzzy	Combined
Reactors (F-001, R-001, R-002, R-003)	Availability of necessary information	2.5	4.5	4.5	5.0
	Development cost	1.0	4.0	3.5	3.0
	Accuracy	4.5	3.0	2.5	4.0
	Applicability as designed	3.5	4.0	3.5	5.0
	Suitable for bundling	4.0	3.5	3.5	3.5
	Adequacy	3.0	3.5	3.5	4.0
	Total	**18.5**	**22.5**	**21.5**	**24.5**
Condensers (boilers) (E-001, E-002, E-004)	Availability of necessary information	3.5	4.0	4.5	4.0
	Development cost	1.5	4.0	4.0	3.0
	Accuracy	4.5	3.5	3.5	3.5
	Applicability as designed	4.0	4.0	4.0	4.5
	Suitable for bundling	4.5	4.0	4.0	4.0
	Adequacy	3.5	3.5	3.5	3.5
	Total	**21.5**	**23.0**	**23.5**	**22.5**
Furnace (F-002)	Availability of necessary information	4.0	5.0	4.5	4.0
	Development cost	3.0	5.0	4.0	4.0
	Accuracy	4.5	4.5	3.5	4.0
	Applicability as designed	4.0	4.0	4.0	4.0
	Suitable for bundling	4.0	4.5	4.0	5.0
	Adequacy	4.0	4.5	4.5	5.0
	Total	**23.5**	**27.5**	**24.5**	**25.0**
Separators (D-001, D-004)	Availability of necessary information	4.5	5.0	4.0	4.5
	Development cost	3.0	5.0	4.0	2.5
	Accuracy	4.5	4.5	2.0	4.0
	Applicability as designed	4.0	4.5	4.5	4.5
	Suitable for bundling	3.5	4.0	3.5	4.0
	Adequacy	4.0	4.0	3.5	4.0
	Total	**23.5**	**27.0**	**21.5**	**23.5**
Pumps (B-001, B-002)	Availability of necessary information	4.5	4.0	4.0	4.5
	Development cost	5.0	4.5	4.0	4.0
	Accuracy	5.0	4.0	4.0	4.5
	Applicability as designed	4.5	4.5	4.0	4.5
	Suitable for bundling	4.5	4.0	4.0	4.0
	Adequacy	4.5	4.0	4.0	4.5
	Total	**28.0**	**25.0**	**24.0**	**26.0**

Note: the scale-based evaluation (ranking) from 1 to 5, where 1 is the lowest estimate, 5 is the highest one. The estimates can be fuzzy.

4. Conclusions

The novelty of the work results is conditioned by the proposed method of mathematical modeling of a chemical and technological system under uncertainty, being applicable to construct an adequate model of a complex facility consisting of a variety of interconnected units. To evaluate the practical applicability of the proposed approach, the paper has analyzed and evaluated possible models of basic sulfur production unit elements at the Atyrau Oil Refinery. A system of mathematical models for sulfur production unit reactors has been developed.

Thus, the work justifies the systematic approach to the development of a set of mathematical models for interconnected technological units of a chemical and technological system. This allows solving basic problems in construction of mathematical models and simulating operating regimes of the processing facility units under conditions of fuzzy initial information. The proposed comprehensive method of model development differs from other approaches in implementation of various information available, including fuzzy information. Different models of the studied objects were constructed that were then combined into a single system of models. This approach was implemented in the construction of the system of models for the main sulfur production units at the Atyrau Oil Refinery. The results helped identifying the structure and parameters of the mathematical models of thermal reactor F-001 and Claus reactor R-001 of the unit. Moreover, the simulation results of the thermal reactor operation were compared and comply well with the experimental and industrial plant data. Thus, the models can be used to evaluate the quality of products in fuzzy environment, which cannot be done by traditional modeling.

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