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Development of mathematical models of R-1 reactor hydrotreatment unit using available information of various types

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Abstract. The structures and model parameters of the hydrotreating reactor of a catalytic reforming unit were identified based on available information of various types. The structural identification of the developed reactor models was carried out on the basis of the ideas of the sequential switching of regressors method, and the parameters were identified using the least squares method modified for working in a fuzzy environment. The developed models have the structure of nonlinear regression models (for output, i.e. hydrogenated) and fuzzy multiple regression equations (for qualitative indicators of hydrogenated). When developing the models with the source information, we used available statistical and experimental data describing the operation of the reactor and fuzzy information representing the knowledge, experience and judgment of experts about the hydrotreatment process. Based on the simulation of the hydrotreatment reactor, a graph of the temperature dependence of the hydrogenate yield of the reactor is constructed. A linguistic model has been constructed that estimates the dependence of the temperature of the hydrotreating process on the quality of the feedstock. This model allows to determine the optimal temperature value in a fuzzy environment depending on the quality of the raw material being cleaned.

1. Introduction

The hydrotreatment process is one of the effective oil refining processes aimed at improving the quality of fuels and oil products by purifying sulfur, unsaturated, resinous compounds, and impurities from their composition [1]. It is known that these compounds and impurities in the composition of petroleum products impair the operational characteristics of technological equipment and metal aggregates. Thus, the hydrotreatment process allows to reduce harmful compounds in the composition of produced petroleum products, i.e. it reduces corrosion of metal equipment and environmental pollution and the atmosphere [2]. Thus, the study and improvement of oil refining hydrotreating processes by means of mathematical modeling methods is a very urgent task of technological science and oil refining.

Improvements in hydrotreating at oil refineries are currently carried out in the following areas [3]:

- The increase in the cycle time of the regeneration of the hydrotreating catalyst and the time of its operation.
- Conducting hydrotreating processes in the optimal mode, for example, based on mathematical models of the process.
- Improving the quality of products.

In this paper, we consider in details the second direction of improving the operation modes of objects, using the hydrotreating unit of the catalytic reforming unit of the Atyrau Oil Refinery as an example, where the hydrotreating process of straight-run gasoline takes place. There are research works on the methods of mathematical modelling and optimization of technological objects and oil refining processes, including hydrotreating process [4, 5]. However, in practice, production situations often arise related to the deficit and fuzziness of the initial information, modelling and optimization of their operation modes, the formulation and solution of which using traditional methods does not provide adequate solutions. Such objects include the hydrotreating unit of the LG unit of the Atyrau Oil Refinery, the main units of which operate under conditions of uncertainty associated with randomness and fuzziness of the initial information [6]. The aim of this work is to build a complex of mathematical models of the R-1 hydrotreating reactor of the catalytic reforming unit, which can be used to optimize process parameters and control the operating modes of the hydrotreating unit.

2. Statement of the problem

In order to create an optimization system and control the operating modes of a hydrotreating unit, it is necessary to develop a set of mathematical models of its main units. This article sets the task of developing mathematical models of the R-1 reactor, where the product of the hydrotreating process is directly produced. Since this reactor is characterized by uncertainty due to deficit, randomness and ambiguity of available information, it will be necessary to apply an appropriate approach to develop its mathematical models, for example, the hybrid method [7], which allows constructing mathematical models based on available information of various nature.

Let $\{\ddot{x}_i,\ i=\overline{1,l}$ и $\tilde{x}_i,\ i=\overline{1,m}\}$ be a variety of available input parameters of the hydrotreatment reactor, which are characterized by the probability - $\ddot{x}$ and fuzziness - $\tilde{x}$. Values $\{\ddot{x}_i,\ i=\overline{1,l}\}$ are determined using measuring instruments, but they are characterized by randomness, but values $\{\tilde{x}_i,\ i=\overline{1,m}\}$ are evaluated by people, i.e. by the experts on the basis of their experience, knowledge and intuition having a fuzzy nature, i.e. by means of words or phrases. Based on this information, it is necessary to identify the structures and parameters of reactor models using the ideas of known methods, for example, the sequential switching of regressors and the least squares method [8], modifying them to work in a fuzzy environment, as well as a hybrid method for constructing models [7]. Thus, using the above methods, we construct mathematical models that allow us to calculate the values of y_1 – the volume of hydrogenate, i.e. the product at the R-1 outlet and evaluate the values of the product's quality indicators: $\tilde{y}_2, \tilde{y}_3$ and $\tilde{y}_4$ – respectively, unsaturated hydrocarbons, sulfur and water-soluble acids and alkalis in the hydrogenate composition.

3. Research results - mathematical models of the R-1 hydrotreating reactor based on statistical data and fuzzy information

To solve the problem, i.e. to construct a complex of mathematical models that allow one to determine the volume of hydrogenate from the outlet of the R-1 hydrotreating reactor, available source information of various types is used, namely experimental statistical data characterized by probability and expert information having a fuzzy nature [9, 10]. For structural identification of R-1 reactor models, the idea of the method of sequential switching on of regressors is used, and for the identification of model parameters it is carried out on the basis of a modified least-squares method. Thus, mathematical models of the R-1 reactor of a hydrotreating unit are developed using statistical data processed by the methods of the theory of fuzzy sets, fuzzy information collected by expert assessment methods, and also based on the equations of material and heat balances.

Based on the processing of experimental statistical data and expert information, as well as using the method of constructing fuzzy models [11], structural identification of models was carried out, describing the product quality of the R-1 hydrotreatment reactor in the form of the following fuzzy multiple regression equations:

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

where $\tilde{y}_2$ – unsaturated hydrocarbons in the composition of the product, i.e. hydrogenate (should be no more, i.e. $\tilde{\leq} 1\%$); $\tilde{y}_3$ – sulfur in the hydrogenate ($\tilde{\leq} 0{,}00005\%$); $\tilde{y}_4$ – water-soluble acids and alkalis in the hydrogenate ($\tilde{\cong} 0\%$); $x_1 -$ raw materials, in our case it is straight-run gasoline (45-80 m^3/h.); $x_2 -$ pressure in the reactor (20-35 kg/cm^2); $x_3 -$temperature in the reactor (300-343 ^oC); $x_4 -$ volumetric raw feed rate (0,5-5 h^{-1}); $x_5 -$ circulating hydrogen-containing gases (HCG) – hydrogen/hydrocarbon ratio (200-500 nm^3); $\tilde{a}_{0j}, \tilde{a}_{ij}, \tilde{a}_{ikj},\ i = \overline{1,5}$ – identifiable fuzzy coefficients, relatively: free member; linear effects; square effects and mutual influence. In parentheses, the permissible fuzzy values of the output parameters are indicated, as well as the intervals for changing the input and operating parameters.

To identify unknown model parameters (coefficients) (1): $\tilde{a}_{ij}$ $(i = \overline{0,5},\ j = \overline{2,5})$ и $\tilde{a}_{ikj}$ $(i, k = \overline{1,5}, j = \overline{2,5})$ – fuzzy sets describing the quality of the hydrogenate are divided into the following level sets α: α=0,5; 0,85; 1. We observed input mode values $x_{ij}, i, j = \overline{1,5}$ and output $\tilde{y}_2, \tilde{y}_3, \tilde{y}_4$ parameters for each chosen α level. Thus, models were obtained that describe the quality of the product from the output of the R-1 reactor in the form of multiple regression for each α level. Since the obtained equations have the form of regression equations, the problem of identifying their unknown coefficients $\alpha_{ij}^{\alpha_q}, i = \overline{0,5},\ j = \overline{2,4},\ q = \overline{1,3}$ is solved as a classical problem of parametric identification, for example, using the least squares method. In this work, to identify the regression coefficients, we used the REGRESS program package, which, based on modified least squares methods, allows us to determine the regression coefficients of linear and nonlinear regression models with any number of input parameters $x_i, i = \overline{1,n}$.

Thus, after parametric identification, mathematical models describing the influence of input, operating parameters $x_i, i = \overline{1,n}$ on the quality of the hydrogenate, i.e. for example, on the content of unsaturated hydrocarbons ($\tilde{y}_2$), for each α level it looks like:

$$y_2 = f_2(x_{12}, x_{22}, \ldots, x_{52}) = \left(\frac{0.5}{0{,}05} + \frac{0{,}85}{0{,}07} + \frac{1}{0{,}08} + \frac{0{,}85}{0{,}09} + \frac{0{,}5}{0{,}095}\right) - \left(\frac{0.5}{0{,}00215} + \frac{0{,}85}{0{,}0029} + \frac{1}{0{,}00324} + \frac{0{,}85}{0{,}00375} + \frac{0{,}5}{0{,}00425}\right)x_{12}$$
$$+ \left(\frac{0.5}{0{,}00591} + \frac{0{,}85}{0{,}00592} + \frac{1}{0{,}00593} + \frac{0{,}85}{0{,}00594} + \frac{0{,}5}{0{,}00595}\right)x_{22} + \left(\frac{0.5}{0{,}0002} + \frac{0{,}85}{0{,}0005} + \frac{1}{0{,}0007} + \frac{0{,}85}{0{,}00095} + \frac{0{,}5}{0{,}0013}\right)x_{32}$$

$$+\left(\frac{0.5}{0,03125}+\frac{0,85}{0,04333}+\frac{1}{0,05333}+\frac{0,85}{0,06333}+\frac{0,5}{0,07333}\right)x_{42}+\left(\frac{0.5}{0,0004}+\frac{0,85}{0,0005}+\frac{1}{0,0006}+\frac{0,85}{0,0007}+\frac{0,5}{0,0008}\right)x_{52}$$
$$+\left(\frac{0.5}{0,00033}+\frac{0,85}{0,00034}+\frac{1}{0,0004}+\frac{0,85}{0,0005}+\frac{0,5}{0,00006}\right)x_{12}^2+\left(\frac{0.5}{0,00215}+\frac{0,85}{0,00217}+\frac{1}{0,00219}+\frac{0,85}{0,00221}+\frac{0,5}{0,00247}\right)x_{22}^2$$
$$+\left(\frac{0.5}{0,0012}+\frac{0,85}{0,0018}+\frac{1}{0,0023}+\frac{0,85}{0,0028}+\frac{0,5}{0,0033}\right)x_{32}^2-\left(\frac{0.5}{0,01675}+\frac{0,85}{0,01727}+\frac{1}{0,01777}+\frac{0,85}{0,01787}+\frac{0,5}{0,01798}\right)x_{42}^2$$
$$+\left(\frac{0.5}{0,000008}+\frac{0,85}{0,00001}+\frac{1}{0,00002}+\frac{0,85}{0,00003}+\frac{0,5}{0,00005}\right)x_{52}^2-\left(\frac{0.5}{0,0003}+\frac{0,85}{0,00035}+\frac{1}{0,0004}+\frac{0,85}{0,00045}+\frac{0,5}{0,0005}\right)x_{12}x_{22}$$
$$+\left(\frac{0.5}{0,00024}+\frac{0,85}{0,0003}+\frac{1}{0,00033}+\frac{0,85}{0,0004}+\frac{0,5}{0,00047}\right)x_{12}x_{32}-\left(\frac{0.5}{0,0068}+\frac{0,85}{0,007}+\frac{1}{0,0072}+\frac{0,85}{0,0075}+\frac{0,5}{0,0077}\right)x_{12}x_{42}$$
$$+\left(\frac{0.5}{0,00012}+\frac{0,85}{0,00019}+\frac{1}{0,00027}+\frac{0,85}{0,00035}+\frac{0,5}{0,00043}\right)x_{22}x_{42}-\left(\frac{0.5}{0,0083}+\frac{0,85}{0,009}+\frac{1}{0,0098}+\frac{0,85}{0,01}+\frac{0,5}{0,015}\right)x_{22}x_{42}$$
$$+\left(\frac{0.5}{0,005}+\frac{0,85}{0,006}+\frac{1}{0,007}+\frac{0,85}{0,008}+\frac{0,5}{0,009}\right)x_{22}x_{52}-\left(\frac{0.5}{0,0001}+\frac{0,85}{0,00015}+\frac{1}{0,00012}+\frac{0,85}{0,00015}+\frac{0,5}{0,00018}\right)x_{32}x_{52}$$

Similarly, for each α level, other qualitative indicators of hydrogenate are determined, i.e. its sulfur content ($\tilde{y}_3$) and water-soluble acids and alkalis ($\tilde{y}_4$). Then, the identified values of the coefficients $a_{ij}^{\alpha_q}, i=\overline{0,5};\ j=\overline{2,4};\ q=\overline{1,3}$ in fuzzy models, using the following expression of theories of fuzzy sets, are combined into a single value [17]:

$$a_{ij} = \bigvee_{\alpha\in[0.5,1]} a_{ij}^{\alpha_q} \text{ или } \mu\tilde{a}_{ij}(a_{ij}) = SUP \min_{\alpha\in[0.5,1]}\{\alpha, \mu a_{ij}^{\alpha}(a_{ij})\}, \text{ где } a_{ij}^{\alpha_q} = \{a_i \mid \mu\tilde{a}_{ij}(a_{ij})\}$$

As a result of the research and processing of the data, it was determined that to find the volume of output from the reactor R-1, i.e. volume of hydrogenate y_1 on the basis of experimental statistical data, it is possible to construct a statistical model, which using the nonlinear regression equation allows us to estimate the values y_1 (m^3/h) from the input and operating parameters $x_i, i=\overline{1,5}$. After identifying the structure and parameters of this model, based on the sequential switching of regressors and least squares methods, the mathematical model that allows to determine the volume of hydrogenate from the output of the R-1 reactor has the form:

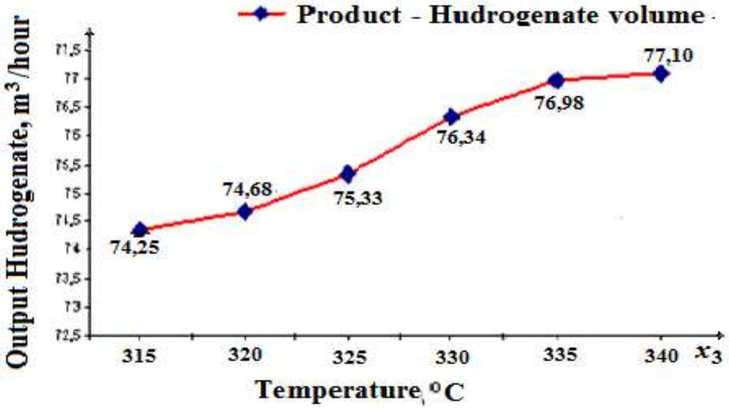
$$y_1 = f_1(x_{11},x_{21},...,x_{51}) = 7,00+0,233x_{11}+0,130x_{21}+0,011x_{31}+2,333x_{41}-0,0175x_{51}+0,0031x_{11}^2+0,0048x_{21}^2$$
$$+0,00003x_{31}^2+0,7778x_{41}^2-0,00004x_{51}^2+0,0017x_{11}x_{21}+0,0015x_{11}x_{31}+0,003111x_{11}x_{41}-0,00023x_{11}x_{51}$$
$$+0,08642\,x_{21}x_{41}-0,00065\,x_{21}x_{51}+0,00730\,x_{31}x_{41}$$

In the above models, input, operating parameters x_{ij} that do not have or have very little effect on y_1, y_2 are zeroed, i.e. not shown.

A graph of the temperature dependence of the yield of hydrogenate in the reactor at fixed values of the input of raw materials x_1 and other operating parameters: параметров: x_2, x_4 and x_5. (figure 1)

By means of modelling, studies are carried out of the influence of other input, operating parameters and their simultaneous influence on y_1, $\tilde{y}_2$, $\tilde{y}_3$ and $\tilde{y}_4$.

To determine the optimal temperature of the hydrotreating process based on expert information and the logical rule of conditional conclusions and the rule base, a linguistic model is constructed. The resulting linguistic model implements the logical dependence "If the raw material is *heavy*, then the process temperature is *low*, otherwise if the raw material is *light*, then the process temperature is *high*."



x_1 = 80 m^3/h – input of raw material; x_2 = 30 kg/cm^2 – pressure in R-1 reactor; x_4 = 3 h^{-1} – volumetric raw feed rate; x_5 = 400 nm^3 – hydrogen containing gas circulation.

Figure 1. Graph of dependence of $y_1 = f_1(x_3)$ at fixed x_1, x_2, x_4 and x_5.

Based on expert judgment and using the methods of theories of fuzzy sets in the form of an exponential dependence, membership functions are constructed that describe the fuzzy parameters of the linguistic model: $\mu_A(ts) = e^{(|(ts-185)^{0.5}|)}$ - heavy raw materials (low thermal stability); $\mu_A(ls) = e^{(|(ls-165)^{0.5}|)}$ - light raw materials; $\mu_B(nt) = e^{(|(nt-300)^{0.5}|)}$ - low temperature; $\mu_B(vt) = e^{(|(vt-400)^{0.5}|)}$ - heat.

Thus, the structure of a linguistic model that evaluates the optimal temperature, depending on the quality of the raw materials: $If\ \tilde{x}_1 \in \ddot{A}_1 \wedge \tilde{x}_2 \in \ddot{A}_2 \wedge ... \wedge \tilde{x}_n \in \ddot{A}_n,\ \ Then\ \ \tilde{y}_j \in \tilde{B}_j,\ j = \overline{1,m}$ is defined using logical rules of conditional output: $If\ \tilde{x} \in \tilde{A}(ts)\ Then\ \tilde{y} \in \tilde{B}(nt),\ else\ If\ \tilde{x} \in \tilde{A}(ls),\ Then\ \tilde{y} \in \tilde{B}(vt)$

The following notation is introduced in the obtained linguistic model: *ts, ls, nt, vt* - respectively, “heavy raw materials”; “Light raw materials”; “Low temperature” and “high temperature”; $\tilde{x}$, $\tilde{y}$, the input and output linguistic variables, that describe the quality of the raw materials and the optimal temperature of the hydrotreatment process; $\tilde{A}$, $\tilde{B}$ - fuzzy subsets describing $\tilde{x}$ and $\tilde{y}$.

4. Discussion of results

The approach to the development of mathematical models based on available information of various types proposed in the work allows us to develop models of real technological objects in conditions of deficiency and fuzziness of the initial information. The structure of the constructed models of the R-1 reforming reactor is identified in the form of nonlinear regression equations. In the conditions of fuzziness of both input and output parameters, i.e. when the input and output of a hydrotreating reactor are described by linguistic variables, it is proposed to build linguistic models based on logical rules of a conditional type. This approach is implemented when constructing a linguistic model that describes the dependence of the optimal temperature of the hydrotreatment process on the quality indicators of the feedstock.

5. Conclusion

Mathematical models of the R-1 hydrotreating reactor have been developed and presented in conditions of a lack of initial information. To solve the problems of lack of initial information and model development, it is proposed to use available information of various nature using the hybrid method of model development. The mathematical models of the hydrotreating reactor are based on experimental statistical data and fuzzy information from expert experts. The model for determining the volume of product from the outlet of the reactor is identified in the form of statistical models of the regression type, and the models that evaluate the fuzzy described quality indicators of the product being produced are identified as fuzzy equations. A graph of the dependence of the yield of hydrogenate on the temperature in the reactor at fixed values of the remaining operating parameters. Using the linguistic rules of conditional inference, a linguistic model has been constructed that allows us to describe the dependence of the optimum temperature on the quality of the feedstock.

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