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# Frame-Production Model of Petroleum Feedstocks Catalytic Processing for the Representation of Knowledge about Process

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**Abstract**

Hydrocarbons secondary refining processes are potentially dangerous, so you need to provide the operator with timely information about the emer-gency situations on the installation in the early stages of their development, and also to get recommendations to correct the technological mode to eliminate these emergency situations. To identify an abnormal situation and identify the cause of it, it is necessary to have a frame-production diagnostic model , which functionally connects the cause with the diagnostic indications that characterize the abnormal situation. If such a situation occurs, the mathematical mode determines the quantitative indicators of the technological regime (temperature, pressure , flow rate) to eliminate deviations from the normal operation of the industrial plant.

***Keywords***: *Catalytic reforming; Octane number; Method of mathematical modeling, Frame.*

## 1. Introduction

Catalytic processes of hydrocarbon feedstocks processing refer to secondary processes of oil refining, i.e. to processes in which oil undergoes chemical changes of the compounds entering it. In the process of catalytic cracking and reforming of hydrocarbon raw materials, gas, gasoline, and diesel fuel are obtained. The main parameters of these processes include temperature, pressure, feedstock l consumption and gas consumption, which affect the formation of a by - product-coke in the reactors. With an increase in temperature and a decrease in flow rate (the contact time increases), higher yields of target and side products are achieved [1-3].

Hydrocarbons secondary refining processes are potentially dangerous, so you need to provide the operator with timely information about the emergency situations on the installation in the early stages of their development, and also to get recommendations to correct the technological mode to eliminate these emergency situations [4].

## 2. Catalytic naphtha reforming

Catalytic naphtha reforming is widely practiced in refineries and in the petrochemical industry to convert low-octane naphtha into high-octane gasoline. In addition, this process is an important source of hydrogen and aromatic substances obtained as by-products. Bifunctional Pt catalysts used in reforming are deactivated by coking during its commercial operation. This leads to a decrease in the yield and octane number. Modeling of the process, taking into account the deactivation of the catalyst and the complex multicomponent composition of the hydrocarbon mixture, allows us to establish quantitative regularities of the transformation of raw materials into a product (Fig.1) [5-8].

In the catalytic reforming process of naphtha coke formation is the most important cause of the catalyst deactivation. Coke is deposited over both metal and acid sites. Even though a large number of scientific papers have been devoted to the study of catalyst coking still this phenomenon remains one of the topical issues [9-10].

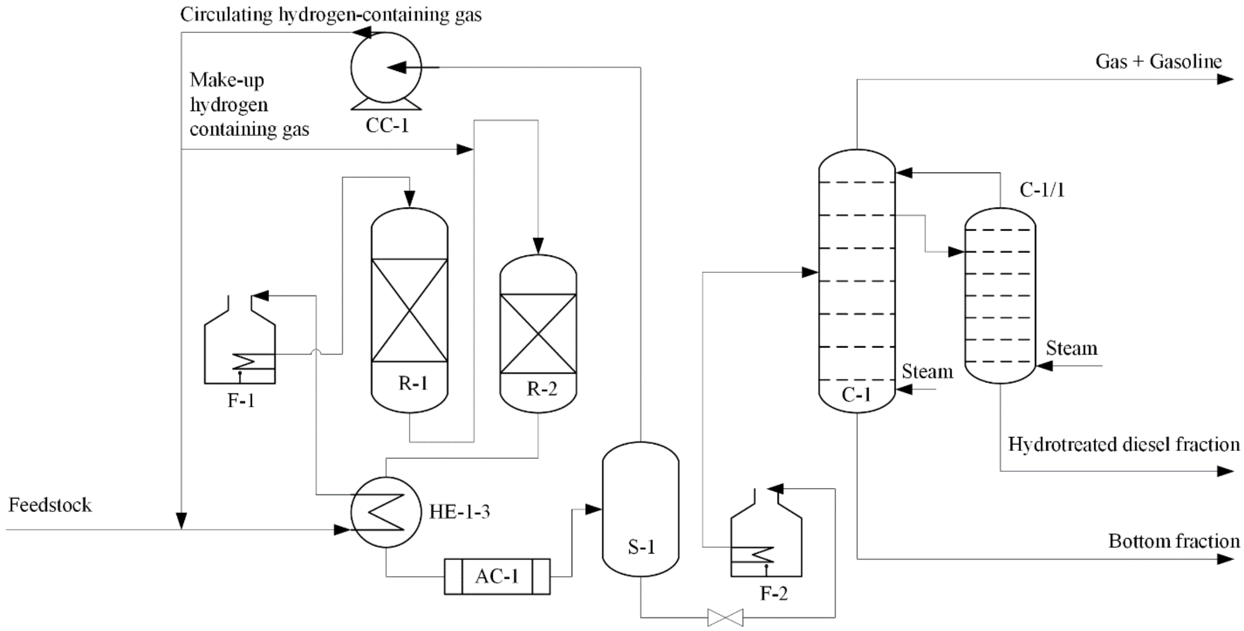


Figure 1. Process flow diagram of a combined unit for the production of low-sulfur diesel fuel with improved cold flow properties

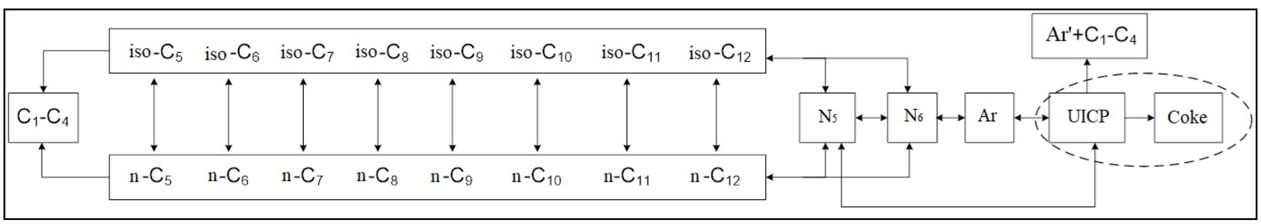


Figure 2. Formalized reaction scheme of naphtha reforming: n-Cn, iso-Cn – normal and iso-alkanes; N-5, N-6 – methylcyclopentane and methylcyclohexanes; Ar – aromatic hydrocarbons; UICP – unsaturated immediate compacting products

Thus, the mathematical model of semi regenerative catalytic reforming of naphtha is presented by a system of equations of material and heat balances:

$$\begin{cases} G_c \dfrac{\partial C_i}{\partial Z} + G_c \dfrac{\partial C_i}{\partial V} = \sum\limits_j k_j \cdot C_i \cdot \eta_j \\ G_c \dfrac{\partial T}{\partial Z} + G_c \dfrac{\partial T}{\partial V} = \dfrac{1}{\rho \cdot C_p^{mix}} \sum\limits_j \Delta H \cdot k_j \cdot C_i \cdot \eta_j \end{cases}$$

The conditions are: at Z=0, $T=T_{en}$, $C_i=C_i$ (at the reactor entrance), at V=0, $T=T_{en}$, $C_i=C_i$ (at the reactor entrance). *Z* is a volume of raw material processed from the moment when the fresh catalyst (new catalyst, no regenerations were done) was loaded, m$^3$; *V* is a catalyst volume in the reactors, m$^3$; *G* is a raw material flow rate, m$^3$/h; *i* is a component's number in a mixture; *j* is a reaction's number due to formalized scheme accepted; $C_i$ is a concentration of i$^{th}$ component, mol/m$^3$; $k_j$ is j$^{th}$ reaction constant; $C_p^{mix}$ is the heat capacity of mixture, J/(kg·K); $\Delta H$ is j$^{th}$ reaction heat, J/mol; ρ is a density, kg/m$^3$; *T* is temperature, K.

## 3. Diagnosis of the causes of emergency situations

To identify an abnormal situation and identify the cause of it, it is necessary to have a frame-production diagnostic model , which functionally connects the cause with the diagnostic indications that characterize the abnormal situation. Let us consider a combined frame-production model based on expert information about the catalytic reforming of gasoline process. The model is a two-level structure with a network of root frames **$FrR_i$** (deviations) at the top level that child frames or slots are associated with **$FrS_j$**, each of which describes the j-th situation. These abnormal situations are created by various types of violations that may occur during the operation of an industrial plant, as well as changes in the chemical composition of raw materials (the operating mode of the rectification column, the presence of impurities of sulfur and nitrogen-containing compounds, heavy metals) [11-13].

Deviation → Diagnosis → Recommendation

The Knowledge Base allows you to collect, accumulate and process information about the functioning of the production process and possible unnormal situations. These are the results of generalizing the work of the devices of an industrial installation or the entire production as a whole. The size of the knowledge base determines the range of tasks to be solved, as well as the duration of information collection and analysis.

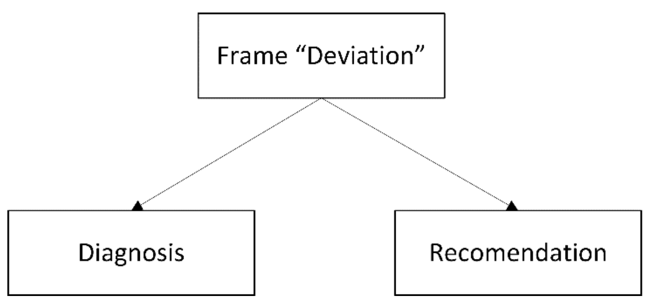


Figure 3.Frame «Deviation»

To use knowledge, it is necessary to formalize and organize all knowledge into a certain system in order to use this knowledge. The choice of a model from among the possible ones is completely determined by the specifics of a particular task. The frame (Fig.3) contains a list of deviations from the regime of the process of catalytic reforming of gasoline and recommendations for their elimination. For example, if < decrease in ON, then <change in hydrocarbon composition> and <increase in temperature>.

In this frame, the list of deviations from the mode of the process of catalytic reforming of gasoline implies a list of appropriate recommendations for their elimination. For example, if < decrease ON>, then <change in hydrocarbon composition> and <increase in temperature>.

Knowledge representation models are always associated with mathematical models. In this example, a mathematical model of the process of processing hydrocarbon raw materials will allow us to quantify how much to raise the temperature. But on the mathematical model in this example, it is impossible to calculate the reason for the rejection and issue a recommendation. In the Frame-production model, in general, the left part is always a rule, and the right part is always an action. Frame-production models are often used in control systems. These models allow you to diagnose deviations and select a specific sequence of actions. The conditions in the production model are associated with each other by certain logical signs. For example, if < concentration of substance A <30%> or <concentration of substance B>10%>, then <operating mode of the unit in the temperature range T1<T<T2>. In this example, depending on the composition of the processed raw materials, the temperature range in the operation of the plant is planned. The numerical values of the temperature T can only be determined on a mathematical model. That is, the combination of mathematical and production models allows us to determine the range of temperature changes at a certain point in time, depending on the composition of raw materials.

A set of rules, facts, and conclusions is formed on the basis of experiments in the operation of industrial installations in an empirical way. These rules must be carefully checked and confirmed in the operation of several industrial plants that operate under different technological conditions and process different raw materials. Then the frame structure at each stage of production can be presented in the following general form.

Fr = f(name, list of attributes that are used to diagnose abnormal situations, list of recommendations).



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To systematize knowledge about the process of catalytic refining of gasoline on the basis of the kinetic and technological laws of the process, the features of its industrial design and purpose, a multi-level hierarchical structure is revealed. The vertical connections of this structure are the basis for considering a typical oil refining process. The upper level of relations characterizes the purpose of the process and is the basic one for further description.

The industrial implementation of catalytic processes is not uniform. On the basis of standard processes, installations that differ in purpose, power, and hardware design function. Depending on the type of installation, the requirements for raw materials are imposed, and the regulatory values of the technological parameters are set. In fact, the second level of relations determines the restriction on changing the technological parameters of the process and the requirements for the fractional composition of raw materials. A fragment of the Knowledge Base of this level of knowledge for the catalytic reforming of gasoline, which combines the regulatory values for input temperatures, system pressure, catalyst loading, volume consumption of raw materials and gas circulation, is designed as an information table containing arrays of boundary values of parameters for typical installations (Table 1).

Table 1. Structured process knowledge

| Process | Catalytic reforming of gasoline | |
|---|---|---|
| Process assignment | Production of gasoline | Production of aromatic carbohydrates |
| Industrial units types | L-35-11/1000<br>LH-35-11/1000<br>L-35-11/600<br>LH-35-11/600<br>L-35-11/300<br>L-35-11/1000 and blocks of LK-6U | LG-35-8/300B<br>L-35-8/300B<br>KPA/300B<br>LH-35-11/600 |
| The feedstock characteristics | Fractional composition and density<br>Hydrocarbon composition | |
| The catalyst activity | Regenerations dates. Coke on the catalyst. The ratio of acid and metal centers on the sur-face of the catalyst | |
| Conditions for processing feedstock | Temperature<br>Pressure<br>Feedstock flow rate<br>Gas circulation | |
| Target products | Gasoline 92, 95,98 | Benzene, Toluene, Xylenes |

To diagnose the causes of deviations in the operation of an industrial units, key concepts are created, on the basis of which a Knowledge Base is formed (Table 2). For example, the hydrocarbon composition of feedstock determines the quality of the product and makes certain requirements for the conditions of its processing. Knowledge about the influence of fractional and hydrocarbon composition on the course of the technological process is allocated to a separate level. This level combines information about the fractional composition and density, the distribution of hydrocarbons by groups, and the content of key components in the feedstock. The components of the level are closely related to each other and describe a single whole, but can be used both in offline mode and in refinement mode. The forecast of technological regimes and schemes of processing of feedstock is based on the knowledge combined at this level. Thus, for the process of catalytic reforming of gasoline, the following concepts can be distinguished about the influence of the fractional composition of the fuel [10]:

1) The presence of light fractions in the feedstock boiling below 85°C (using a fraction of 62-180°C):

a) Determines the production of low-octane gasoline and low product yield due to gas formation;

b) To increase the depth of processing of light feedstock , it is recommended to increase the temperature at the entrance to the reactors with an increase circulation of gas circulation and a decrease in the volumetric feed rate of feedstock.

2) The weighting of feedstock contributes to:

a) Increase in the octane number of the reformate;
b) Increase in the yield of the reformate;
c) Increase of coke formation and deactivation of the catalyst.

Table 2. Fragment of the Knowledge Base for the process of catalytic reforming of gasoline

| Deviations | Signs of the cause of deviations | Recommendations |
|---|---|---|
| The octane number of the reformate decreased | The content of naphthenic hydrocarbons in the product has increased | Check the raw material heat exchangers for tightness |
| | The temperature at the entrance to any reactor has dropped by more than 5C | Check the fuel gas pressure |
| | The sulfur content in the hydrogenate is higher than normal-deactivation of the catalyst due to selective sulfur etching | Check the operating mode of the hydrotreating unit<br>Increase the frequency of gas circulation<br>Reduce the volume feed rate of feedstock<br>Calculate the optimal amount of dichloroethane on the model |
| | The value of the boiling point of the raw material fraction increased - deactivation of the catalyst due to coking | Raise the temperature of the entrance to the 1st and 2nd reactor<br>Reduce the volume feed rate of feedstock |
| | The $H_2$ content in gas circulation increased – the acidity of the catalyst was decreased | Include organochlorine additives in the feedstock<br>Reduce the supply of water vapor to the reactors |
| | The service life of the catalyst exceeds 3/4 of the run - deactivation of the catalyst | Raise the temperature of the entrance to the 1st and 2nd reactor<br>Reduce the volume feed rate of raw materials |
| | There were sharp temperature jumps-deactivation of the catalyst due to coking | Raise the temperature of the entrance to the 1st and 2nd reactor<br>Reduce the volume feed rate of raw materials |
| The reformate yield decreased | The value of the boiling point of hydrocarbons in the fractional composition of raw materials has increased - change in the quality of footstock | Optimization of the operating parameters of the plant on a mathematical model, taking into account changes in the quality of feedstock |
| | The content of $Cl_2$ in the catalyst exceeds 0.9% by weight - change in the acidity of the catalyst | Stop the supply of organochlorine compounds to the raw material, increase the water vapor content in the system |
| | The pressure in the system increased by more than atm | To reduce gas circulation |
| | The temperature at the entrance to the third reactor increased by more than 5°C | Lower the temperature at the entrance to the 3rd reactor |
| | The H2 content in the circulating gas is below normal (less than 70% vol.)- change in the acidity of the catalyst | Stop the supply of organochlorine compounds to the raw material, increase the water vapor content in the system |

## 4. Frame for diagnosing the causes of deviations in the operation of industrial units for catalytic reforming of gasoline

The procedure for making decisions consists in sequentially considering the situations that lead to a particular deviation, selecting the most significant sign of the reasons for the deviation in the dialog mode, and then using the rules laid down in the knowledge base, getting recommendations for their elimination. At the same time, the set of rules is formed on the basis of the experience of operating industrial units an empirical way. These rules, called heuristics, must be thoroughly tested and validated when running multiple industrial installations. Quantitative recommendations of changes in technological parameters can be calculated using a mathematical model of the process of catalytic reforming of gasoline.



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The considered situation will be a fragment of the knowledge base of catalytic reforming of gasoline. In this case, "reduction of octane number of reformate" will be introduced into the slot of the frame "deviations", "Number of paraffin hydrocarbons i feedstock has increased" in the slot frame "Diagnosis", "Changing technological conditions of the process" in the slot "Recommendations". The entire set of identified situations is systematized in accordance with the probability of occurrence of a particular cause in the order of consideration of deviations, the contents of the selected frames are presented in Table 2.

## 5. Conclusion

Thus, frame-production model of petroleum feedstocks catalytic processing can be used as a computer simulator for training technical personnel in the regularities of the research process aimed at: improving the knowledge, skills and competencies of personnel in order to increase the degree of readiness of the personnel of technological installations and working out actions when detecting malfunctions and emergency situations. If such a situation occurs, the mathematical model (2) determines the quantitative indicators of the technological mode(temperature, pressure , flow rate) to eliminate deviations from the normal operation of the industrial plant.

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