Strategy of transition to advanced digital intellectual production technologies of catalytic processes of transformation of hydrocarbon raw materials

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***Abstract*—in the gasoline preparation process, various products are used, such as catalytic reforming, isomerization, hydrocracking, hydrodewaxing, catalytic cracking, liquid-phase catalytic alkylation processes, as well as additives such as gasoline. As a result of the catalytic activity of a bifunctional catalyst in isomerization and aromatization reactions. The yield of liquid products (C_{5+}), the composition of the reformate and the octane number can be adjusted by optimizing the independent variables (temperature, pressure, consumption of raw materials) or by adding different promoters to the reaction catalytic zone (water, chlorine). Optimization of this process is a very complex multi-stage technology for processing hydrocarbon feedstock into high-octane components, and increasing its efficiency reduces the cost of the product.**

Keywords—mathematical modelling, oil refining, thermodynamics, kinetics

I. INTRODUCTION (*HEADING 1*)

Research in the field of catalytic processes, the study of the mechanism and kinetic laws of the catalytic reactions in industrial conditions with the involvement of a complex of modern research methods, both experimental and mathematical modeling methods, the creation of computer systems for processing large amounts of data is a priority. The main feature of these studies is their interdisciplinarity at the intersection of chemistry, physics, mathematics and computer science.

In the field of catalytic processes of hydrocarbon processing, the integration of Sciences is associated with the transition to system analysis and problem solving using intellectual computer systems as complex systems that combine databases and knowledge bases, as well as program codes built on the basis of predictive models.

In the report the results of creation of import-substituting system of technological modeling of processes and devices of technologies of oil processing in motor fuels and biodegradable surfactants are considered. "Russian Hysys" will include mathematical models of the main processes of processing of hydrocarbon raw materials, built on the basis of physical and chemical laws of transformation of individual components, as well as taking into account the unsteadiness of industrial processes caused by the dynamic change in the hydrocarbon composition of the processed raw materials, as well as the deactivation of the catalytic systems used.

The application of the proposed integrated modeling system allows to increase the resource efficiency of industrial production, as well as to solve the problem of supply of quality marketable products. The methodological basis for the development of fundamental mathematical models of processes of processing of petroleum raw materials created for interrelated processes – catalytic cracking,reforming,alkylation,isomerization – the most important stages of production of components of high-octane gasoline and diesel fuel, as well as for the production of synthetic detergents – biodegradable alkylbenzosulfonates (LABS).

The fundamental bases of creation of resource-efficient technology of production of high-energy low-density hydrocarbon fuels with the use of mathematical models, based on the chemical interaction of reagents at the production stage and at the compounding stage, taking into account changes in the composition of the processed raw materials and the activity of the catalyst in the processes of reforming, isomerization, alkylation and catalytic cracking, as well as the intensity of intermolecular interactions of components in the compounding process. Mathematical models make it possible to quickly and accurately predict the hydrocarbon composition of the mixing flows and determine the optimal ratio of components that ensure the production of hydrocarbon fuels that meet all modern requirements with a minimum margin for quality.

In the existing technologies of preparation of motor fuels (gasoline and diesel fuels) there is no account of the chemical interaction between the individual components of the mixture (hydrocarbon flows, anti-knock additives, oxygenates, etc.), which leads to a divergence of important indicators (octane numbers, pour point, etc.), calculated and experimental. The principal consequence of this is the deterioration of the quality of products – commercial

gasoline, diesel fuel and a decrease in economic indicators due to the cost overruns of expensive components used in the preparation. With large volumes of production of commodity products, economic indicators reach a significant value.

The solution of this multifactorial problem is possible using the method of mathematical modeling on the physico-chemical basis, i.e. taking into account the thermodynamics and kinetics of hydrocarbon transformations on the surface of the catalyst, as well as the unsteadiness of the processes due to coking, aging and poisoning by harmful impurities of the catalyst, changes in the chemical composition of the processed raw materials.

Multistage processes of preparation of motor fuels proceed according to the following scheme (Fig. 1).

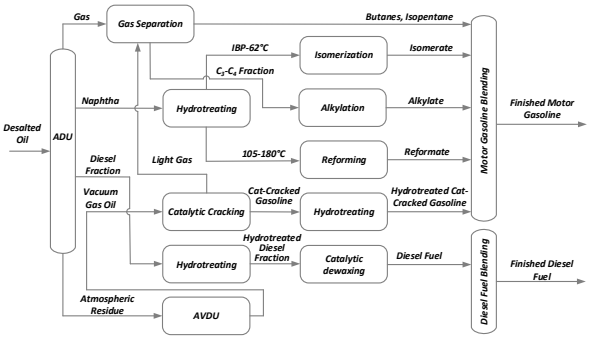

Fig.1 Diagram of the process of preparation of motor fuels

The mathematical description of the processes of catalytic reforming and isomerization of straight-run gasoline fractions, as well as catalytic dewaxing of medium distillates is made in the form of a system of differential equations of material and thermal balance and is described in detail in the following works[1, 3].

$$\begin{cases} G \cdot \dfrac{\partial C_i}{\partial z} + G \cdot \dfrac{\partial C_i}{\partial V} = \sum_{j=1}^{m} a_j \cdot r_j \\ G \cdot \dfrac{\partial T}{\partial z} + G \cdot \dfrac{\partial T}{\partial V} = \dfrac{1}{\rho \cdot C_p^m} \cdot \sum_{j=1}^{m} Q_j \cdot a_j \cdot r_j \end{cases} \quad (1)$$

initial conditions: $z = 0$, $C_i = C_{i0}$, $T = T_{en}$

$$V = 0, T = T_{en}, C_i = C_{i0}$$

where G is the volume flow rate of raw materials, m^3/h; z = G*t (t catalyst operating time since loading into the reactor, h); Ci is the concentration of the i-th component, mol/m^3; V - volume of catalyst, m^3; a is the catalyst activity, ρ is the density of the hydrocarbon mixture, kg/m^3; Cmp hydrocarbon mixture heat capacity, j/(kg*K); Q_j is the heat effect of the j-th reaction, j/mol, T is the temperature, K; r_j - rate of j-th reaction, $mol/(m^3 h)$.

Mathematical modeling of the processes of production of commercial petroleum products (gasoline, diesel and boiler fuels) [4-6] should be made on the basis of models of individual flows from reforming plants, isomerization, alkylation, dewaxing, catalytic cracking, hydrocracking, which changes the quantitative and qualitative parameters of the processes. In this case, the procedure of mixing several products from common components is implemented. To establish a connection between the quality of the resulting mixture and the quantitative and qualitative characteristics of the mixing components, it is necessary to solve the problem of multi-criteria optimization.

The optimization process has to deal with many conflicting product release requirements. The values of some indicators need to be increased while others need to be reduced. The problem is compounded by the fact that these indicators are not independent. They are interrelated, interdependent and the increase in some indicators leads to a decrease in others. The search for the optimal solution is associated with finding a reasonable compromise in the conditions of conflicting demands. For this purpose, compromise schemes based on the principle of uniformity are used. In this case, the solution is the result of a uniform increase in the quality of the optimized object for all private standardized criteria. This principle is of three kinds: the equality-normalized partial criteria, quasirent and fair concession. A compromise is considered fair, in which the total level of decline in some indicators does not exceed the total level of increase in other indicators. Let in descending order of their importance or significance. Let each of them be minimized. For compounding flows from installations, both primary and secondary oil refining are directed. In the General case, the most significant components are reformate, gasoline to catcracking, alkylate, isomerizate and MTBE. Depending on the production capacity of the units, 92, 95 and 98 gasoline are produced. The optimization algorithm consists of two main blocks: a block for calculating the detonation resistance of both individual flows and their mixtures with additives and additives, and a block for calculating the optimal ratio of components to achieve a given value of the octane number of gasoline based on Pareto optimization.

From the economic point of view, the optimal mixing scheme meets the following conditions:

1. Maximum utilization of resources;

2. Maximum use of the reformed, because the reforming unit are at the same time production capacity for hydrogen, which is necessary in the process of Hydrotreating as gasoline and diesel fractions.

TABLE I. PARTICULAR COMPONENTS OF THE EFFICIENCY CRITERION

Criterion	Name	Value
ψ_1	Yield of gasoline, t	max
ψ_2	Flow rate of the reformate, t	max
ψ_3	Benzene content, %	1 max
ψ_4	Sulphur, ppm	10 max
ψ_5	RON	80, 92, 95, 98
ψ_6	Aromatic hydrocarbon, %	35 max
ψ_7	Olefins, %	17 max
ψ_8	SSP, KPa	50-100

Thus, the optimized parameters $\vec{X}$ are the flow rates for compounding. According to the requirements of gasoline at the same time must meet the following particular components of the criterion. The space of criteria is represented by a vector $\vec{\Psi}(\vec{X})$, each private component of which is represented by the yield of gasoline or its quality.

By changing the optimized parameters represented by the components of the vector $\vec{X}$, we will change the values of all particular criteria. The purpose of multi-criteria optimization is to determine such values X_1, X_2, …, X_n, that provide the required values Ψ_1, Ψ_2, ..., Ψ_8 . Private criteria contradict each other, so the solution must be a compromise. To find a compromise solution, we introduce the concept of ideal value for all particular components of Ψ_i. Then the criterion of efficiency will be written as follows:

$$\vec{\psi} = \left(1 - \frac{\psi_i}{\psi_{i,\ идеал.}}\right)^2 \rightarrow \min \qquad (2)$$

Since the requirements of the standards impose restrictions on the content of individual components in gasoline of different brands, such as benzene, the amount of aromatic or olefin hydrocarbons. Then determination of the General Pareto optimality criterion for the compounding process:

$$\psi = (1 - \frac{\psi_1}{\psi_{1,идеал.}})^2 + (1 - \frac{\psi_2}{\psi_{2,идеал.}})^2 + (1 - \frac{\psi_3}{\psi_{3,идеал.}})^2 + (1 - \frac{\psi_4}{\psi_{4,идеал.}})^2 + \\ + (1 - \frac{\psi_5}{\psi_{5,идеал.}})^2 + (1 - \frac{\psi_6}{\psi_{6,идеал.}})^2 + (1 - \frac{\psi_7}{\psi_{7,идеал.}})^2 + (1 - \frac{\psi_8}{\psi_{8,идеал.}})^2 \qquad (3)$$

where Ψ_1 - yield of gasoline, t; Ψ_2 – the flow rate of the reformate, t; Ψ_3 – benzene,%; Ψ_4 - sulfur, ppm; Ψ_5 - RON; Ψ_6 - aromatic hydrocarbons, %; Ψ_7 – olefins, %; Ψ_8– SSP, KPa.

Development of the formulation is carried out taking into account the involvement of the maximum amount of the cheapest and most used basic component of gasoline – reformate and the minimum involvement of the most expensive components – alkylbenzenes and oxygenates. Thus, an approach to optimizing the compounding process based on a comparison of planned and actual mixing formulations is proposed. The main recommendations are to increase the octane number of the product, reduce the excess supply of octane number and expensive fuel components.

According to the developed technology, on-line reading of a large array of data of the technological mode of operation of the units for obtaining components of motor fuels – reforming, isomerization, alkylation, catalytic cracking, dewaxing, etc. will be carried out and the calculation of the optimal operating modes of industrial devices depending on the composition of the processed raw materials and the activity of the catalysts used. The results of the calculations will be transmitted as initial data from the system of modeling the process of mixing hydrocarbon flows to determine the optimal fuel compositions of the components of high-octane gasoline and diesel fuels, which are determined by the composition and intensity of the chemical interaction of the components of hydrocarbon mixtures. On the basis of the developed mathematical models, an intelligent system for the management, optimization and forecasting of industrial plants for processing oil into high-octane gasoline, diesel fuel and LABS was created.

Improving the efficiency of the use of raw materials in the process of preparing commercial gasolines is possible through the development and use of an intelligent computer system that improves the quality of products by optimizing the mixing flow rates, including in accordance with the requirements of the Technical Regulations and environmental friendliness of production.

The main goal of optimizing the process of scheduling the preparation of motor fuels is to predict the optimal volumes and formulas for mixing components to obtain gasoline of the required quality, taking into account changes in the composition of the feedstock and the activity of reforming catalysts, isomerization, alkylation and catalytic cracking.

For the purpose of forecasting the scheduling process, an integrated computer-aided modeling system for the preparation of commercial gasolines from products of gasoline reforming, isomerization, alkylation and catalytic cracking processes is being developed, which is suitable for predicting the performance of industrial installations. The developed system should be able to respond quickly to the following changes:

- the composition of the raw material at the entrance to the catalytic reactors;

- technological mode;

- catalyst activity.

The system should take into account the non-additive mixing of hydrocarbon streams with the issuance of recommendations for adjusting the gasoline preparation recipe for optimal consumption of components.

The prediction of the optimal mixing formulas was carried out when compounding the flows, taking into account changes in the hydrocarbon composition of the processed raw materials in the reforming and isomerization processes and the activity of catalysts to solve the problem of octane conversion.

Predicted calculations of the performance properties of domestic and imported catalysts for the processes of reforming and isomerization were made, with recommendations for improving the resource efficiency of their work.

Reformats differ in aromatics and benzene, and also have different RON. The properties of the used reformates are presented in table 2.

TABLE II. THE PROPERTIES OF REFORMATES

Parameter	Fixed bed of catalyst		Moving bed of catalyst	
	Reformate 1	Reformate 2	Reformate 1	Reformate 2
RON	94.80	95.80	103.60	106.40
Benzene content,wt. %	2.09	3.26	2.30	2.10
Aromatics content, wt. %	60.86	59.77	79.51	81.81

Predictive calculation of the optimal recipes for mixing gasoline brands Regular 92, Premium 95 and Super 98 was carried out for a given amount of gasoline (table 3), based on the specified daily performance of the plants (table 4).

TABLE III. SPECIFIED GASOLINE YIELD

Flow	Tonne
Regular 92	9016
Premium 95	4260
Super 98	349

TABLE IV. AVERAGE DAILY INSTALLATION CAPACITY

Flow	Tonne
Catalytic cracking gasoline	2034
Hydrotreated catalytic cracking gasoline	3773
Reformate (moving catalyst bed)	2820
Reformate (fixed catalyst bed)	969
Alkylate	1027
Isomerate	960
Isopentane	1200
MTBE	150
Straight-run gasoline	333
Toluene	210

When calculating the optimal mixing recipes, the following tasks were solved:

1) obtaining gasoline of a given quality;

2) the production of the maximum amount of gasoline of each brand.

The quality indicators of the calculated gasoline, depending on the properties of the reformate are presented in table 5.

TABLE V. INDICATORS OF THE QUALITY OF GASOLINE, DEPENDING ON THE PROPERTIES OF REFORMATES

Parameter	Reformate 1			Reformate 2		
	Regular 92	Premium 95	Super 98	Regular 92	Premium 95	Super 98
RON	92	95	98	92	95	98
Benzene content, wt. %	0.97	0.88	0.79	0.99	0.97	0.92
Aromatics content, wt. %	34.93	34.64	32.62	33.04	34.30	32.44
Olefins content, wt. %	11.22	10.16	4.70	11.22	9.85	4.56
Sulfur content , ppm	10.00	10.00	7.00	10.00	9.00	7.00

According to the data presented in table 4, the properties of the calculated gasoline meet the established quality standards and have a stock on the content of benzene and aromatic hydrocarbons.

Estimated gasoline recipes are presented in table 6.

TABLE VI. RECIPES MIXING GASOLINE, DEPENDING ON THE PROPERTIES OF REFORMATES

Flow, wt. %	Reformate 1			Reformate 2		
	Regular 92	Premium 95	Super 98	Regular 92	Premium 95	Super 98
Catalytic cracking gasoline	31.79	27.80	8.37	31.79	26.95	8.13
Hydrotreated catalytic cracking gasoline	13.48	13.59	12.37	13.48	13.18	12.01
Reformate (moving catalyst bed)	22.06	20.46	22.28	22.33	22.64	22.28
Reformate (fixed catalyst bed)	7.70	6.94	7.90	3.82	4.76	7.90
Toluene	0.00	2.46	3.39	0.93	2.68	4.02
Isomerate	7.27	8.05	11.00	7.37	8.30	11.00
Isopentane	8.98	9.12	11.53	9.49	9.63	11.53
Alkylate	5.86	8.00	15.17	7.98	8.00	14.54
MTBE	0.00	3.57	7.97	0.00	3.85	8.57
Straight-run gasoline	2.85	0.01	0.00	2.80	0.01	0.00

The calculated mixing formulations change depending on the properties of the streams used, in this case, on the properties of reformate. Reducing the content of benzene in the composition of the reformate ensures its more complete involvement in the production of gasoline. The higher the reformate RON, the less the involvement of costly high-octane streams.

Along with the properties of the streams involved, an important condition is the maximum involvement of catalytic cracking and reforming gasoline.

Forecast calculations for the production of gasoline were carried out taking into account changes in the properties of reformate, based on the following criteria:

• Criterion 1: the maximum production of gasoline brand Regular 92;

• Criterion 2: Maximum production of Premium 95 gasoline;

• Criterion 3: Maximum production of Super 98 gasoline.

The estimated amount of gasoline is presented in table 7.

TABLE VII. ESTIMATED AMOUNT OF GASOLINE

Gasoline grade	Criterion 1		Criterion 2		Criterion 3	
	Reformate 1	Reformate 2	Reformate 1	Reformate 2	Reformate 1	Reformate 2
Regular 92, t	9016	9016	8210	8575	8811	9000
Premium 95,t	3227	3227	4260	3958	3458	3169
Super 98, t	325	295	0	0	349	349
Total, t	12568	12538	12470	12533	12618	12518

According to the results of the forecast calculation, the highest total gasoline output is achieved subject to the production of the maximum amount of gasoline Super 98 using reformate 1. When using reformate with high benzene content and low RON, the maximum production of gasoline Premium 95 (Criterion 2) is limited to the available daily production of MTBE.

Thus, the use of reformates with a low benzene content and high RON can reduce the involvement of expensive high-octane streams in the production of motor fuels, as well as increase the involvement of catalytic cracking gasoline.

On the basis of the studies that have been carried out, optimal formulations for mixing material flows of industrial refineries have been developed, ensuring the solution of a multifactor task and increasing the efficiency of gasoline production using schedules.

The solution will meet the requirements for octane number, the content of aromatic hydrocarbons, including benzene, as well as the content of sulfur, olefinic hydrocarbons, etc.

The functionality of the system is as follows:

- tracking in the continuous recipe of gasoline mixing;

- corrective mode (output values for making adjustments) when changing: the quality, the volume of the batch of preparation, the calendar plan for the production of gasoline, the operation of installations;

- checking the correctness of the task of recipes (comparison of raw materials costs);

- calculation of the formulation, taking into account the quality and quantity of raw materials, including taking into account the tanks;

- the system is able to control the component streams used for mixing and the flow change with the subsequent adjustment of the formulations;

- the system is able to provide for the interchangeable calculation of branded gasolines according to the monthly mixing plan, taking into account the periods of operation and the operational mixing plan for a given number of days;

- the intelligent system takes into account the nonlinear laws of mixing octane numbers, the values of dipole moments for polar molecules.

Thus, the proposed strategy for the transition to the "Russian Hysys" solves the problem corresponding to the direction of the Strategy of the transition to advanced digital, intelligent production technologies, robotic systems, new materials and methods of construction, the establishment of systems for processing large volumes of data, machine learning and artificial intellect.

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