Petroleum and Coal

Article **Open Access**

DEVELOPMENT OF GASOLINE BLENDING RECIPES TAKING INTO ACCOUNT VOLUME AND COMPOSITION OF THE INVOLVED FEEDSTOCK

Maria V. Kirgina, Elizaveta V. Sviridova, Bogdan V. Sakhnevich, Nikita V. Chekancev, Yury A. Chursin*

Department of Fuel Engineering and Chemical Cybernetics, Tomsk Polytechnic University, Russia

Received October 12, 2017; Accepted December 23, 2017

Abstract

The process of gasoline blending is a sophisticated multistage industrial technology. In this paper, blending recipes of different gasoline brands were developed using computer modeling system "Compounding" considering the volume and changing composition of the involved feedstock. The developed modeling system allows increasing the efficiency of the gasoline production using only internal resources of the refinery with no additional investments and expenses.

Keywords: gasoline; mathematical modeling; blending recipes; octane number.

1. Introduction

Automobile fuels, primarily, gasoline and diesel fuel are the most significant part of petroleum products which play a crucial role in the economics of Russian Federation. On a modern refinery, the most part of the crude oil is being refined into motor fuels, primarily in gasoline. This makes gasoline blending an important process for petroleum industry with the main goal to mix products of refinery processes in specific proportions and obtain a final blend that complies all quality requirements [1-2].

This multi-staged process is one of the most sophisticated technologies from the standpoint of economic efficiency. The key point lies in the complexity of feedstock mixtures which consist of large quantities of individual hydrocarbons, in conditions of ever-changing feedstock composition. In addition, detonation resistance does not follow the law of additivity (octane number is a non-linear characteristic), so this makes it more difficult to optimize the process.

Considering all above-mentioned factors, it appears to be impossible to formulate a universal blending recipe; existent recipes need to be revised in real time to correspond the changing conditions of blending.

Thus, optimization of trade gasoline blending process is an urgent industrial-oriented research direction in terms of the modern trends of annual increase in demand for high-octane gasoline. There is a large number of research works of domestic and foreign scientists dedicated to the study of aspects of this problem [3–5].

However, the most efficient way of optimization and of gasoline blending process and prediction of operational properties of blended gasoline is to apply modeling systems which use physic-chemical properties of hydrocarbons as a basis for calculations.

The main role of such systems is to formulate economically feasible recipes of gasoline blending considering the composition of the involved feedstock.

2. Complex modeling system for optimization of gasoline blending

During the research, complex system for optimization of gasoline production was developped. The following interconnected modules are presented in the system: Module of chromategraphic data systematization; Module of detonation and physic-chemical characteristics calculation; The module of optimal gasoline blends.

The developed modeling system provides the user with calculations of detonation properties and a wide range of physical and chemical characteristics of gasoline and gasoline components including octane number, vapor pressure, density and viscosity of mixtures and precise hydrocarbon composition of each stream based on chromatographic analysis data. On the basis of this data, the system calculates an economically optimal gasoline recipe for different brands of gasoline.

A detailed description of modules is provided in the following sub-chapters.

2.1. Module of chromatographic data systematization

In this modeling system, chromatography data of feedstock streams serve as an input data for calculations of detonation characteristics.

In view of the fact that hydrocarbon composition gasoline component streams vary significantly in set and number of hydrocarbons, the module of chromatographic data systematization "UniChrom" has been introduced into the system for unification and standardization of experimental chromatography data.

Systematization of the chromatography is an automatic process constituting the reclassification of hydrocarbons in the initial mixture to the set of 110 key components. This set serves as a baseline for high accuracy calculations of octane numbers of blending gasoline. This set includes both individual hydrocarbons and pseudo-components [6].

2.2. Module of detonation and physic-chemical characteristics calculation

The module of detonation and physic-chemical characteristics calculation provides calculations for the following detonation characteristics of gasoline:

1. Octane numbers (RON, MON) of hydrocarbon stream involved in the blending process taking into account their non-additivity;
2. Mixture density, by the Mendeleev formula;
3. Mixture viscosity, by the Orrick and Erbar formula;
4. Saturated vapor pressure (SVP) by the Antoine equation;
5. Aromatics, olefins hydrocarbons, and benzene percentage.

The main module is developed in Borland "Delphi 7" workspace combining a user-friendly interface, coordination, integrity of sub-components and stable functioning of the system in general. It is possible to manually change flow rates of input streams [7-8].

2.3. Module of optimal gasoline blends

From the standpoint of economic profitability of the refinery, optimal blend of gasoline must ensure the biggest economic effect: Refinery has to use the cheapest raw materials for blending of gasoline with low market value (low-octane brands) and the cheapest raw streams, and high-octane raw streams for the most commercially demanded brands, respectively. Refinery tends to produce the maximum possible volume of gasoline, using available stocks of the raw stream; the product must comply with the demands of the Russian Technical Regulations and State Standard R 51866-2002.

In the research, a logical algorithm was compiled on purpose to formulate optimal blending recipes. In this algorithm, 12 typical hydrocarbon streams are involved in the blending process:

1. Hydrotreated catalytic cracking gasoline (HYT FCC);
2. Catalytic cracking gasoline (FCC);
3. Reformate from catalytic gasoline reforming unit with continuous catalyst regeneration (Reformate (moving-bed));
4. Reformate from catalytic gasoline reforming unit with periodic catalyst regeneration (Reformate (fixed-bed));
5. Toluene concentrate on the complex production of aromatic hydrocarbons (Toluene);

6. Isomerate from the isomerization unit of light gasoline fractions (Isomerate);
7. The fraction of the isopentane from the isomerization unit of light gasoline fractions (Isopentane);
8. Alkyl gasoline with the unit of the sulfuric acid alkylation (Alkylate);
9. Methyl tertiary butyl ether (MTBE);
10. Straight-run gasoline fraction from atmospheric and vacuum pipe stills (Straight-run gasoline);
11. Gasoline fraction from complex production of aromatics hydrocarbons (Feedstock for aromatics production);
12. Gasoline-raffinate from the complex production of aromatic hydrocarbons (Raffinate of aromatics production).

Limiting conditions in recipes formulation are strictly regulated characteristics as RON, MON, SVP and content of benzene, aromatic and olefin hydrocarbons, sulphur and MTBE in trade gasoline of a specific brand.

The module of optimal gasoline blends formulation was developed in the workspace Borland "Delphi 7" on the basis of the algorithm flowchart of the logical algorithm is presented in Figure 1.

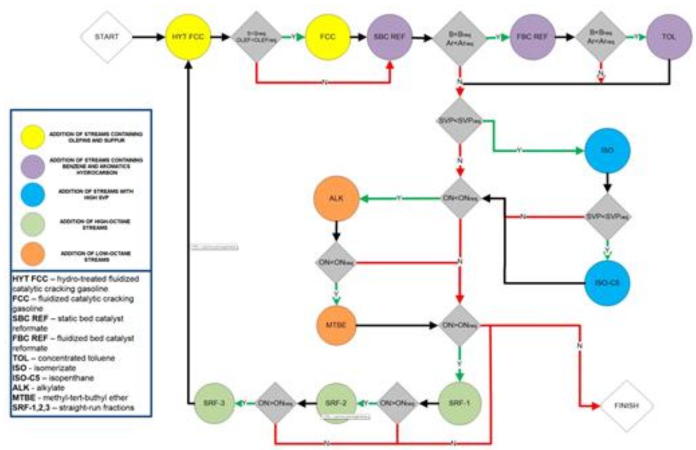

Fig. 1. Flowchart of the logical algorithm for optimal gasoline blends formulation

The developed algorithm automatically optimal gasoline blends on the basis of a formalized hydrocarbon composition of involved streams and predict all detonation characteristics of blended gasoline. Gasoline blending is carried out step-by-step as well as a recalculation of required quality characteristics.

Priority of using streams is chosen to the way of the biggest resource saving production. So first use the lowest-quality (and therefore least expensive) components, and then, when that streams are consumed, or used as much as possible, involve more expensive components.

The proposed approach has several advantages: first of all, it becomes possible to respond to changes in the composition of raw materials, develop "flexible" blending recipes and formulate recommendations for the involvement of streams with different composition when the blended to different gasoline brands.

Secondly, the algorithm is aimed to the efficient solution of several technological situations: production of the certain volume of gasoline, maximization of the particular brand yield, and the combination of several gasoline brands with an ability to set "the priorities of the sequence."

Thirdly, the algorithm reflects the concept of resource-saving blending, which allows to saving the most expensive components, involving unspent reserves only into the production of high quality fuels and reducing of unwanted quality giveaways and production of off-grade gasoline. These measures are able to increase the economic efficiency of blending, using only internal resources of the refinery without additional investments.

3. Formulation of gasoline blending recipes considering the volume of involved feedstock

For this research, blending recipes of different gasoline brands were developed using computer modeling system "Compounding." The recipes were formulated on the basis of data on configuration and composition of feedstock for one of the largest refineries in Russian Federation.

Here, we demonstrate calculated blending recipes for gasoline of Premium-95 brand corresponding to the Euro-5 quality standard of yield rate: 100, 500, 1000 and 2000 tons, respectively. In each case, the volume of each feedstock component equals 200 tons (hereafter refers to gasoline pool). Calculated recipes of Premium-95 gasoline for 100 (I), 500 (II), 1000 (III) and 2000 (VI) tons are shown in Figure 2 and in Table 1.

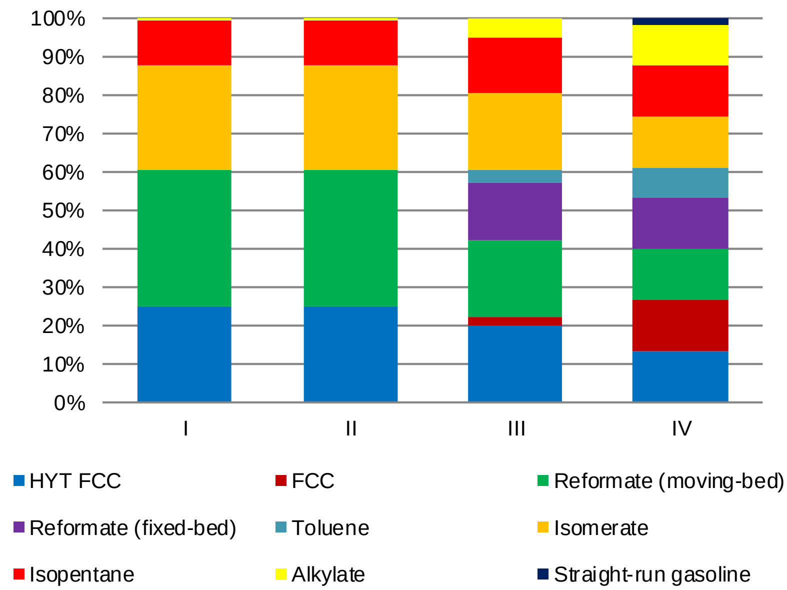

Fig. 2. The recipes of Premium-95 brand gasoline blending (Euro-5 quality standard)

Table 1. The main properties of gasoline of Premium-95 brand (Euro-5 quality standard)

Characteristics	Weight, tons			
	100	500	1000	2000
RON	95.0	95.0	95.0	95.2
MON	88.7	87.3	88.5	88.5
SVP, kPa	50.2	50.1	51.7	50.1
Density, kg/m^3	727.9	726.3	720.0	724.8
Benzene, wt. %	0.89	0.74	0.98	0.83
Aromatic hydrocarbons, wt. %	34.98	34.98	34.98	34.98
Olefins, wt. %	6.72	12.35	5.80	6.25

As it can be seen from Figure 2 and Table 1, calculation of blending recipes was conducted in such way that the values of benzene, aromatic hydrocarbons contents, as well as the SVP values, were maximized most closely to the values regulated by Russian Technical Regulations, but not exceeding them. The logic of algorithm is a multi-step mixing of available feedstock components in the order of the increased value. Such an approach tends to formulate gasoline blending recipes for required volume and quality of the product in a resource-efficient way.

On the basis of obtained results, it can be concluded that the structure of blending recipes depends on the required volume of product: in case of small volumes, the constraining factors are quality requirements for certain gasoline characteristics, and in case of large volumes availability of feedstock plays the crucial role in the structure of blend.

Consider another practical task which consists in the production of several gasoline brands from a limited volume of feedstock in a certain time period of scheduling horizon and specific sequence of blending. The developed logical algorithm of complex modeling system is able to formulate blending recipes for simultaneous production of gasoline brands from the total available gasoline pool.

In this case, the task is to produce trade gasoline brands from gasoline pool volume of 200 tons in the following order and quantity: Regular-92, Euro-5 – 500 tons; Premium-95, Euro-5 – 500 tons; Super-98, Euro-5 – 500 tons.

All calculations for this case including the actual volume of gasoline blended by this algorithm are provided in Figure 3 and in Table 2.

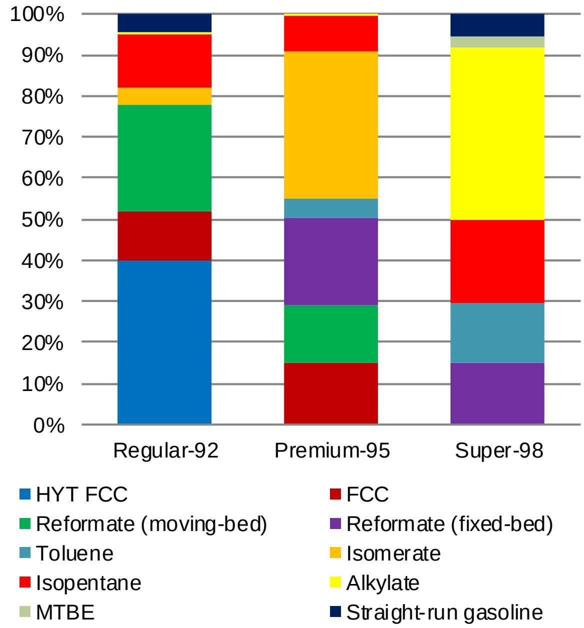

Fig. 3. The recipes of gasoline of Regular-92, Premium-95 and Super-98 brand gasoline blending in case of joint production

Table 2. The main properties of gasoline of Regular-92, Premium-95 and Super-98 brand gasoline blending in case of joint production

Characteristics	Regular-92	Premium-95	Super-98
RON	92.0	95.0	98.0
MON	84.2	89.4	93.1
SVP, kPa	50.2	50.1	58.4
Density, kg/m3	731.3	723.1	720.3
Actual product amount, tons	500	500	460
Benzene, wt. %	0.89	0.74	0.98
Aromatic hydrocarbons, wt. %	34.98	34.98	34.98
Olefins, wt. %	6.72	12.35	5.80

As it can be seen from in Table 2, all quality properties of blended gasoline comply with the requirements of Russian Technical Peculations and State Standard R 51866-2002. During the recipes formulation, the involvement of basic refinery products such as reformate, catalytic cracking gasoline, and straight-run gasoline fraction is maximized that ensures the economy of expensive components such as MTBE (188 tons), toluene (111 tons).

Such an approach in the formulation of gasoline recipes reflects the strategy of economically-efficient blending. It tends to obtain gasoline brands with the maximum possible involvement of the less valuable and surplus components while minimizing percent of the most valuable, scarce ones. The latter components are added after all the other in order to comply with the requirements or can be saved for the next blending operations.

4. Formulation of gasoline blending recipes considering the composition of the involved feedstock

During the production cycle, hydrocarbon composition of refinery products is ever-changing; in its turn, it leads to changes in detonation characteristics of the obtained gasoline. Thus, resource-efficient gasoline production requires continuous real-time correction of blending recipes. In this section, calculations of optimal blending recipes depending on the composition of the involved feedstock are presented.

The main properties of feedstock components involved in gasoline production are shown in Table 3. For components demonstrating the most significant deviations of the detonation characteristics (Reformate m/b, Reformate f/b, Isomerate, and Isopentane), additional samples of the worst (I) and the best (II) quality are provided.

Table 3. The main properties of feedstock gasoline streams

Stream	RON	SVP, kPa	Characteristics Density, kg/m^3	Summary content, wt.%	
				Benzene	Aromatic hydrocarbons
HYT FCC	89.1	43.2	722.4	0.70	23.76
FCC	91.0	53.6	741.4	0.80	34.49
Reformate m/b	105.4	14.0	820.8	2.00	81.40
Reformate m/b I	102.6	20.5	812.7	2.50	78.68
Reformate m/b II	106.3	16.5	826.0	1.50	81.85
Reformate f/b	95.7	21.6	790.2	2.70	65.40
Reformate f/b I	90.7	27.7	780.3	1.20	58.57
Reformate f/b II	97.5	24.0	791.7	1.30	66.57
Toluene	117.0	7.2	854.7	0.00	100.00
Isomerate	90.0	62.0	636.8	0.00	0.00
Isomerate I	89.5	61.2	638.5	0.00	0.00
Isomerate II	93.6	67.4	637.3	0.00	0.00
Isopentane	92.4	146.3	600.9	0.00	0.00
Isopentane I	92.0	143.7	601.4	0.00	0.00
Isopentane II	93.0	141.4	601.8	0.00	0.00
Alkylate	96.6	34.7	678.6	0.00	0.00
MTBE	125.0	40.3	717.5	0.00	0.00
Straight-run gasoline	59.3	26.1	716.3	0.30	5.05

In the previous calculations, it was accepted that gasoline pool is constant; however, often in a real production situation, the volumes of available components are unequal due to different capacities of refinery units and volumes of product tanks.

The trends of feedstock availability were calculated for one production cycle (1 week) with a focus on the quantitative data from refineries. The average index of availability of feedstock for gasoline blending is shown in Table 4.

In this way, unequal amounts of feedstock were used for calculations of gasoline blending recipes depending on the composition of feedstock. The total gasoline pool is set to 2 400 tons; such situation (Table 4) reflects the average real situation of production of refinery products in the refinery.

Table 4. The average index of availability of feedstock for gasoline blending

Streams	The average index of availability of feedstock	Streams	The average index of availability of feedstock
HYT FCC	0.2763	Isomerate	0.0759
FCC	0.1220	Isopentane	0.0897
Reformate m/b	0.2215	Alkylate	0.0695
Reformate f/b	0.0631	MTBE	0.0119
Toluene	0.0163	Straight-run gasoline	0.0256
Total			1.0

Blending recipes for Premium-95 gasoline corresponding to the Euro-5 quality standard with a total yield of 1000 tons and various compositions of the involved feedstock (I – worse, II – medium, III – best feedstock) are shown In Table 5 and Figure 4.

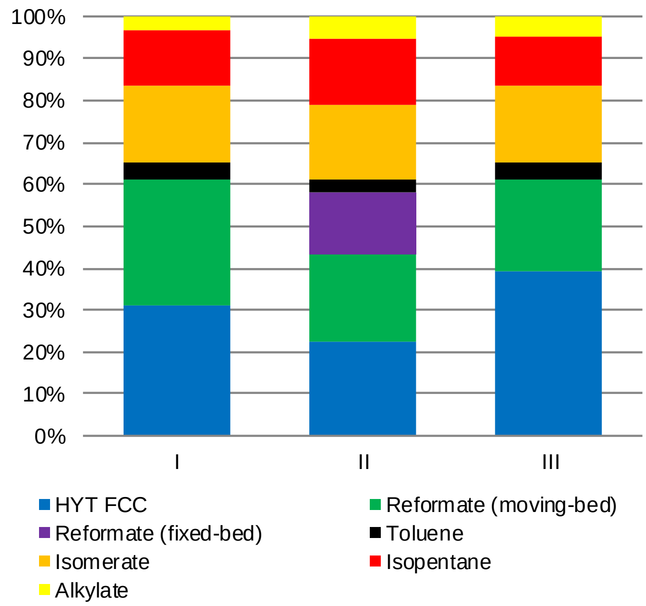

Fig. 4. The recipes of gasoline of Premium-95 brand gasoline blending considering various compositions the involved feedstock

Table 5. The main properties of gasoline of Premium-95 brand (Euro-5 quality standard) blending considering various compositions the involved feedstock

Characteristics	I	II	III
RON	95.0	95.0	95.0
MON	87.9	87.6	88.0
SVP, kPa	51.2	51.6	51.6
Density, kg/m^3	721.8	720.2	720.6
Actual product amount, tons	1000	1000	1000
Benzene, wt. %	0.98	0.98	0.61
Aromatic hydrocarbons, wt. %	34.94	34.98	31.34
Olefins, wt. %	8.52	6.03	10.61

As it can be seen from Tables 4 and 5, changes in hydrocarbon composition influence the detonation characteristics of streams; in its turn, it leads to a reformulation of blending recipes. For ensuring of the efficient gasoline blending refinery has to respond to changes in feedstock composition and adjust blending recipes to produce trade gasoline avoiding extra quality giveaways, as well as overruns of expensive high-quality hydrocarbon streams and production off grade gasoline batches.

In this case, at the beginning of the production cycle, Premium-95 gasoline brand (Euro-5) was produced using feedstock with average quality (Feedstock No. II, Table 5). As the composition of feedstock has been changing continuously within the certain limits during refinery operations, that influenced the quality of the obtained product. Calculations of detonation characteristics of produced gasoline in conditions of changes in composition are shown in Table 6. Feedstock No. I represent changes to the worst quality of components and Feedstock No. II, to the best quality, respectively.

Table 6. The main properties of gasoline considering various compositions the involved feedstock

Characteristics	Feedstock I	Feedstock II
RON	93.9	95.9
MON	87.3	89.2
SVP, kPa	53.6	52.9
Density, kg/m3	717.3	721.7
Benzene, wt. %	0.90	0.70
Aromatic hydrocarbons, wt. %	33.40	35.24
Olefins, wt. %	6.10	6.08

As it can be seen from Table 6, production of gasoline by averaged ("universal") recipes is not economically profitable because there are unwanted deviations of operational characteristics of gasoline brands are observed throughout the changes in hydrocarbon composition.

Thus, in case of a decline in the feedstock quality (Feedstock I) gasoline, produced by the averaged recipes demonstrates drop in octane number down to 93.93 points as well as a decrease in density. Such deviations are not allowable for product certification, so the quality of gasoline needs to be additionally raised up to requirements Russian Technical Regulations demands and State Standard R 51866-2002. In case of an increase in the feedstock quality, unwanted RON giveaway (95.85) is observed, which is evidence of an overrun of high-quality components.

In order to avoid these issues, correction of gasoline blending recipes was automatically performed by the use of developed integrated modeling system (Table 5). In every single case, formulated blending recipes reflect the concept of the most resource-efficient distribution of available gasoline pool of certain quality and volume.

Considering the revealed data above we can suggest that using the modeling system for correction of gasoline blending in respect to changes in feedstock composition leads to positive results, such as:

1. In case of the worst feedstock, correction of recipes allows avoiding off-grade gasoline production; however, it becomes impossible to use Reformate F/B due to high contents of benzene and aromatic hydrocarbons. The necessity to compensate the shortage of octane number forces to involve 88 additional tons of the Reformate M/B.
2. In case of the best feedstock, correction of recipes allows saving scarce, high-quality components: 6 tons of Alkylate and 37 tons of Isopentane. Also, the involvement of 170 tons of FCC gasoline is an effective decision due to its low detonation characteristics and availability at refinery tanks.

5. Conclusion

1. It was established that for resource-efficient maintenance of gasoline blending process it is necessary to correct blending recipes considering the hydrocarbon composition of involved feedstock and non-linear nature octane numbers throughout blending operations.
2. For this research, the logical algorithm for the formulation of the optimal gasoline blending recipes was created. It ensures economically efficient blending as well as obtaining of the required amount of gasoline which meets contemporary environmental and technical standards.

3. In this work, optimal blending recipes for Premium-95 gasoline brand (Euro-5 quality) were formulated using the developed complex modeling system. Joint and separate production regimes are simulated.
4. Influence of changes in hydrocarbon composition of feedstock on detonation characteristics of gasoline is shown. In case of a change to the worst-quality feedstock, correction of recipes allows avoiding production of off-grade gasoline; it is also possible to save high-quality components in case of a change to the best-quality feedstock.
5. The developed modeling system allows increasing the efficiency of the gasoline production using only internal resources of the refinery with no additional investments and expenses. Corrections of gasoline blending recipes considering changes in the composition of the involved feedstock allow avoiding undesirable quality giveaways trade gasoline and overruns of expensive components. The results show the concept of the resource-efficient gasoline production which makes a large economic effect for the refinery.

Acknowledgements

The study is supported by the Ministry of Education and Science of the Russian Federation, project 2.3649.2017 / 4.6.

References

[1] Braginsky OB. Prediction of the Russian automotive fuels market. Open seminar Economic problems of energy comple" (seminar of A.S. Nekrasov). One hundred and twenty-ninth meeting of 24 April 2012.

[2] Smolikov MD. The production trade gasoline at domestic refineries. Problems and solutions. Chemistry under the SIGMA sign: investigations, innovations, technologies: all-Russian youth school-conference, Omsk, 2010, pp. 251-252.

[3] Kulkarni-Thaker S, Mahalec V. Multiple optima in gasoline blend planning. Industrial and Engineering Chemistry Research, 2013; 52(31): 10707-10719.

[4] Pasadakis N, Gaganis V, Foteinopoulos C. Octane number prediction for gasoline blends", Fuel Processing Technology, 2006; 87: 505-509.

[5] Caixia G, Jinbiao G, Lei Z. Application of mathematical programming in off-line formulation optimization of gasoline blending. Petroleum Refinery Engineering, 2013; 43(3): 61-64.

[6] Sakhnevich BV, Kirgina MV, Chekantsev NV, Ivanchina ED. Development module of chromatographic data systematization to improve the efficiency of the process compounding trade gasoline. Izvestia of the Tomsk Polytechnic University, 2014; 324(3): 127-136.

[7] Maylin MV, Kirgina MV, Sviridova EV, Sakhnevich BV, Ivanchina ED. Calculation of gasoline octane numbers taking into account the reaction interaction of blend components. Procedia Chemistry, 2014; 10: 477-484.

[8] Ivanchina ED, Kirgina MV, Chekantsev NV, Sakhnevich BV, Sviridova EV, Romanovsky RV. Complex modeling system for optimization of compounding process in gasoline pool to produce high-octane finished gasoline fuel. Chemical Engineering Journal, 2015; 282: 1-12.

To whom correspondence should be addressed: Nikita V. Chekancev, Department of Fuel Engineering and Chemical Cybernetics, Tomsk Polytechnic University, 30, Lenin Avenue, Tomsk, 634050, Russia; e-mail: Chekancev@tpu.ru