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APPLICATION OF COMPOUNDING PROCESS MATHEMATICAL MODEL FOR GASOLINE QUALITY IMPROVING

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Abstract

The paper presents the simulation results for the octane number and the saturated vapor pressure of commercial gasoline of various grades. The compounding process mathematical model was veryfied by comparison of simulation results and laboratory data. The results confirmed the appropriateness of computer simulation system use for the development of high-octane gasoline blending formulations.

Keywords: gasoline; compounding; octane number; product quality.

1. Introduction

Improving the quality of oil products and the efficiency of refining is one of the main tasks at the present stage of development of oil refining industry. For the formation of quantitative and qualitative commercial gasoline indicators, the process of compounding is the most important [1-4].

The components entering for mixing, are products of primary and secondary refining processes and have different quality and cost. In order to avoid substandard consignments, it is necessary to observe strict quality standards of commercial gasoline, and this leads to increase in the use of expensive high-quality components.

The improvement of compounding process permits to increase the quality of the fuel and its yield. However, the optimization process is complicated by the large number of the components involved. However, the major difficulty in the compounding process modeling is that the knock characteristic of gasoline does not have the property of additivity, but it is the major operational characteristic for fuel. Also blending octane numbers differ from the weighted sum of the octane numbers. This fact can be explained by the presence of intermolecular interactions between hydrocarbons forming the gasoline [5-7].

The polarity of the molecules affects the strength of intermolecular interaction of the components in the gasoline mixture. At the Department of chemical technology of Fuels and Chemical Cybernetics, Institute of Natural Recourses of Tomsk Polytechnic University, we found the regularity that explains the deviation of octane numbers of mixtures, depending on the concentration of hydrocarbons, which are most prone to intermolecular interaction: equations (1, 2) and equation for calculating the octane number of the mixture (3):

$$B = \frac{1}{100}\sum_{i=1}^{n-1}\sum_{j=2}^{n} B_i B_j C_i C_j \,, \qquad (1)$$

$$B_i = \alpha \left(\frac{D_i}{D_{\max}} \right)^n , \quad (2)$$

$$ON_{mix} = \sum_{i=1}^{n} (ON_i \cdot C_i) + C_i \cdot B , \quad (3)$$

here *Ci* – concentration of hydrocarbons in the mixture; *a* and *n* – kinetic parameters that determine the intensity of intermolecular interactions in dependence on the dipole moment; *D, Bi , Bj* – values characterizing the propensity to intermolecular interaction between *i*-th and *j*-th molecules; *Dmax* – maximum dipole moment of hydrocarbon molecules; *ONmix* – octane number of gasoline.

2. Experimental

We used the «Compounding» computer program to calculate the main indicators of the quality of commercial gasoline and to compare with laboratory data. The program allows to forecast the octane number of gasoline considering the intermolecular interactions of hydrocarbons, as opposed to commercial software packages such as: Blend Ratio Control, Aspen PIMS, Refinery and Petrochemical Modeling System, Blend Optimization and Supervisory System, that does not take non-additivity of blending octane numbers into account. Application of these programs in some cases is difficult, as conditional mixing characteristics are used for calculations and this leads to significant errors.

Intelligent computer system «Compounding» allows you:

- to calculate the optimum recipes of components mixing for commercial gasoline brands required to meet the requirements of technical and environmental standards;
- to calculate detonation resistance and saturated vapour pressure of components of comercial gasoline;
- to calculate the influence of additives and supplements on the knock resistance of gasoline.

The calculation results are the octane number of gasoline, saturated vapour pressure considering intermolecular interactions, as well as the cost of the resulting product and its componentwise composition [8-11].

3. Results and discussion

To confirm the accuracy of the calculations obtained with use of the «Compaunding» computer modeling system, we used data of industrial plant for production of commercial gasoline. We selected 17 brands of commercial gasoline and performed calculations and comparison of such quality indicators as: the octane number by research method; saturated vapor pressure;- density; weight content of sulfur, benzene, aromatic and olefinic hydrocarbons.

The «Compounding» program data base contains the octane numbers of individual hydrocarbons forming the gasoline. The investigated brands of gasolines are presented in Table 1.

Table 1**.** Gasoline brands

No.	Brand	No.	Brand	No.	Brand
1	Normal 80 3 (1)	7	Premium 95B(2)	13	Regular 92BPF (2)
2	Normal 80 3 (2)	8	Super 98B	14	Premium 95B3 (1)
3	Regular 92	9	Normal 80B3	15	Premium 95B3 (2)
4	Regular 92B(1)	10	Regular 92KK	16	Super 98B3 (1)
5	Regular 92B(2)	11	Regular 92B3PF	17	Super 98B3 (2)
6	Premium 95B(1)	12	Regular 92BPF (1)		

Fig. 1-3 present the results of model verification on following parameters: the octane number by research method; saturated vapor pressure; weight content of sulphur. The discrepancy between the experimental and calculated values of sulphur content is not more than 0.01 wt. %, which corresponds to the requirements of GOST-R 51859-2002.

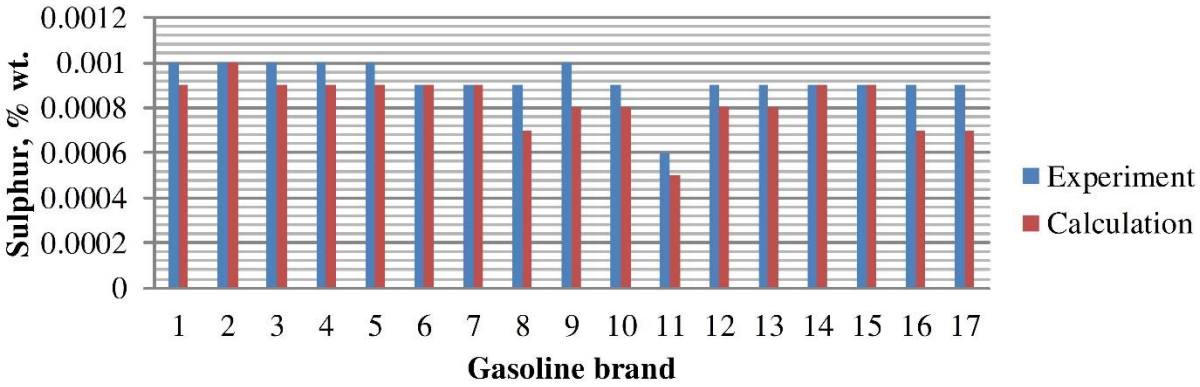

Figure 1. The experimental and calculated values of octane number by research method

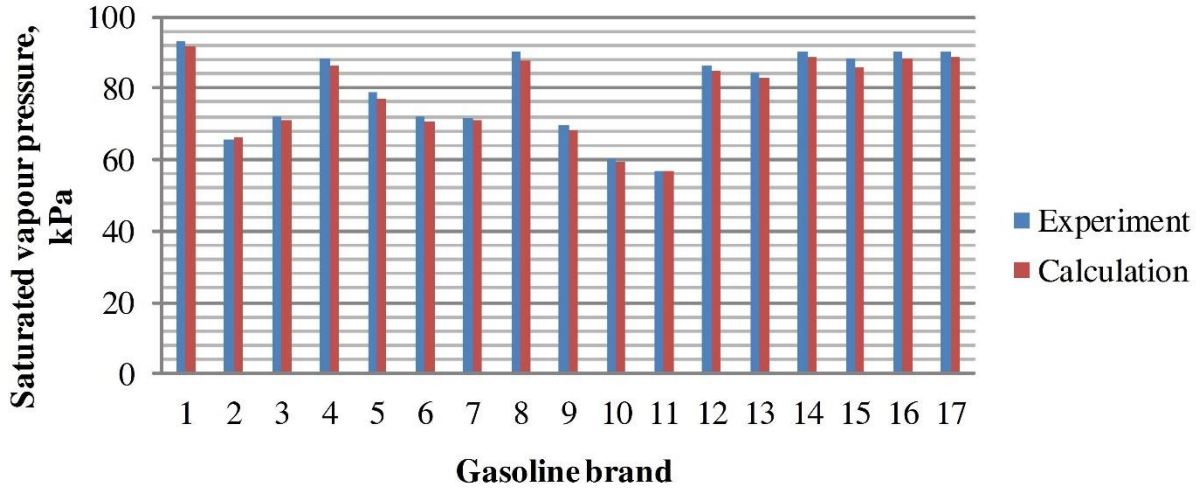

Figure 2. The experimental and calculated values of saturated vapor pressure

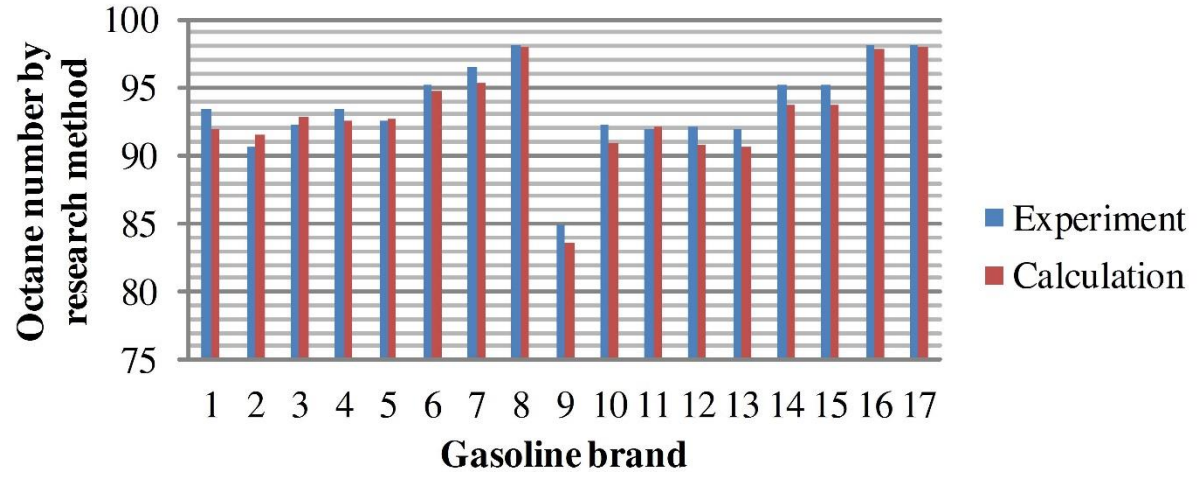

Figure 3. The experimental and calculated values of Sulphur content

3.1. Obtaining gasoline of formulations using substandard product

Substandard gasoline is product that does not meet all the requirements of environmental and technological standards. The use of substandard petrol can harm the environment and human health. To improve the quality of substandard product, it is possible to re-involve it in the com-

pounding process, considering the basic characteristics and composition. Indicators of sub-standard quality product involved in the process of blending for production of high-quality commercial gasoline, are shown in Table 2.

Table 2. Quality indicators of substandard gasoline

Parameter	Value
Octane number by research method	94.63
Octane number by motor method	87.41
Saturated vapor pressure, kPa	64.96
Density, kg/m^3	736.64
Viscosity, ·Pa s	42.23
Content of n-parafins, % wt.	6.60
Content of iso-parafins, % wt.	41.54
Content of naftenes, % wt.	7.13
Content of olefines, % wt.	10.37
Content of benzene, % wt.	0.90
Content of aromatic hydrocarbons, % wt.	34.39
Content of sulphur, % wt.	0.001
Cost, rub/t	25 718.77

We developed gasolines formulations with octane numbers 92 and 95, containing 50 % of substandard product by weight. The results of rebounds of formulations and their cost are presented in Table 3. The lowest cost recipe for AI-92 is 21255 rubles, and for AI-95 - 22971 rubles. Quality parameters of obtained formulations are presented in Table 4**.**

Table 3 The results of rebounds of formulations with octane numbers 92 and 95

	Formulations, % wt.							
	Octane number 92				Octane number 95			
	1	2	3	4	1	2	3	4
GO BKK	17.3	18	20	20	4	0	3	13
Kreking KT-1	7.2	7.2	6.2	6.2	8	6	6	7
Reformate L-35-11-1000	10	6	6	4	10	10	13	11
Reformate L-35-11-600	2	6.5	6.5	8.5	6	7	8	4
Toluene concentrate	0	0	0	0	1	2	0	1
Isomerization Isomalk-2	4.5	4.5	4.5	4.5	4.5	4.5	4.5	2.5
Isopentane	2.5	2.5	2.5	2.5	5.5	10	6.5	2.5
Alkylbenzene	0	0	0	0	5	6.5	4	6
MTBE	0	0	0	0	4	2	3	2
AVT-10 fraction 62	2	2	2	2	0	0	0	0
KPA C-100 fraction 62-85	1	1.3	1.3	1.3	0	0	0	0
KPA C400 Rafinate	1	0	0	0	0	0	0	0
n-butane	2.5	2	1	1	2	2	2	1
Substandard gasoline	50	50	50	50	50	50	50	50
Cost, rub/t	21512	21366	21316	21255	24066	24077	23746	22971

Table 4 Quality indicators of gasolines

Characteristic of gasoline	AI – 92				AI – 95				Required value (max.)
	1	2	3	4	1	2	3	4	
Saturated vapor pressure, kPa	70.7	69.7	65.8	70.0	64.1	73.3	70.1	70.2	maximum 100
Benzene content, vol. %	0.9	0.9	0.9	0.9	0.9	0.9	0.9	1	1
Aromatic hydrocarbons, vol. %	33.2	33.0	33.2	32.8	35.0	33.8	33.8	35	35
Olefines, vol. %	11.3	11.4	11.8	11.8	10.1	6.4	7.8	7.2	18
Sulphur content, mg/kg	10	10	10	10	10	8	9	8	10

4. Conclusions

To verify the mathematical we compared the calculated and experimental values for developed formulations. We used data from the installation of gasoline blending. The discrepancy between the results meets the standard. We developed gasolines formulations with octane numbers 92 and 95, containing 50 % of substandard product by weight, and calculated their cost. The lowest cost recipe for AI-92 is 21255 rubles, and for AI-95 - 22971 rubles.

Analysis of the results confirms the feasibility of substandard re-engaging of product into the compounding process.

Acknowledgments

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