Correction of gasoline blending recipes with the use of computer modelling system

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Abstract. The process of gasoline blending is a difficult multistage industrial technology. In this paper gasoline blending recipes for one of the largest refineries in Russian Federation were corrected by using of developed computer modelling system «Compounding». As the result of correction, production volume of high-octane and high-quality gasoline was increased on 47 wt. %.

1. Introduction

Since the January, 1-st, 2015, all refineries in Russian Federation have to switch their technologies to produce automobile gasoline of ecological class no below Euro-4 quality standard. One year later, only Euro-5 gasolines can be produced and presented in the domestic market. In order to solve this problem, trade gasoline producers perform upgrades of existent refineries by inputs of the new secondary refinery units and reconstruction of the old ones. As a result, the total production volume of oil-products increases, along with the increase of oil conversion ratio; in turn, it leads to upgrades in ecological and operational qualities of automobile gasolines.

From year to year, the total production volume of low-octane gasoline brands such as Normal-80 (RON 80) reduces, at the same time, high-octane gasoline (for example, brands Premium-95 and Super-98 have RONs 95 and 98, respectively) production increases permanently. In order to decrease the percent of low-octane gasoline brands production, it is necessary to revise existent gasoline blending recipes, redistribute the raw between the secondary refinery units, and their products – between different gasoline brands.

Solution of this problem is extremely difficult due to list of technological features, which take place at industrial gasoline production, as this process reflects the idea of blending of different hydrocarbon streams, such as: products of catalytic reforming, isomerization, catalytic cracking, alkylation with octane boosters and special anti-knock additives.

This multi-staged process is one of the most sophisticated technologies from the economical optimization point of view. The key point lies in complexity of mixtures, consisting of large quantities of individual components, in conditions of constant changes in feedstock composition. In addition, detonation resistance does not subject to the law of additivity [1-4], so it makes it more difficult to optimize the process. All above mentioned factors counteract developing of a universal blending recipe; existent recipes require for revisions and constant corrections due to changes in external factors.

Solution of such a multi-factorial and multi-criteria optimization task could be carried out in the most effective way by means of a mathematical modelling approach, and applying of computer modelling systems using a physic-chemical basis of the blending process [5, 6].

2. Computer modeling system «Compounding»

Previously, at the Chemical Engineering of Fuels and Chemical Cybernetics Department of Tomsk Polytechnic University, Russia, the mathematical model for gasoline blending process was developed. It described the nature of blending taking into the account deviations from the law of additivity of octane numbers caused by intermolecular interactions in a mixture. It provides calculations for main detonation characteristics of gasoline streams and anti-knock additives influence on octane number values. On a basis of this model, the computer modeling system «Compounding» was developed [7-9]. It provides calculations for:

1) Octane numbers of hydrocarbon stream involved into the blending process taking into account their non-additivity by the research and motor method (RON, MON);

2) Mixture density, by the Mendeleev formula:

$$\rho_4^t = \rho_4^{20} - \Delta t \cdot (t - 20) \quad (1)$$

where ρ_4^t – density for temperature t, kg/m^3; ρ_4^{20} – density for temperature of 20 °C, kg/m^3; Δt – temperature correlation for density by 1 °C.

3) Mixture viscosity, by the Orrick and Erbar formula:

$$\ln(\eta/(\rho \cdot M)) = \alpha + \beta/T \quad (2)$$

where η – viscosity, sP; T – temperature, K; ρ – density for T = 20 °C; M – molar mass; α, β – constants depending on the substance nature.

4) Saturated vapor pressure (SVP) by the Antuan equation:

$$\ln P_T = A - B/(T + C) \quad (3)$$

where T – temperature, K; A, B, C – physic-chemical constants.

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 system in general. The module has open database for detonation and physic-chemical characteristics of individual components.

In this modeling system, the input data for calculations are the actual industrial data and chromatography data of streams involved in the blending process. For unification of an experimental chromatography data, the module of chromatographic data systematization has been introduced into the system. During the chromatographic data systematization, all chromatograms are basically considered sets of 110 key components, and this set is a baseline for the high accuracy calculations of the blending gasoline octane numbers.

There is a possibility to calculate detonation characteristics of hydrocarbon mixtures by inputting the volumetric ratios of components, and calculates gasoline blending recipes with required brand and quality.

3. Results and discussion

For this study, by using of computer modelling system «Compounding», gasoline blending recipes for one of the largest refineries in Russian Federation were investigated. We explored 19 real hydrocarbon streams involved into the blending process for different brands of gasoline. During the research, blending recipes were reproduced, and all detonation characteristics including RON and MON and composition of streams, were calculated and analyzed.

Oil refinery produces such gasoline brands as Normal-80, Regular-92, Premium-95 and Super-98 alongside with gasoline for industrial purposes (GIP), which is semi-finished product.

Table 1.Volume of gasoline production.

Brand	Production volume, tons
Normal-80	12742
Regular-92	145592
Premium-95	70656
Super-98	7006
GIP	35814

As it can be seen from Table 1, the main part of produced gasoline is Regular-92 (53 wt. %), Premium-95 brand amounts to the quarter part, and remaining volume relates to Super-98, Normal-80 gasolines and GIP. In addition, the results shown in Table 1 demonstrate large amounts of produced gasoline falls up to GIP, which is not a trade product, wherein amount of high-octane Super-98 gasoline is small. This ratio doesn't represent a resource saving strategy, thus upgrading the quality of trade oil products is a top-priority aim for all producers. The main properties of gasoline produced at oil refinery by existing recipes are shown in the Table 2.

Table 2. The main properties of gasoline produced at oil refinery by existing recipes.

Characteristic	**GIP**	**Normal-80**	**Regular-92**	**Premium-95**	**Super-98**
RON	56.3	80.8	93.5	96.4	99.0
SVP, kPa	24.1	40.7	46.7	65.3	58.8
Density, kg/m^3	696.1	732.0	728.0	722.3	721.8
Viscosity, sP	35.9	44.7	41.3	39.6	38.6
Olefins, wt. %	0.8	11.3	13.6	7.4	3.0
Benzene, wt. %	0.7	0.9	1.0	0.9	1.0
Aromatic hydrocarbons, wt. %	1.1	27.4	35.3	38.0	34.7

As it can be seen from Table 2, several properties of producing gasoline do not comply with the demands of the Russian Technical Regulations and State Standard R 51866-2002. It can be observed that gasoline octane number is always higher than it is required. It is not economically profitably, that is why in this case there is a high-octane feedstock over expenditure. That feedstock can be used for production of other brands of gasoline. At the same time, in Regular-92 and Premium-95 gasolines the aromatic hydrocarbons content exceeds the maximum allowable standards (according to the Russian Technical Regulations, the maximum of aromatic content is 35 wt. %), thus they do not correspond the established demand. Thus, according to the data from Table 1 and Table 2, the existing recipes used at oil refinery do not allow obtaining trade product, corresponding with the Russian Technical Regulations demands and State Standard R 51866-2002. Moreover, the ratio of volumes in gasoline production is not reasonable, thus it is necessary to correct existing recipes for increasing the quality of trade product and the part of high-octane brand.

The aim of correction was to decrease the volumes of is semi-finished product (GIP) and to increase the volumes of high-octane and high-quality Super-98 brands production. Table 3, 4 show corrected recipes for gasoline blending. GIP is semi-finished product and it is used for further usage on the filling station, thus the task of correction recipes is to decrease its production volumes in favor of increasing production of Normal-80 gasoline, which has higher operational and ecological properties. As it can be seen from Table 3, the corrected recipe for GIP blending is practically the same as the existing one. The main part of feedstock consists of straight run gasoline No.2 streams and raffinate of aromatics production. It can be noticed that in existing recipes there are streams of straight run gasoline No.1, and aromatics production feedstock streams, but in corrected recipes they were excluded.

Table 3. Corrected blending recipes of Normal-80 and GIP gasoline brands, wt. %.

Feedstock streams	Normal-80 (cor.)	Normal-80 (ex.)	GIP (cor.)	GIP (ex.)
Catalytic cracking gasoline No.1	17.17	55.72	–	–
Catalytic cracking gasoline No.2	3.90	1.09	–	–
Reformate (fixed-bed)	8.05	6.25	–	–
Reformate (moving-bed)	5.09	–	–	–
Izomerizate	–	0.97	–	–
Isopentane No.1	6.36	–	–	–
n-butane	0.53	–	–	–
Straight run gasoline No.1	0.31	0.09	–	0.29
Straight run gasoline No.2	23.84	15.89	49.39	51.72
Aromatics C_8	3.97	–	–	–
Aromatics C_9	1.19	–	–	–
Feedstock for aromatics production	0.08	0.03	–	0.08
Raffinate of aromatics production	19.85	14.72	50.61	47.91
Condensate of aromatics production	1.01	3.01	–	–
Toluene	8.66	2.24	–	–

Table 4. Corrected blending recipes of Regular-92, Premium-95 and Super-98 gasoline brands, wt. %.

Feedstock streams	Regular-92 (cor.)	Regular-92 (ex.)	Premium-95 (cor.)	Premium-95 (ex.)	Super-98 (cor.)	Super-98 (ex.)
Gasoline of catalytic cracking No.1	4.54	3.93	7.41	7.21	4.08	4.01
Gasoline of catalytic cracking No.2	48.77	45.46	18.72	21.05	7.78	7.65
Reformate (fixed-bed)	15.09	16.73	8.49	6.85	15.05	14.80
Reformate (moving-bed)	3.81	4.66	14.73	15.47	13.36	13.13
Izomerizate	11.76	13.59	6.80	1.24	1.57	1.54
Isopentane No.1	4.00	3.82	20.10	23.82	20.33	20.00
Isopentane No.2	0.10	0.24	1.44	1.53	3.85	1.28
n-butane	0.34	0.49	1.67	1.63	1.39	1.38
Alkylate	0.82	1.30	5.02	4.60	16.54	16.26
Aromatics C_8	3.27	2.70	5.87	8.97	7.75	7.62
Aromatics C_9	0.88	1.22	4.15	4.04	3.48	3.43
Straight run gasoline No.2	0.77	–	2.04	–	–	–
Platformate of aromatics production	–	0.40	2.31	1.32	–	1.11
Raffinate of aromatics production	1.63	–	–	–	–	–
Toluene	4.12	5.47	–	0.96	0.80	0.79
MTBE	0.10	–	1.26	1.31	4.00	6.99

According to the data from Table 3, in correct recipes amounts of raffinate of aromatics production and straight run gasoline No.2 were significantly increased due to increase in production volumes of this gasoline brand. That streams were saved at the expense of reducing volume of GIP production. In this regard for enhancing the main property (RON) of gasoline, the following streams were involved: reformate (moving-bed), aromatics C_8, aromatics C_9; contents of the following streams were increasing: reformate (fixed-bed), catalytic cracking gasoline No.2, toluene. The isopentane stream No.1 and n-butane were involved in the blending scheme in order to increase SVP.

The aim of the recipes correction for Regular-92 gasoline blending was to reduce RON to the desired (from 93.5 to 92 points) and, in the same time, to decrease amount of aromatic hydrocarbons. Corrected volume of Regular-92 gasoline production affects the corrected recipes. As the part gasoline, that was previously used to produce Regular-92 gasoline, was switched to produce Normal-80 gasoline, the production volume of this brand was reduced to 10 000 tons (6.23 wt. %).

The amount of the next streams, such as toluene, reformate (moving-bed), reformate (fixed-bed) was decreased and streams of raffinate of aromatics production and straight run gasoline No.2 was involved to reduce contents of aromatics hydrocarbons and ON.

The task of blending recipes correction was to decrease the ON to the desired values and to decrease high contents of aromatics (from 38 wt. % to 35 wt. %). For reducing of aromatics hydrocarbons amount mainly the contents of aromatics C_8 streams were decreased (from 8.97 wt. % to 5.87 wt. %), that surplus was used to the Regular-92 brand production. Also, the toluene stream was excluded, but the content of not-aromatics isomerizate stream was increased. For increasing SVP of Normal-80 gasoline the isopentane No.1 stream taken from recipes Premium-95 gasoline was used, thus the content of isopentane No.1 stream was decreased. At the expense of increasing volume production Super-98 gasoline volume production Premium-95 gasoline was reduced to the 3 wt. %.

As it can be seen from Table 4 change of Super-98 gasoline recipes is insignificant in spite of increasing volume production on 47 wt. %. ON in existing recipes was enhanced, thus amount of supplements-oxygen was decreased in corrected recipes. That surplus was used to increase ON of other brand gasoline.

Table 5 shows the main properties of gasoline producing by correct recipes.

Table 5. The main properties of gasoline produced at oil refinery by corrected recipes.

Characteristic	Normal-80	Regular-92	Premium-95	Super-98	GIP
RON	80.0	92.0	95.1	98.0	56.1
SVP, kPa	37.1	46.6	63.5	62.1	24.1
Density, kg/m^3	733.17	725.49	718	717.85	695.03
Viscosity, sP	41.38	41.11	39.47	38.38	35.55
Olefins, wt. %	4.74	14.66	6.77	3.05	0.84
Benzene, wt. %	0.9	1.0	1.0	0.9	0.7
Aromatic hydrocarbons, wt. %	30.4	33.2	35.0	34.5	1.1

As it can be seen from Table 5 all properties of gasoline comply the Russian Technical Peculations demands and State Standard R 51866-2002. It means that recipes can be used for gasoline preparation. The amount of aromatic hydrocarbon was decreased in Regular-92 and Premium-95 gasoline as a result of correction. Also it can be noticed that there is not a surplus of primary streams, because ONs consistent with the stated. It allows save high-quality streams to using them for high-octane gasoline production.

Table 6 shows the data about gasoline volume changes, which is produced by corrected recipes.

As it can be seen volume of production GIP was decreased on 48 wt. % while the volume of production of Super-98 gasoline was increased on the 47 wt. %.There are a volume changes of production of GIP due to the involving in the production part of Normal-80 gasoline, because of the volume of production Normal-80 gasoline increases on the 196 wt. %. As in the production of Normal-80 gasoline low-octane streams, such as straight run gasoline No.1 and raffinate of aromatics production were involved, it was necessary to use high-octane streams from Regular-92 gasoline production. In this regard there is a reduction volume of production of Regular-92 gasoline on the 6 wt. %. Volume changing of production Super-98 gasoline was due to decreasing high-octane components in existing recipes and involving the part of Premium-95 gasoline. Because of this there is a reduction volume of production Premium-95 gasoline on the 2 wt. %.

Table 6. Changing volumes of gasoline production.

Brand	Existing recipes, tons	Correct recipes, tons	Volume changing, wt. %
Normal-80	12 742	37 750	+196.26
Regular-92	145 592	136 526	-6.23
Premium-95	70 656	68 791	-2.64
Super-98	7 006	10 332	+47.47
GIP	35 814	18 411	-48.59

4. Conclusion

In this paper, a novel computer modelling system «Compounding» was developed. Practical importance of this system consists in increasing of the resource efficiency of gasoline blending process, by maximizing the yield and quality of high-octane trade gasoline. Such an effect is achieved by using only internal oil refinery resources, and this is beneficial in terms of economy and gasoline production technology.

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