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CALCULATION METHOD FOR PREDICTION OF THE CETANE INDEX OF BLEN DED DIESEL FUELS

Maria V. Kirgina*, Ilya A. Bogdanov, Andrey A. Altynov, Nataliya S. Belinskaya

National Research Tomsk Polytechnic University, Russia

Received October 1, 2018; Accepted December 21, 2018

Abstract

The article considers modern calculation methods for determining the cetane index of diesel fuels. The most accurate calculation method was established. The non-additivity of the cetane index and the fractional composition of diesel fuels was experimentally proven. The method for calculating the cetane index of blended diesel fuels was developed based on the true boiling points. The method takes into account the non-additivity of the cetane index.

Keywords: diesel fuel; calculation method; cetane index; fractional composition; true boiling point.

1. Introduction

Over the last years, a rapid increase in the number of motor transport equipped with diesel engines has been observed all over the world. Majority of the industrially developed countriesimporters of petroleum products are focused on the quality of diesel fuels and are bent on reduction of harmful emissions. Thus, strict control and improvement of the diesel fuel quality, produced these days, is one of the most crucial tasks.

The key quality indicators of diesel fuels, which are strictly imposed by requirements, include cetane index, flash point, density, kinematic viscosity and low-temperature properties (cloud point, cold filter plugging point, pour point).

The most important characteristic of diesel fuel when used in internal combustion engines is the cetane index. The optimal operation of modern engines is provided by diesel fuels with cetane index ranged from 45 to 55 points. In case of using the diesel fuel with the cetane index of less than 45 points, the ignition delay (the time between the injection and ignition of fuel) and the rate of pressure rise in the combustion chamber increase sharply resulting in enhancement of engine wear. When diesel fuel has the cetane index of more than 55 points, the combustion efficiency decreases, the smoke opacity increases, and fuel consumption in creases.

The essence of the experimental method for determination of cetane index is as follows: the cetane index of diesel fuel is determined by comparing its combustion characteristics in the test engine with the characteristics of blends of control fuels with a known cetane index under standard operating conditions. However, the experimental determination of the cetane index is a multi-stage and labor-intensive process, which requires certain skills, special equipment, as well as time and money costs. For these reasons, the selection of the most accurate calculation method and development of a new calculation method for prediction of cetane index are relevant tasks ^[1-5].

2. An overview of correlations for the quantitative prediction of the cetane index and selection of the most accurate calculation method

The cetane index (CI) of diesel fuels can be calculated using a number of correlations ^[6]. According to the formula presented in the international standard ISO 4264 "Petroleum products – Calculation of cetane index of middle-distillate fuels by the four-variable equation" ^[7], the calculation is performed according to the following equation with four variables:

$$CI_{ISO} = 45.2 + 0.0892 \cdot T_{10N} + (0.131 + 0.901B) \cdot T_{50N} + + (0.0523 - 0.42B) \cdot T_{90N} + [0.00049 \cdot (T_{10N}^2 - T_{90N}^2)] + 107B + 60B^2 T_{10N} = T_{10\%} - 215 T_{50N} = T_{50\%} - 260 T_{90N} = T_{90\%} - 310 B = [\exp(-0.0035 \cdot D_N)] - 1 D_N = D - 850$$
(1)

 $T_{10\%}$, $T_{50\%}$, $T_{90\%}$ are the boiling points of 10 % vol., 50 % vol., and 90 % vol. fraction, °C; D is the density at 15°C.

Also, the cetane index of diesel fuels can be calculated by the formula presented in the National State Standard 27768-88 "Diesel fuel. Determination of cetane index by calculation method" ^[8]. The method consists in measuring the density of diesel fuel at the temperature of 15°C and the average boiling point of the 50% vol. fraction of diesel fuel. In this method the cetane index is calculated by the equation:

$$CI_{NS} = 454.74 - 1641.416 \cdot \rho_4^{15} + 774.74 \cdot (\rho_4^{15})^2 - 0.554 \cdot t + 97.803 \cdot (\lg t)^2$$
(2)

 ρ_4^{15} is density at 15°C measured according to the National State Standard 3900-85 "Petroleum and petroleum products. Methods for determination of density", g/sm³; *t* is the boiling point of 50% vol. fraction corrected for the normal barometric pressure of 101.3 kPa, °C; *t* is measured according to the National State Standard 2177-99 "Petroleum products. Methods for determination of distillation characteristics".

To calculate the cetane index of oil fractions, the following equation, presented in the standard ASTM D976 "Standard test method for calculated cetane index of distillate fuels", can also be used ^[9]:

$$CI_{ASTM} = 0.49083 + 1.06577 \cdot x - 0.0010552 \cdot x^{2}$$

$$x = 97.833 \cdot (\log(T_{50\% F}))^{2} + 2.2088 \cdot API \cdot \log(T_{50\% F}) +$$

$$+0.01247 \cdot API^{2} - 423.51 \cdot \log(T_{50\% F}) - 4.7807 \cdot API + 419.59$$

$$API = \frac{141.5}{2} - 131.5$$
(3)

 $T_{50\%F}$ is the boiling point of 50 % vol. fraction, F; API is the relative specific gravity.

Using the data obtained by the experimental measurements at industrial production of diesel fuels, the cetane index was calculated by equations (1) – (3) (CI_{ISO} , CI_{NS} , CI_{ASTM}) to determine the most accurate calculation method. The results of the calculation were compared with experimentally measured cetane index of diesel fuels ($CI_{exp.}$) and the calculation errors (Δ_{ISO} , Δ_{NS} , Δ_{ASTM}) were determined. The results of the calculations are given in Table 1.

No.	T _{10%}	T _{50%}	T _{90%}	Density at 15°C	CI _{exp.}	CI_{ISO}	CI _{NS}	CIASTM	Δ_{ISO}	Δ_{NS}	Δ_{ASTM}
		°C		kg/m³				points			
1	187	222	266	826.0	43.30	43.31	42.97	43.52	0.01	0.33	0.22
2	194	223	265	825.6	44.10	44.08	43.46	44.00	0.02	0.64	0.10
3	198	234	278	831.6	45.00	44.96	44.87	45.07	0.04	0.13	0.07
4	201	237	283	831.5	46.10	46.06	45.81	46.02	0.04	0.29	0.08
5	192	229	285	823.3	47.10	47.08	46.28	46.80	0.02	0.82	0.30
6	221	285	339	857.4	47.20	47.17	48.42	49.48	0.03	1.22	2.28
7	228	283	337	856.0	48.10	48.12	48.50	49.49	0.02	0.40	1.39
8	228	287	341	856.2	48.60	48.62	49.15	50.45	0.02	0.55	1.85
3 4 5 6 7	198 201 192 221 228	234 237 229 285 283	278 283 285 339 337	831.6 831.5 823.3 857.4 856.0	45.00 46.10 47.10 47.20 48.10	44.96 46.06 47.08 47.17 48.12	44.8745.8146.2848.4248.50	45.07 46.02 46.80 49.48 49.49	0.04 0.04 0.02 0.03 0.02	0.13 0.29 0.82 1.22 0.40	0 0 0 2 1

Table 1. Results of calculating the cetane index of diesel fuel by different methods

No.	$T_{10\%}$	$T_{50\%}$	T _{90%}	Density at 15°C	CI _{exp.}	CI_{ISO}	CINS	CIASTM	Δ_{ISO}	Δ_{NS}	Δ_{ASTM}
9	231	283	339	853.9	49.30	49.31	49.17	50.28	0.01	0.13	0.98
10	261	305	340	865.7	50.30	50.32	49.03	51.39	0.02	1.27	1.09
11	262	312	338	866.3	50.70	50.67	49.77	52.85	0.03	0.93	2.15
12	260	299	345	862.1	51.40	51.36	49.26	51.25	0.04	2.14	0.15
13	271	315	346	868.1	51.70	51.73	49.60	52.89	0.03	2.10	1.19
14	269	314	350	866.2	52.30	52.36	50.05	53.36	0.06	2.25	1.06
15	272	314	355	865.9	53.10	53.08	50.14	53.47	0.02	2.96	0.37
16	268	312	355	863.1	53.50	53.55	50.74	54.04	0.05	2.76	0.54
17	280	320	353	867.2	54.10	54.12	50.45	54.40	0.02	3.65	0.30
							avera	ige error	0.03	1.33	0.83

According to the data in Table 1, the most accurate calculation method for determining the cetane index is the method presented in ISO 4264 since the average error of this method is 0.03 points, while the average errors of the methods presented in the National State Standard 27768-88 and ASTM D976 are 1.33 and 0.83 points, respectively. The method presented in the ISO 4264 standard is used for further calculations.

3. Non-additivity of the cetane index and the fractional composition of diesel fuels

In this work, the cetane indices of the components of diesel fuels were calculated according to the equation ISO 4264 "Petroleum products – Calculation of cetane index of middle-distillate fuels by the four-variable equation" using the data from Russian industrial enterprise ^[10]. The results of the calculation are presented in Table 2.

Component	T10%	T50%	T90%	Density at 15°C	CIISO
	170	0C	256	kg/m ³	45.0
Straight-run diesel fraction	176	198	256	801.3	45.9
Kerosene fraction	159	180	211	787.4	43.6
Hydrotreated diesel fraction	258	292	336	844.9	57.4
Dewaxed diesel fraction	208	243	283	835.0	46.3

Table 2. Calculated cetane indices of commercial diesel fuels components

Further, the calculations of cetane indices of commercial diesel fuels blends, were performed. Cetane indices for mixtures were also determined experimentally. The calculation was performed according to the rule of additivity, assuming that each of the components contributes to the total cetane index of the blend in proportion to its mass fraction in this blend:

$$CI_{mix.} = \sum_{i=1}^{n} CI_i v_i$$

(4)

 $CI_{mix.}$ is the cetane index of the blend, points; CI_i is the cetane index of i^{th} component of the blend, points; v_i is the mass fraction of i^{th} component in the blend, % wt.

Table 3 shows the ratios of the blending components of diesel fuel (blending recipes), the cetane indices of the blends determined experimentally ($CI_{mix.exp.}$), cetane indices of the blends calculated according to the rule of additivity ($CI_{mix.add.}$), as well as the error ($\Delta_{add.}$) and the average calculation error ($\Delta_{add.av.}$) of the cetane index of the blends determined by the rule of additivity.

As a result, the difference between the cetane index of the blend, determined experimentally, and the cetane index of the blend, calculated according to the rule of additivity, varies from 1 to 3 points. This fact evidences the non-additivity of the cetane index of diesel fuels. Thus, there is the necessity to develop methods for calculating the cetane indices of blended diesel fuels, taking into account the non-additivity.

		Ble	nds	
Components	1	2	3	4
		vi, %	6 wt.	
Straight-run diesel fraction	0.40	0.40	0.37	0.40
Kerosene fraction	0.12	0.00	0.00	0.00
Hydrotreated diesel fraction	0.30	0.35	0.40	0.50
Dewaxed diesel fraction	0.18	0.25	0.23	0.10
CImix.exp.	47	49	48	50
CImix.add.	49	50	51	52
Δ add.	2	1	3	2
Δ add.av.		-	2	

Table 3. Calculated cetane indexes of blended diesel fuels

Calculation of the cetane index of blended diesel fuel, taking into account the non-additivity, is possible by using the fractional composition of blend. However, when solving the problems of production planning (the development of blending recipes), the blend is not yet exist, and it is impossible to determine its fractional composition. At the same time, the fractional composition of the blending components is usually known. A further stage of the study was to establish whether the fractional composition of diesel fuel is subject to the rule of additivity.

For this purpose, 4 samples of commercial diesel fuel were taken from fuel station located in Russia. Each sample was assigned a numerical cipher from 1 to 4. For all 4 samples, the fractional composition was determined experimentally (Table 4).

No.	IBP	T10%	T20%	T30%	T40%	T50%	T60%	T70%	T80%	T90%
NO.										
1	142	177	203	225	244	263	281	301	322	353
2	172	198	214	231	246	260	275	291	311	339
3	130	202	225	242	260	275	294	314	334	331
4	162	214	239	256	268	278	290	304	318	336

Table 4. Fractional composition of diesel fuels

Using the 4 samples of commercial diesel fuel, the blends were prepared according to the recipes presented in Table 5. Each prepared blend was assigned a numerical number from 1 to 9.

No of the		Compos	sition, %	
blend	1	2	3	4
1	50	20	30	-
2	50	50	_	-
3	70	30	-	-
4	80	20	-	-
5	_	33.3	33.3	33.4
6	-	50	30	20
7	-	50	20	30
8	_	30	50	20
9	-	20	30	50

Table 5. Blending recipes of commercial diesel fuels

Based on the fractional composition, presented in Table 4, and the blending ratios of diesel fuel, presented in Table 5, the fractional composition of blends 1-9 was calculated by the rule of additivity. The calculation results were compared with the experimentally determined fractional composition of blends 1-9 (Table 6).

As a result, the fractional composition of the blended diesel fuels is also a non-additive value, the average calculation error by the rule of additivity varies from 2 to 9°C.

			Experim	nentally o	letermin	ed fracti	onal com	position		
No.	IBP	T 10%	T20%	T30%	<i>T</i> 40%	T 50%	T 60%	<i>T</i> 70%	T 80%	T 90%
					0	С				
1	147	186	207	231	250	266	282	303	325	339
2	139	184	204	221	240	256	270	290	310	326
3	147	185	205	223	240	259	276	294	314	344
4	140	180	203	222	240	258	276	295	318	346
5	155	201	219	244	257	271	285	301	319	320
6	168	202	222	237	254	268	283	300	319	344
7	167	205	221	239	254	268	283	300	318	342
8	167	207	226	244	259	274	289	306	329	348
9	166	210	226	249	262	275	289	305	324	344
Fractional composition calculated according to the rule of additivity										
No.	IBP	<i>T</i> 10%	T20%	T 30%	<i>T</i> 40%	<i>T</i> 50%	T 60%	T 70%	T 80%	<i>T</i> 90%
						С				
1	144.4	188.7	211.8	231.3	249.2	266.0	283.7	302.9	323.4	343.6
2	157.0	187.5	208.5	228.0	245.0	261.5	278.0	296.0	316.5	346.0
3	151.0	183.3	206.3	226.8	244.6	262.1	279.2	298.0	318.7	348.8
4	148.0	181.2	205.2	226.2	244.4	262.4	279.8	299.0	319.8	350.2
5	153.1	202.6	223.7	240.6	255.4	268.3	283.5	300.0	317.8	332.0
6	157.4	202.4	222.3	239.3	254.6	268.1	283.7	300.5	319.3	336.0
7	160.6	203.6	223.7	240.7	255.4	268.4	283.3	299.5	317.7	336.5
8	149.0	203.2	224.5	241.5	257.4	271.1	287.5	305.1	323.9	334.4
9	154.4	207.2	229.8	246.8	261.2	273.5	288.2	304.4	321.4	335.1
					Δa	dd.				
No.	IBP	T 10%	T20%	T 30%	<i>T</i> 40%	T 50%	T 60%	T 70%	T 80%	T 90%
					0	С				
1	2.6	2.7	4.8	0.3	0.8	0.0	1.7	0.1	1.6	4.6
2	18.0	3.5	4.5	7.0	5.0	5.5	8.0	6.0	6.5	20.0
3	4.0	1.7	1.3	3.8	4.6	3.1	3.2	4.0	4.7	4.8
4	8.0	1.2	2.2	4.2	4.4	4.4	3.8	4.0	1.8	4.2
5	1.9	1.6	4.7	3.4	1.6	2.7	1.5	1.0	1.2	12.0
6	10.6	0.4	0.3	2.3	0.6	0.1	0.7	0.5	0.3	8.0
7	6.4	1.4	2.7	1.7	1.4	0.4	0.3	0.5	0.3	5.5
8	18.0	3.8	1.5	2.5	1.6	2.9	1.5	0.9	5.1	13.6
9	11.6	2.8	3.8	2.2	0.8	1.5	0.8	0.6	2.6	8.9
∆av.	9.0	2.1	2.9	3.0	2.3	2.3	2.4	2.0	2.7	9.1

Table 6. Comparison of the fractional composition calculated according to the rule of additivity with experimentally determined fractional composition

4. Calculation method for prediction of the cetane index of blended diesel fuels taking into account non-additivity

As the fractional composition of diesel fuel does not subject the rule of additivity, the developed calculation method uses the true boiling points of the fractions.

Data obtained by atmospheric distillation of petroleum fractions, as a rule, do not represent the actual boiling points of the components in the fraction. Therefore, technologists are more

interested in the true boiling points (TBP) of the components in the petroleum product. TBP is obtained by distillation of petroleum products using a tray distillation column with 15-100 theoretical plates with a relatively high reflux ratio (1-5 or higher). A high degree of fractionation in these columns gives accurate separation of the components of the mixture. However, the lack of unified equipment and the complexity of the procedure itself are significant drawbacks of the laboratory measurement of the TBP. The determination of the TBP is more complex procedure than the determination of the fractional composition in terms of time and money. However, there are calculation methods for converting the fractional composition (FC) to the true boiling point [11]:

$$TBP = a(FC)^b$$

(5)

TBP is true boiling point, °K; *FC* is fractional composition, °K; *a*, *b* are empirical coefficients. The values of coefficients *a* and *b* are presented in Table 7.

<i>FC</i> , % vol.	а	Ь	<i>FC</i> , % vol.	а	b
0	2.9747	0.8466	70	8.2873	0.6871
10	1.4459	0.9511	90	10.6266	0.6529
30	0.8506	1.0315	100	7.9952	0.6949
50	3.2680	0.8274			

Table 7. Coefficients for converting the fractional composition to the true boiling point

Using equation (5), TBP was calculated for the components of diesel fuels produced at one of the Russian refineries (Table 2). Using the obtained correlations, the initial boiling point (0%) and the end boiling points (100%) of fractions were determined (Table 8).

Table 8. TBP of diesel fuel components

Component		FC				TBP		
Component	10%	50%	90%	0%	10%	50%	90%	100%
Straight-run diesel fraction	449	471	529	423	433	473	541	559
Kerosene fraction	432	453	484	405	415	455	495	505
Hydrotreated diesel fraction	531	565	609	507	520	569	624	638
Dewaxed diesel fraction	481	516	556	454	467	519	569	582

In view of the absence of information on the initial and the end boiling points of fractions, the correlations of distillation yield of the fraction versus the boiling point were founded. These correlations were used to obtain necessary data (Figures 1-8).

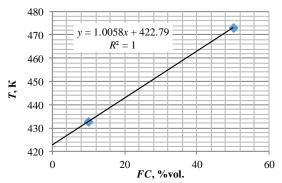


Figure 1. Distillation yield of straight-run diesel fraction versus initial boiling point dewaxed diesel fraction versus end boiling point

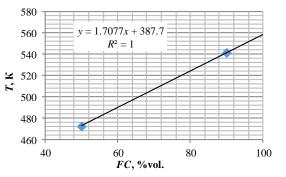


Figure 2. Distillation yield of straight-run diesel fraction versus end boiling point versus end boiling point

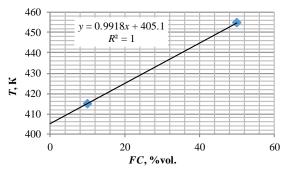


Figure 3. Distillation yield of kerosene fraction fraction versus initial boiling point of dewaxed diesel fraction versus end boiling point

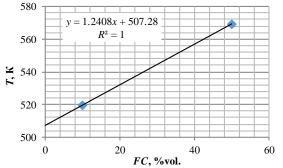


Figure 5. Distillation yield of hydrotreated diesel fraction versus initial boiling point

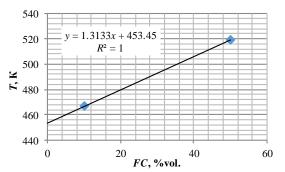


Figure 7. Distillation yield of dewaxed diesel fraction versus initial boiling point

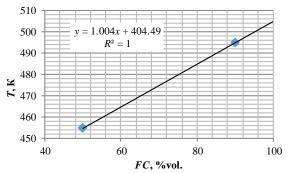


Figure 4. Distillation yield of kerosene fraction versus end boiling point

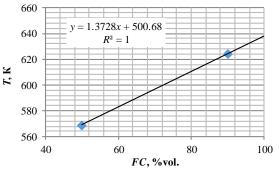


Figure 6. Distillation yield of hydrotreated diesel fraction versus end boiling point

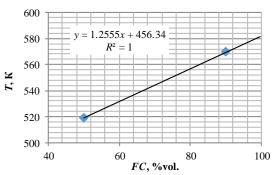


Figure 8. Distillation yield of dewaxed diesel fraction versus end boiling point

Using the data presented in Table 8, the distillation yields of fractions were calculated at the temperature from the initial boiling point to the end boiling point in increments of 1°K.

To calculate the cetane index of the blended diesel fuel, the key component of the blend are determined, i.e. the component whose proportion in the blending recipe is greatest. Further, the true boiling point of 90 % vol. fraction of the key component are determined (Table 8). Then, at the temperature obtained from the correlations, presented in Figures 1-8, the distillation yields of the remaining components involved in blending (μ_i) are determined. Then the obtained values are multiplied by the volume content of the components in the blend (v_i) and the obtained values are normalized (X_i). The obtained values (Y_i) represent the proportion of each component contributes to the cetane index of the blend.

Let's consider an example of calculation of the cetane index of the blended diesel fuel, produced according to the blending receipt No. 1, presented in Table 3.

The key component of diesel fuel produced according to the blending receipt No. 1 is straight-run diesel fraction. The true boiling point of 90 % vol. fraction of this component is

541 °K (Table 8). From the correlations presented in Figures 3-8, we determine that at the temperature of 541 °K, 27 % vol. hydrotreated diesel fraction, 67.5 % vol. dewaxed diesel fraction, and 100 % vol. kerosene fraction are distilled.

The values of X_i are determined as follows:

 $X_{i} = \mu_{i} \cdot \nu_{i}$ Thus, we obtain: $X_{1}=0.4.0.9=0.360$; $X_{2}=0.1.1=0.120$; $X_{3}=0.3.0.27=0.081$; $X_{4}=0.18.0.675=0.122$; Then we normalize the values of X_{i} : $Y_{i} = X_{i} / \sum_{i=1}^{n} X_{i}$ Thus, we obtain: $Y_{1}=0.527$; $Y_{2}=0.176$; $Y_{3}=0.119$; $Y_{4}=0.179$ (6)

The cetane idex is calculated according to the rule of additivity. Using the developed calculation method, the cetane indices of the blended diesel fuels ($CI_{mix.met.}$) were calculated for the four blending recipes presented in Table 3 (Table 9).

Table 9. Calculated cetane indices using the developed method

Component	Vi	μ_i	Xi	Yi	CI_{ISO}	CI mix.met.
	R	eceipt No	. 1			
Straight-run diesel fraction	0.40	0.900	0.360	0.527	45.9	
Kerosene fraction	0.12	1.000	0.120	0.176	43.6	47
Hydrotreated diesel fraction	0.30	0.270	0.081	0.119	57.4	47
Dewaxed diesel fraction	0.18	0.675	0.122	0.179	46.3	
	R	eceipt No	. 2			
Straight-run diesel fraction	0.40	0.900	0.360	0.578	45.9	
Hydrotreated diesel fraction	0.35	0.270	0.095	0.152	57.4	48
Dewaxed diesel fraction	0.25	0.675	0.169	0.271	46.3	
	R	eceipt No	. 3			
Straight-run diesel fraction	0.37	1.000	0.370	0.380	45.9	
Hydrotreated diesel fraction	0.40	0.900	0.360	0.370	57.4	50
Dewaxed diesel fraction	0.23	1.000	0.230	0.240	46.3	
	R	eceipt No	. 4			
Straight-run diesel fraction	0.40	0.900	0.360	0.640	45.9	
Hydrotreated diesel fraction	0.50	0.270	0.135	0.240	57.4	49
Dewaxed diesel fraction	0.10	0.675	0.0675	0.120	46.3	

Calculated values were compared with experimentally determined cetane indices of blends, as well as with cetane indices of blends, calculated according to the rule of additivity (Table 10).

Receipt	CImix.exp.	CImix.add.	CImix.met.	Δ add.	∆met.
1	47	49	47	2	0
2	49	50	48	1	1
3	48	51	50	3	2
4	50	52	49	2	1
			∆ av.	2	1

Thus, the developed method allows calculating the cetane index of blended diesel fuels with an average error ($\Delta_{met.}$) not exceeding 1 point, while the calculation according to the rule of additivity has an average error of 2 points.

5. Conclusion

1. Based on the experimental data, it was established that the most accurate method for calculating the cetane index of diesel fuel is the method proposed by the ISO 4264 "Petroleum products – Calculation of cetane index of middle-distillate fuels by the four-variable equation". This method can be used for the successful quantitative prediction of cetane indices of diesel fractions. 2. Using the industrial blending recipes for the production of diesel fuels, it was shown that the cetane index of blended diesel fuels is non-additive value. The average deviation from the calculation according to the rule of additivity is 2 points.

3. On the basis of laboratory studies, it was established that the fractional composition of the blended diesel fuels does not subject the rule of additivity. The average error of calculation by the rule of additivity varies from 2 to 9 °C.

4. The developed calculation method for prediction of the cetane index of the blended diesel fuels is based on the true boiling points of blending components. The method takes into account non-additivity of the cetane index. The absolute error of calculating the cetane index according to the developed method does not exceed 1 point.

Acknowlegements

The work was performed within the framework of the state task №10.13268.2018/8.9.

List of symbols

CI – cetane index, points;

T10% – boiling point of 10%vol. fraction, °C;

T50% – boiling point of 50%vol. fraction, °C;

T90% – boiling point of 90%vol. fraction, °C;

 $D - density at 15 \,^{\circ}C, kg/m^3;$

 $\rho^{4^{15}}$ – density at 15 °C, g/sm³;

t – boiling point of 50 % vol. fraction corrected for the normal barometric pressure of 101.3 kPa, °C. T_{50%F} – boiling point of 50 % vol. fraction, °F;

API – relative specific gravity;

CIIso – cetane index proposed by the ISO 4264 "Petroleum products – Calculation of cetane index of middle-distillate fuels by the four-variable equation", points;

CINS – *cetane index proposed by the National State Standard* 27768-88 "*Diesel fuel. Determination of cetane index by calculation method*", *points;*

CIASTM – cetane index proposed by the ASTM D976 "Standard test method for calculated cetane index of distillate fuels", points;

Clexp. - cetane index determined experimentally, points;

 Δ _{ISO} – calculation error of cetane index according to the ISO 4264 "Petroleum products – Calculation of cetane index of middle-distillate fuels by the four-variable equation", points;

 ΔNS – calculation error of cetane index according to the National State Standard 27768-88 "Diesel fuel. Determination of cetane index by calculation method", points;

 Δ ASTM – calculation error of cetane index according to the ASTM D976 "Standard test method for calculated cetane index of distillate fuels", points;

CImix. - cetane index of the blend, points;

CIi – cetane index of *i*th component of the blend, points;

vi – *mass fraction of ith component in the blend, % wt.;*

CImix.exp. – *cetane index of the blend determined experimentally, points;*

CImix.add. - cetane index of the blend calculated according to the rule of additivity, points;

 $\Delta_{add.}$ – calculation error of the cetane index by the rule of additivity, points;

 $\Delta_{add.av.}$ – average calculation error of the cetane index by the rule of additivity, points;

TBP – true boiling point, °K;

FC – fractional composition, °K;

a, b – empirical coefficients for calculation of true boiling point;

 μ_i – distillation yield of ith component at true boiling point of 90 % vol. fraction of the key component, % vol.;

 X_i – coefficient for converting the content of ith component in the blend used to calculate cetane index taking into account non-additivity;

Yi – proportion of each component contributes to the cetane index of the blend;

CImix.met. – cetane index of the blend, calculated according to the developed method, points;

 $\Delta_{met.}$ – calculation error of cetane index of the blend according to the developed method, points.

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To whom correspondence should be addressed: Dr. Maria V. Kirgina, Division for Chemical Engineering, School of Earth Sciences & Engineering, National Research Tomsk Polytechnic University, 30, Lenin Avenue, Tomsk, 634050, Russia; e-mail: mkirgina@tpu.ru