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Short communication

RELATIONSHIP BETWEEN THE AVERAGE BOILING TEMPERATURES OF PETROLEUM DISTILLATE FRACTIONS AND THEIR STOICHIOMETRIC BURNING COEFFICIENTS

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ABSTRACT

An experimental correlation for calculating of the stoichiometric burning coefficient of petroleum distillate fractions from their average boiling temperature is derived. The obtained dependency is applicable for the individual hydrocarbons.

Keywords: Petroleum fractions, stoichiometric burning coefficient.

INTRODUCTION

To calculate some of the indicators for fire hazard of substances, such as concentration limits of ignition, heat of combustion, flame temperature, etc., a stoihiometric burning coefficient is used [1-3]. Analytically it is determined by the type and number of atoms that take part in the burning process, which is why, it is necessary to know the elemental composition of the compound.

The calculation of the stoichiometric burning coefficient of petroleum products, on the basis of the number of atoms taking part in the burning, is difficult. The petroleum products are a mixture of hydrocarbons. Their average empirical formula provide information about the molecular mass and elemental composition which however, are usually not determined in the production process.

Bearing this in mind, we set ourselves the task of checking the possibilities for calculation of the stoichiometric burning coefficient of petroleum distillate fractions with the help of their average boiling temperature, a parameter experimentally controlled in their production.

EXPERIMENTAL

In order to study the targeted dependency, we used experimental data about the elemental composition, molecular mass and fractional composition of 63 petroleum fractions [4, 5]. If we neglect the content of nitrogen, oxygen and sulphur in the petroleum distillate fractions, the stoichiometric burning coefficient can be calculated as follows [1]:

$$\beta_1 = m_c + 0.25 m_H \qquad (1)$$

where m_c and m_H are the number of hydrocarbon and hydrogen atoms in the average carbon molecule of the fraction.

The number of carbon and hydrogen atoms in their average molecules, resp. the stoichiometric burning coefficients were calculated from the data for the elemental composition and molecular mass. The data for the fractional composition were used to determine the average boiling temperatures.

The graphic analysis of the results for stoichiometric burning coefficient, calculated with equation [1], and the average boiling temperature of the 63 petroleum fractions showed that in a half-logarithmic coor-

Table 1. Chemical composition, molecular mass, average boiling temperatures and stoichiometric burning coefficients for the different petroleum fractions.

No	Petroleum oil fraction	Elemental composition		Molecular mass, M	Average boiling temperature, $T_{Cp.k.}$, °C	Stoichiometric burning coefficient	
		% C	% H			β_1	β_2
1	Pyrolysis oil fraction	91,39	8,49	83,7	85	7,5	9,65
2	Pyrolysis oil fraction	90,34	9,23	86,4	114	7,5	10,87
3	Pyrolysis oil fraction	85,65	13,04	236,0	350	24,0	23,31
4	Pyrolysis oil fraction	90,47	9,35	97,0	175	9,0	13,96
5	Pyrolysis hidrated oil fraction	89,40	10,40	97,0	175	8, 57	13,96
6	Hydrogenated pyrolysis mixture	86,23	13,77	80,0	67	7,50	8,98
7	Hydrogenated pyrolysis mixture	89,19	13,81	105,0	116	10,50	10,96
8	Hydrogenated pyrolysis mixture	85,99	14,01	139,0	175	13,50	13,96
9	Hydrogenated pyrolysis mixture	86,99	14,01	172,0	219	18,00	16,72
10	Hydrogenated pyrolysis mixture	86,14	13,86	122,0	139	12,00	12,04
11	Hydrogenated pyrolysis mixture	86,21	13,79	91,0	91	9,00	9,89
12	Hydrogenated pyrolysis mixture	86,09	13,91	120,0	145	12,00	12,34
13	Hydrogenated pyrolysis mixture	85,99	14,01	154,0	197	13,70	15,28
14	Hydrogenated pyrolysis mixture	86,16	13,84	113,0	127	12,00	11,47
15	Hydrogenated pyrolysis mixture	86,07	13,93	130,0	157	13,50	12,97
16	Hydrogenated pyrolysis mixture	84,14	13,86	107,0	132	9,00	11,70
17	Hydrogenated pyrolysis mixture	86,08	13,92	134,0	162	13,50	13,24
18	Hydrogenated pyrolysis mixture	86,11	13,89	124,0	142	12,50	12,20
19	Hydrogenated pyrolysis mixture	86,89	13,11	83	76	7,50	9,30
20	Hydrogenated pyrolysis mixture	86,70	13,30	101	112	9,00	10,78
21	Hydrogenated pyrolysis mixture	86,38	13,62	134	171	13,5	13,74
22	Hydrogenated pyrolysis mixture	86,63	13,37	120	139	12,0	12,04
23	Oil fraction from Borneo	87,30	11,99	233	299	24,0	23,21
24	Oil fraction from Borneo	88,05	11,35	248	327	25,5	26,04
25	Oil fraction from Borneo	88,43	10,93	267	345	25,0	28,03
26	Oil fraction from Borneo	88,42	10,71	281	365	26,25	30,43
27	Oil fraction from Borneo	88,26	10,63	305	385	28,75	33,03

dination system, the dependency between them can be approximated with the following equation:

$$\beta_2 = A.e^{B.t_{Cp}.K} \quad (2)$$

where A and B are coefficients and t_{Cp}. - the average boiling temperature of the petroleum distillate fraction.

The values of the coefficients A and B were determined by the least-sguare-method and equation (2) became:

$$\beta_2 = 6.8132.e^{0.0041.t_{Cp}.K} \quad (3)$$

Table 1 shows the chemical composition, molecular mass, average boiling temperatures and stoichiometric burning coefficients for the different petroleum fractions.

RESULTS AND DISCUSSION

The accuracy of equation (3) can be estimated by the difference between the values of β calculated from the element of composition and the equation. For 46,5 % of the used data, the absolute differences are below one unit, for 36,0 % of the data – between one and three, and for 17,5 % of them there were absolute differences between one and three.

Equation (3) is applicable for individual hydrocarbons as well. The validation done with different hydrocarbons (normal and isosaturated, non-saturated- with double and triple bond, paraffin hydrocarbons, aromatic, alkyl-cyclopentane and alkyl-cyclohexane hydrocarbons) with boiling temperatures from 162°C to 330°C showed that in these cases, the deviations are the same as with the petroleum distillate fractions.

CONCLUSIONS

An exponential correlation for prediction of the stoichiometric burning coefficients of the petroleum distillate fractions from their average boiling temperatures is derived. With sufficient accuracy the obtained correlation is applicable for individual hydrocarbons as well.

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