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REGRESSION EQUATIONS FOR CALCULATING THE SOLUBILITY OF HYDROGEN IN LIQUID FUELS

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The efficiency of combustion of liquid fuels in heat engines is determined by their hydrocarbon composition. The rate of combustion and the completeness of combustion depend on the hydrocarbon composition of the fuel. One of the ways to increase the efficiency of combustion of fuel is to use fuel-hydrogen mixtures. The use of such mixtures gives prerequisites for low-temperature self-ignition of fuel droplets (about 590 °C). Preheating of the fuel gives the possibility of "explosive" combustion with increasing of the temperature up to 2500 K in 0.02 –. 0.04 ms. This leads to the intensification of heavy fuel combustion. The use of fuel-hydrogen mixtures allows to obtain a low level of harmful emissions with flue gases and to reduce emissions: CO and CH – not less than 15%, CO_2 – not less than 20%. A promising direction for the creation of such mixtures is the direct dissolution of hydrogen in liquid fuel. This simplifies the flow of the fuel-hydrogen mixture into the combustion chamber of the heat engine or into the cylinders of the internal combustion engines. Analysis of previous studies showed the possibility of obtaining a single form of regression dependence for calculations of the dissolution of hydrogen in liquid fuels. The processing of the literature data and the results of our own research gave a set of regression equations for calculating the solubility of hydrogen in liquid fuels: gas, diesel, fuel oil, LVGO, HVGO, GDAR, ABVB. The obtained regression dependencies show that with increasing average molecular weight the solubility of hydrogen in the fuel decreases. These regression dependencies make it possible to obtain baseline data for the design of fuel systems for supplying fuel and hydrogen mixtures to combustion chambers of heat engines. Studies of hydrogen-diesel have shown a decrease in the flash fuel temperature by 10 – 15 ^{o}C by comparison with pure fuel. For heavy fuels, this level of reduction of the fuel round is not sufficient. Therefore, it is necessary to conduct further studies on the intensification of the process of dissolution of hydrogen in heavy fuels. This will significantly reduce energy costs for the organization of the combustion process.

Keywords: hydrogen, fuel, solubility, regression dependences.

INTRODUCTION. The combustion efficiency of liquid fuels in thermal installations is determined primarily by the hydrocarbon composition of the fuel. The combustion rate and completeness of combustion depend on the hydrocarbon composition of the fuel. Therefore, the intensification of fuel combustion processes is an urgent task to improve the efficiency of heat engines.

One way to solve this problem is to use hydrogen-fuel mixtures [1]. The experimental results show that at low concentrations of hydrogen in fuel – air mixtures an abnormal increase in the completeness of fuel combustion is observed. The intensification of the combustion processes of fuel - air mixtures with hydrogen additives is confirmed by the data [2–4].

Research [1–4] was conducted on internal combustion engines, in which the fuel supply system was modernized. Hydrogen was supplied to the engine cylinders simultaneously with the supply of liquid fuel. This required the provision of a hydrogen pressure in the supply system exceeding the pressure of compressed air in the cylinder. This reduces the reliability of the internal combustion engine.

The obtained data [1] on the intensification of the process of burning liquid fuel with small additions of hydrogen to the fuel – air mixture allow us to make an assumption about the possibility of using fuel-hydrogen mixtures in heat engines. In this case, we can consider the process of obtaining fuel-hydrogen mixtures by pre-dissolving hydrogen in fuel. This simplifies the supply of fuel-hydrogen mixture to the combustion chamber of a heat engine or to the internal combustion engine cylinders.

Studies of the solubility of hydrogen in liquid fuel [5–10] allow us to conclude that the use of fuel-hydrogen mixtures in heat engines is promising. However, the process of dissolving hydrogen in liquid fuel is not well understood. The possibility of using hydrogen-fuel mixtures in heat engines requires additional research.

The solubility of hydrogen in liquid fuel substantially depends on the hydrocarbon and fractional compositions of the fuel. These parameters depend on the oil field and the characteristics of the rectification process. In addition, the constant hydrocarbon and fractional composition of the fuel is extremely difficult to ensure during operation of the heat engine. Therefore, it is advisable to have integral characteristics for estimating the amount of hydrogen dissolved in liquid fuel when it is saturated with hydrogen.

The aim of the work is to obtain regression dependences for calculating the saturation of light fuels (diesel fuel and kerosene) with hydrogen at atmospheric pressure and a temperature of up to 60 °C.

EXPERIMENT AND DISCUSSION OF THE RESULTS. Liquid fuel is a multicomponent mixture of organic substances Henry's law [11] for a multicomponent mixture, taking into account the Wohl’s expansion [12], can be represented as:

$$\ln(H_{2M}) = x_1 \cdot \ln(H_{21}) + x_3 \cdot \ln(H_{23}) - \mathrm{a}_{13} \cdot x_1 \cdot x_3 \quad (1)$$

where $H_{2,\mathrm{M}}$ – Henry's constant for a gas 2; x_1 and x_2 – share of solvents 1 and 3 in the mixture, respectively; H_{21} and H_{23} – Henry's constants for individual solvents, respectively ; a_{13} – the interaction parameter of the solvents from Wohl’s expansion of the excess chemical potential of the ternary mixtures.

Improving the modeling of hydrogen solubility in heavy oil cuts using an Augmented Grayson-Streed (AGS) approach gives a significant deviation from experimental data [7]. This is due to the difficulty in determining the exact proportions of organic matter in the fuel.

Another important factor is the achievement of an equilibrium state between the gas and liquid phases. The intensity of mass transfer between phases during the absorption of hydrogen by fuel is described by Fick's law [13]:

$$J = D \cdot ({}^{dc}\!/_{dn}), \qquad (2)$$

where J is the diffusion flux; D is the diffusion coefficient of hydrogen in fuel; c is the concentration of hydrogen in fuel; n is position in the fuel layer.

The rapid achievement of equilibrium between the phases can be achieved with $D \to \infty$ or contact time $\tau \to \infty$. Parameters (D and τ) values cannot be reached equal to infinity in real experiments .Therefore, the experiment time [10] was determined based on the ratio of the dissolution time of a fixed volume of hydrogen at the beginning τ_b of the experiment to the time of dissolution of the same volume of hydrogen at the end of the experiment τ_e as $\tau_e / \tau_b = 15$ – based on the recommendations [14].

The value of the dosed hydrogen volume was taken equal to 0.01 + 0.0002 L. The time of complete dissolution of hydrogen bubbles was recorded. During the experiment, the data obtained were entered into a program for calculating the dynamics of hydrogen dissolution. As a result of the calculation, a graph of hydrogen solubility and a regression dependence of solubility were obtained. An example of processing experimental data is shown in fig. 1: the abscissa axis is the logarithm of the time of dissolution of hydrogen in the fuel ($\log(\tau 10)$); the ordinate axis is the logarithm is the amount of dissolved hydrogen in the fuel ($\log(m1)$); the vertical line is the predicted maximum amount of hydrogen in the fuel.

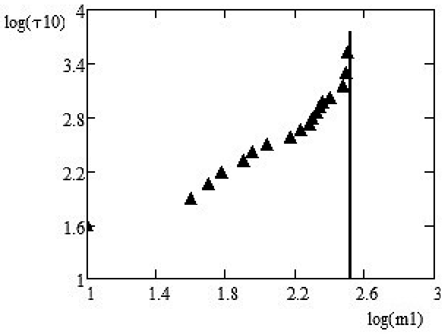

Fig. 1. An example of processing experimental data.

The graph (fig.1) showed the hydrogen solubility curve and the predicted limit value of the concentration of hydrogen in the fuel. The experiment ended when the solubility of hydrogen became equal to 0.97 from the equilibrium.

Based on the foregoing, it becomes appropriate to obtain regression equations for calculating the solubility of hydrogen in each fuel grade based on a regression analysis of experimental data [6–8, 10] and own experiments. Relevant physical properties for these fuels are given in table 1.

The data on hydrogen solubility in fuels (table 1) are summarized in the temperature range $T = 293 – 653$ K and pressures $P = 0 – 10$ MPa by the following regression dependence :

$$\begin{aligned} R(P,T) &= A \cdot B \\ A(T) &= a0 + a1 \cdot T + a2 \cdot T^2 \\ B(P) &= b0 + b1 \cdot P + b2 \cdot P^2 \end{aligned} \qquad (3)$$

Table 1

Characterization of fuels and experimental conditions

Name of fuel, source	Density, kg / *l*	*T*, K	*P*, MPa
Kerosene (K) [6]	0.840	298 – 573	4.7 – 30
Fuel oil (FO) [6]	0.930	473 – 573	10.0 – 30
Light Virgin Gas Oil (LVGO) [7]	0.892	353 – 653	2.2 – 11
HeavyVirgin Gas Oil (HVGO) [7]	0.973	353 – 653	1.0 – 11
GuDao Atmospheric Residuum (GDAR) [7]	0.922	353 – 653	0.9 – 11
Athabasca Bitumen Vacuum Bottoms (ABVB) [7]	1.050	353 – 653	0.9 – 10
Diesel fuel (DF) [10]	0.847	295 – 333	Atmospheric
Fuel oil [10]	0.937	295 – 333	Atmospheric

Table 2

The coefficients in equation (3)

Fuel	*a*0	*a*1	*a*2	*b*0	*b*1	*b*2
K [6]	1.69	$-7.0{\ast}10^{-3}$	$1.19{\ast}10^{-5}$	0.55	0.46	$1.54{\ast}10^{-3}$
FO[6],[10]	0.45	$-2.75{\ast}10^{-3}$	$5.9{\ast}10^{-6}$	2.00	0.55	$5{\ast}10^{-3}$
LVGO [7]	3.4	-0,011	$8.53{\ast}10^{-6}$	0.40	1.49	0,013
HVGO [7]	3.77	-0.011	$7.88{\ast}10^{-6}$	0.40	0.77	0.042
GDAR [7]	2.6	$-6.22{\ast}10^{-3}$	$4.81{\ast}10^{-6}$	0.083	0.954	-0.036
ABVB [7]	3.7	-0,012	$7.9{\ast}10^{-6}$	0.113	0.85	-0,026
DF [10]	3.3	-0.0105	$8.2{\ast}10^{-6}$	0.45	1.49	0,013

Table 3

The solubility of hydrogen in various fuels at atmospheric pressure and *T* = 298 K

Parameter	K	DF	FO	LVGO	HVGO	GDAR	ABVB
Solubility, l/l	0.363	0.405	0.309	0359	0.198	0.097	0.099
Mean molar mass, g/mol	162	144	310	250	350	1678	1700

The coefficients in equation (3) are shown in table 2. The error in determining the amount of hydrogen dissolved in the fuel according to the given regression does not exceed ± 8.3%. What is quite acceptable for the predictive assessment and design of fuel systems for such mixtures [15].

A graphical interpretation of experimental data processing in the form of paired regression (the dependence of hydrogen solubility on temperature and pressure) for LVGO [7] is shown in fig. 2.

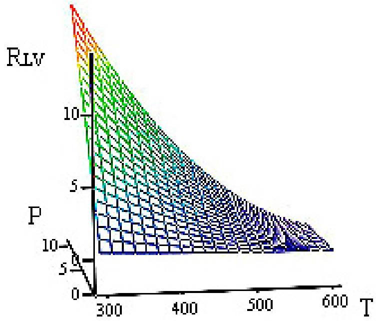

Fig.2. The dependence of hydrogen solubility on temperature and pressure) for LVGO [7].

Table 3 presents data on the solubility of hydrogen in various fuels at atmospheric pressure and T = 298 K. The data in table 3 show that the solubility of hydrogen in the liquid fuel depends on the average molecular weight of the fuel. As the average molecular weight of the fuel increases, the solubility of hydrogen in it decreases. The amount of dissolved hydrogen in light grades of fuel is quite sufficient to reduce the flash point by 10 – 15 K. Further increase of the concentration of hydrogen in light fuel is not appropriate based on the safety requirements of the heat engine.

CONCLUSIONS. The obtained regression equations allow us to predict the solubility of hydrogen in liquid fuel. Light grades of fuel do not require special preparation before the process of dissolution of hydrogen at atmospheric pressure.For heavy fuels it is necessary to develop methods of intensification of the process of dissolution of hydrogen in the fuel.

РЕГРЕСИВНІ РІВНЯННЯ ДЛЯ РОЗРАХУНКУ РОЗЧИННОСТІ ВОДНЮ В РІДКИХ ПАЛИВАХ

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Ефективність горіння рідких палив у теплових установках визначається їх вуглеводневим складом. Від вуглеводневого складу палива залежить швидкість його горіння і повнота згорання. Одним із шляхів підвищення ефективності згорання палива є використання паливно-водневих сумішей, що створює передумови до виникнення низькотемпературного самозаймання крапель палива (близько 590 °С). Попередній розігрів палива дає можливість виниканню «вибухового» горіння з підвищенням температури до 2500 К за 0,02 –. 0,04 мс. Це веде до інтенсифікації згорання важких палив. Застосування паливно-водневих сумішей дозволяє отримати низький рівень шкідливих викидів з димовими газами, і знизити викиди: СО і СН не менше 15, CO_2 – не менше 20 %. Перспективним напрямком створення таких сумішей є пряме розчинення водню в рідкому паливі. Це спрощує подачу паливно-водневої суміші в камеру згорання теплового двигуна або в циліндри двигунів внутрішнього згорання. Аналіз попередніх досліджень показав можливість отримання єдиної форми регресійної залежності для розрахунків розчинення водню у рідких паливах. Обробка літературних даних та результатів власних досліджень дала сукупність регресійних рівнянь для розрахунку розчинності водню в рідких паливах: гасі, дизельному паливі, мазуті, LVGO, HVGO, GDAR, ABVB, Отримані регресійні залежності показують, що з ростом середньої молекулярної маси палива розчинність водню в ньому знижується. Ці регресійні залежності дозволяють одержати вихідні дані для проектування паливних систем подачі паливо-водневих сумішей у камери згорання теплових машин. Дослідження насиченого воднем дизельного палива показали зменшення температури початку спалаху на 10 – 15 °C порівняно з чистим паливом. Для тяжких палив такий рівень зменшення температури палива недостатній. Тому необхідно вести подальші дослідження по інтенсифікації процесу розчинення водню в важких паливах. Це значно знизить витрати енергії на організацію процесу горіння палива.

Ключові слова: водень, паливо, розчинність, регресійна залежність.

РЕГРЕССИОННЫЕ УРАВНЕНИЯ ДЛЯ РАСЧЕТА РАСТВОРИМОСТИ ВОДОРОДА В ЖИДКИХ ТОПЛИВАХ

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Эффективность горения жидких топлив в тепловых установках определяется прежде всего углеводородным составом топлива. От углеводородного топлива зависит скорость его горения и полнота сгорания. Поэтому интенсификация процессов горения топлива является актуальной задачей повышения эффективности тепловых двигателей. Одним из путей повышения эффективности сгорания топлива является использование топливно-водородных смесей. Перспективным направлением создания таких смесей является прямое растворения водорода в жидком топливе. Это упрощает подачу топливно-водородной смеси в камеру сгорания теплового двигателя или в цилиндры ДВС. Анализ литературных данных и результатов собственных исследований показал возможность получения совокупности регрессионных уравнений для расчета растворимости водорода в жидких топливах: керосине, дизельном топливе, мазуте, LVGO, HVGO, GDAR, ABVB, анализ полученных регрессионной зависимости показал, что с ростом средней молекулярной массы топлива растворимость водорода в нем снижается. Полученные регрессионные зависимости позволяют получить исходные данные для проектирования топливных систем подачи топливно-водородных смей в тепловые машины.

Ключевые слова: водород, топливо, растворимость, регрессионная зависимость.

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