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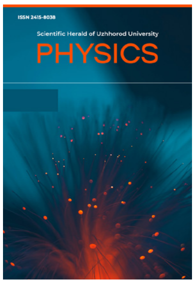

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Diffusion flames and a semi-empirical method for estimating the distribution of hydrogen molecules in propane flames

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Abstract

Relevance. The greatest effectiveness in determining the main characteristics in gas burning was shown by optical methods due to their high speed and accuracy. Despite all the advantages of these methods, their main disadvantage is the price and folding of implementation. Therefore, today it is necessary to improve approaches to solve this problem.

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Purpose. The research is devoted to the study of diffusion flame by a semi-empirical method.

Methods. The data of the experimental study of the diffusion flame of hydrocarbons on the example of propane are presented. To visualize the invisible part of the structure of this flame, namely, the afterburning zone of hydrogen molecules formed in the flames in nonequilibrium quantities and, due to the large value of the diffusion coefficient, leaving the flame zone and creating a new combustion zone, molecules containing atoms of alkali metals (NaCl and Na_2CO_3) are vaporized in the flame zone.

Results. The method of delivery of molecules of alkali metal salts from outside was applied for the first time, which allowed the investigation of this phenomenon more thoroughly. Based on the research results, a method for determining the concentration of hydrogen atoms and the relative distribution of the concentration of hydrogen molecules along the axis of propagation of the flame after the burning zone was proposed. The research method combines experiments with mathematical modeling. The application of the method described in the article makes it possible to determine the distribution of hydrogen molecules over the glow zone of the main fuel.

Conclusions. The results obtained will help to better understand the phenomena of hydrocarbon combustion under diffusion flame conditions, as well as to search for new ways of obtaining hydrogen fuel from domestic waste treatment

Keywords: atom; fuel; sensors; physical effects; gas

Introduction

The rapid growth of the industry in the modern world and the climate changes caused by it make the tasks of controlling the concentration of harmful gases in production and at home topical. It is also important to determine the parameters of gases in various industrial processes [1-3]. In practice, when it is necessary to determine the concentrations of certain gases, it is necessary to choose the method which best meets the requirements and can solve the task. Optical methods showed the greatest efficiency in determining the main characteristics of the combustion of gases because of their high speed and accuracy. Despite all the advantages of these methods, their main disadvantage is the price and folding of implementation [4-6]. Therefore, today it is necessary to improve approaches to solve this issue. It is known that in diffusion flames of organic compounds in the gas phase hydrocarbon fuels form a nonequilibrium large concentration of intermediate H_2 products, which create a second (invisible) flame zone in the neighborhood of the luminous flame zone.

Theoretical simulations of hydrocarbon combustion under diffusion flame conditions show that the flame has a complex structure; it consists of clearly defined zones that differ from each other in character [7; 8]. Namely, the zone of contact and mutual diffusion of the combustible and oxidizer can be divided into a zone of combustible flow, followed by a new zone of radical formation [9]. In the same work, the profiles of concentrations of radicals and H_2, CO, H_2O, and O_2 were obtained in the case when the stoichiometric ratio between methane and oxygen is achieved. The afterburning zone of H_2 and CO after the complete consumption of methane is visible. The data of Zh. Wang *et al.* [10] also show that the structure of the diffusion methane flame includes a thin zone of reaction of CH_4 with OH, H, and O and a fairly wide zone of weak combustion of H_2 and CO. To explain the asymptotic structure of the methane flame in [11-13], it can be found an example of a discussion of the three-stage mechanism commonly used to explain the reaction process in the steady state approximation and partial equilibrium for intermediate products. For the oxidation of methane (1):

$$\begin{array}{c} 1.\, \mathrm{CH_4 + O_2 \rightarrow CO + H_2 + H_2O} \\ 2.\, \mathrm{CO + H_2O \rightarrow CO_2 + H_2} \\ 3a.\, \mathrm{O_2 + 2H_2 \rightarrow 2H_2O} \\ 3b.\, \mathrm{O_2 + 3H_2 \rightarrow 2H + 2H_2O} \end{array} . \tag{1}$$

In dimensionless coordinates, the flame structure is calculated, and several zones are highlighted, namely, a thin zone of methane flow and a fairly wide zone of weak hydrogen flame, the length of which is determined by the reaction $H+O_2+M \rightarrow HO_2+M$ from the list of reactions (2):

$$\begin{array}{c} 1.\, \mathrm{H + O_2 + M \rightarrow HO_2 + M} \\ 2.\, \mathrm{H + HO_2 \rightarrow H_2 + O_2} \\ 3.\, \mathrm{HO_2 + HO_2 \rightarrow H_2O_2} \\ 4.\, \mathrm{H_2O_2 + H \rightarrow H_2 + HO_2} \end{array} . \tag{2}$$

In the work of A. Hamins and K. Seshadri [14] determined the dependence of concentrations of H_2, CO, methanol, and heptane on the distance behind the luminous flame zone under countercurrent conditions. For hydrogen molecules in all experimental cases, the width of the zone of their penetration in the direction of oxygen due to diffusion is about 1-2 millimeters. It is reasonable to describe the contribution of the diffusive transfer of constituents in a complex four-component system within the framework of the nonlinear multicomponent diffusion formalism developed by the authors of the following works [15-17]. Due to the experimental difficulties of forming and maintaining diffusion flames for a long time, the use of visual (photographic) methods in their study is very effective for establishing the concentration distribution of intermediate products in this flare [18]. Methods of photographic imaging capture an instantaneous picture of a continuously fluctuating process and make it possible to determine the concentration distribution of the flame participants. It is also possible to continuously monitor the progression of the process [19].

It is known that NaCl vapor in a mixture of combustible gases, such as H_2, hydrocarbons, and various organic compounds, causes flame coloring caused by excited sodium atoms [1]. To explain the mechanism of the formation of excited sodium atoms, the authors of many studies propose different mechanisms [20; 21]. Since sodium atoms have low electronic levels, only a portion of the recombination heat released by the reaction is sufficient to excite them, and the presence of low-lying ionic terms increases the probability of energy transfer between them. Several are known to explain the coloring of hydrogen-burning flames by the addition of sodium atoms and the addition of sodium to the stream of hydrogen atoms coming out of the electric discharge tube [20-22]. Two elementary acts leading to the manifestation of excited sodium atoms are considered:

$$H + OH + Na \rightarrow H_2O + Na\ (2P), \tag{3}$$

$$H + H + Na \rightarrow H_2 + Na\ (2P)\,. \tag{4}$$

Kinetic analysis of the results for reactions (3) and (4) showed satisfactory agreement with experimental data and the rate constants of these reactions 2·1010 and 8·109 l^2/mol^2s, respectively, were obtained [21]. At present, the absorption spectroscopy method based on the phenomenon of selective absorption of radiation by gases is widely used [23; 24]. Selective absorption can be achieved if the radiation frequency is resonant for the molecules of a given gas.

The phenomenon of flame coloration is mainly used to determine the flame temperature, and therefore, in all works, salt molecules, as usual, were fed into the flame together with the flow of oxidizer or combustible gas [1]. But until now, due to the complexity of calculation, the distribution of the concentration of intermediate products depending on the flow rate cannot be obtained accurately. In this paper, authors propose a method for determining the concentration of atoms and the concentration distribution of hydrogen molecules behind the glow zone of the main combustible by feeding sodium-containing salt vapor into the flame from the outside.

The main goal of the study was to conduct an experiment that would confirm the effectiveness of using the semi-empirical method in the study of diffuse flames.

Materials and Methods

The diffusion flame of propane (used in domestic conditions) is obtained by feeding the combustible through a capillary 1 cm long and 0.5 mm in diameter into the atmosphere. To study the invisible combustion zone of hydrogen formed in nonequilibrium quantities during the combustion of hydrocarbons, in this work authors use molecules of NaCl and drinking soda $NaHCO_3$ (transformed into Na_2HCO_3 by the reaction $2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$). The method of delivery of the molecules of these substances to the flame was carried out as follows. A schematic of the experimental setup is shown in Figure 1.

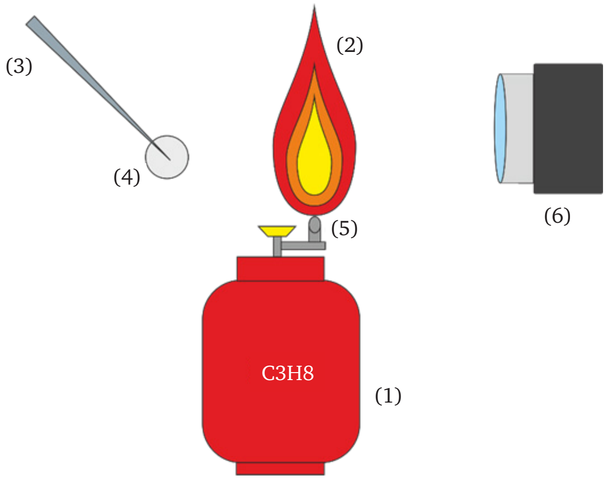

Figure 1. Schematic of the experimental setup

Note: 1 – propane cylinder; 2 – propane diffusion flame; 3 – steel needle; 4 – sodium salt crystals; 5 – fuel capillary; 6 – photo camera

Source: [24]

The edge of the steel needle was pre-wet with water, after which NaCl or $NaHCO_3$ crystals were collected on it. Then this part of the needle was preheated until a liquid drop of these substances appeared on it. After cooling, a plate or a ball of the above-mentioned substances was formed at the end of the needle. Before the probing process, this part of the needle was preheated to intensify the evaporation rate.

The needle was then fixed at different distances from the propane flame. The NaCl or $NaHCO_3$ molecules from the surface of the steel needle evaporated into the combustion zone. Due to the recombination of H and OH radicals on sodium atoms, which are the products of the reaction of NaCl and $NaHCO_3$ with the flame H_2, $CO+O_2$, which sodium atoms are formed in electronically excited states, carrying away with their part of the recombination energy. Some of these molecules are stabilized by collisions with atmospheric gas, while others emit light quanta in the wavelength range λ=5889-5899 A. In this case, a luminous zone is formed around the hydrocarbon flame, making it possible to visually observe the magnitude of hydrogen combustion.

Results

The diffusion propane flame was photographed using a digital camera. The results are shown in Figures 2. At the bottom of the figures, the conditions of the experiment are shown. In Figure 2a, the case of NaCl molecules evaporating over the luminescent flame zone of propane. There is an image of a fragment of the hydrogen afterburning zone as a yellow luminescent zone. Figure 2b gives an image of the propane flame in the case where the salt molecules evaporate into the flame from the side, outside the luminescent zone. A legible image is drawn of the invisible part of the flame structure as a second flame surrounding the luminous zone. It can be seen that the width of the hydrogen afterburning zone is about 2 millimeters on the side. At the top of the flame, the hydrogen afterburning zone extends to about 6 millimeters.

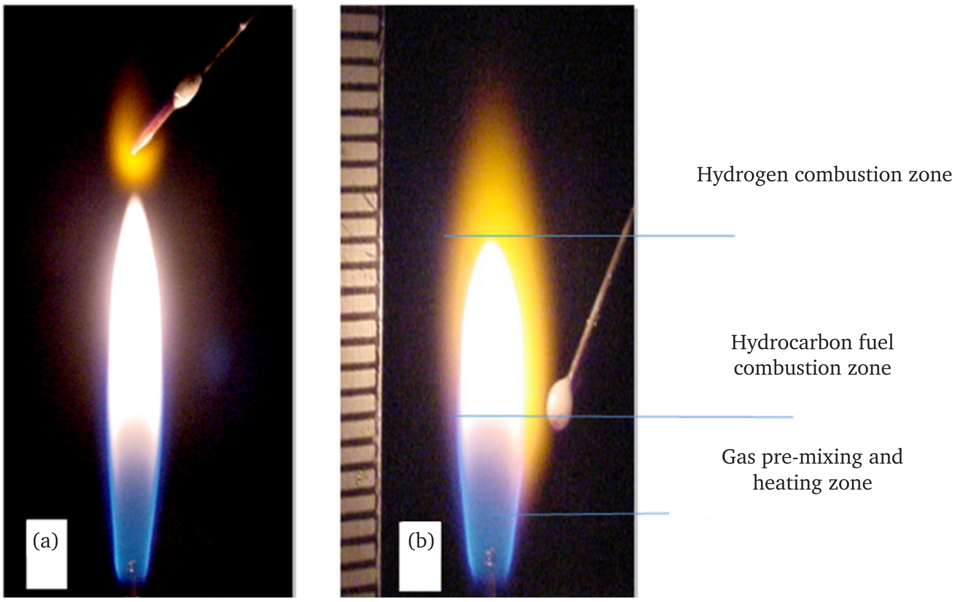

Figure 2. Visualization of the H_2 flame fragment during evaporation of NaCl molecules in a diffusion propane flame (a); visualization of a fragment of flame H_2 by evaporation of NaCl molecules in a diffusion propane flame from the side of the flame (b)

Note: a – flow velocity from tube v=4.6 m/s, tube diameter d=0.5 mm, and the volumetric flow rate in the evaporation zone of the flow from tube Q=0.9 cm^3/s; b – flow velocity from the tube v=4.6 m/s, tube diameter d=0.5 mm, the temperature in the zone of evaporation of salt molecules T=906K, the volume flow rate from the tube Q=0.9 cm^3/s

Source: developed by the authors

When the salt vapor is supplied from the side by the width of the hydrogen afterburning zone, the main contribution is given by diffusion, and from the side of flow propagation it is supplemented by the contribution due to the flow velocity, which is dominant. The expansion of the hydrogen after the burning zone following the flow direction of the gas mixture is related to this. The effect of the dependence on the flow velocity is particularly clear when comparing the pictures in Figure 3-4.

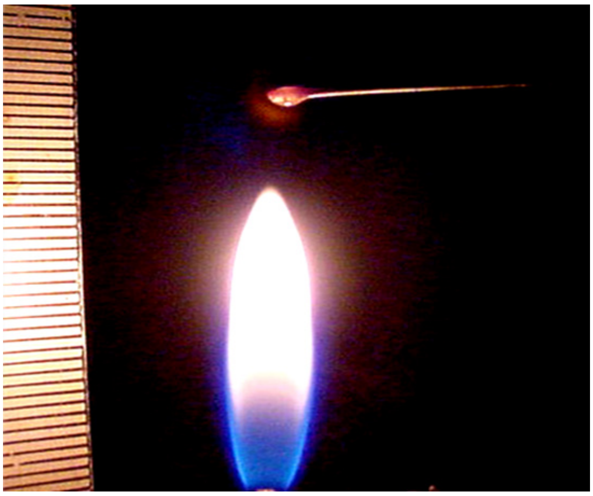

Figure 3. Visualization of the H_2 flame fragment by evaporation of NaCl molecules in a diffusion propane flame from the upper side of the flame

Note: Flow velocity from the tube v=6.07 m/s, tube diameter d=0.5 mm, the temperature in the zone of evaporation of salt molecules T=1406K, the volume flow rate from the tube Q=1.15 cm^3/s

Source: developed by the authors

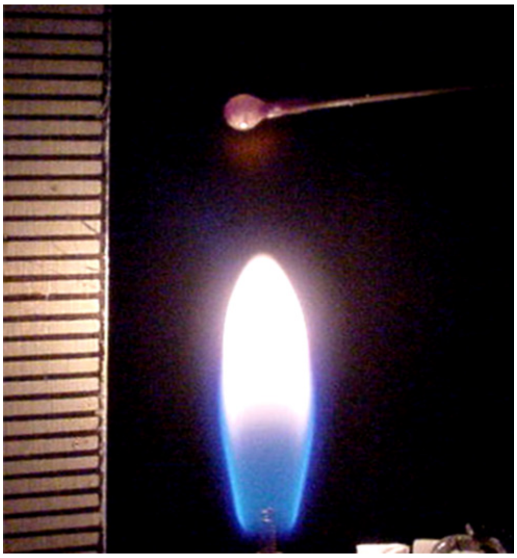

Figure 4. Visualization of the H_2 flame fragment by the evaporation of NaCl molecules in a diffusion propane flame from the side of the flame

Note: flow velocity from the tube v=4.6 m/s, tube diameter d=0.5 mm, the temperature in the zone of evaporation of salt molecules T=906K, the volume flow rate from the tube Q=0.9 cm^3/s

Source: developed by the authors

In Figure 3, when the volumetric flow rate Q=1.1 cm^3/s and the flow rate from the capillary v=6 m/s the hydrogen flame expands conditionally to 8 mm, and in the case of Figure 4, when the volumetric flow rate Q=0.9 cm^3/s and the flow rate from the capillary v=4.6 m/s the hydrogen flame spreads by only 6 mm. From this, it is easy to estimate the contribution of the flow velocity to the distribution of hydrogen concentration in its combustion zone.

The problem of the distribution of the concentration of hydrogen molecules over the distance behind the combustion zone of the main hydrocarbon fuel is of great interest. The proposed method of probing diffusion hydrocarbon flames and the experimental data obtained in this work allows us to develop a new method for studying the visible and invisible hydrogen afterburning zones in these flames. The balance equations for describing the kinetic regularities of the reaction medium development and describing the length of the second zone caused by the processes of substance transfer due to diffusion, convection, and kinetics of the combustion process, can be obtained by solving the corresponding diffusion-kinetic equations. Following the notations of Zh. Wang *et al.* [10], this equation can be represented in the following form (5):

$$\rho\frac{\partial Y_i}{\partial_t}+\rho V_x\frac{\partial Y_i}{\partial_x}+\frac{\partial}{\partial x}\left(\frac{J_{i,x}}{M_i}\right)+\sum_{k=1}^{r}\lambda_{ik}W_k\ , \qquad (5)$$

where: Y_i– species mass fraction, M_i – its molecular mass, ρ – density, t – time coordinate, v_i – speed in the x direction, $J_{i,x}$ – diffusion flux, λ_{ik}– stoichiometric coefficient of i-th reaction participant k, W_k– speed of this reaction.

When the values of all characteristic parameters are known, this equation allows us to obtain the structure of the flame. The method is based on the following considerations: if the concentration of sodium atoms in the reaction zone is known, the density of excited sodium atoms in the reaction zone, due to the processes $H+H(OH)+Na \rightarrow H_2O(H_2)+Na$ can be determined and with a known minimum value of the concentration of excited sodium atoms, whose glow can be registered visually, it can be estimated the concentration of hydrogen molecules in the zone where the glow comes to end. After that, from equation (5) it is possible to determine the distribution of hydrogen molecule concentration from the far along the course of H_2 flame propagation.

As shown in the works of Y. Chen *et al.* [9], and A.E. Long [12], using the generally accepted scheme of hydrocarbon oxidation, at atmospheric pressures above, when the length of the combustion zone of hydrogen molecules determines the reaction $H+O_2+M \rightarrow NO_2+M$, there is one rate describing the process, namely the reaction rate (6), in the right part of the equation (5), which describes the concentration distribution of H_2 at steady-state conditions:

$$W_{III}=k_6[O_2][M][H]. \qquad (6)$$

And in the combustion zone of intermediates, when the main fuel will be completely consumed, there is a relation of the type (7) [9; 10] for the value of hydrogen atom concentration where β is a proportionality factor:

$$[\mathrm{H}] = \beta\,[\mathrm{O_2}]^{1/2}[\mathrm{H_2}]^{3/2}/[\mathrm{H_2O}], \qquad (7)$$

In the general case, when the mutual diffusion process of H_2 and O_2 is dominant, the concentrations of O_2 and H_2O will depend on the distance of hydrogen flame propagation. However, if the flow velocity dominates over the longitudinal diffusion, then at some distance from the zone of full consumption of the main fuel, when the diffusion penetration of oxygen and the delivery of H_2O by the jet into the H_2 flame zone dominates over the process of its flow rate, it can be assumed that the O_2 and H_2O flow in this zone can be neglected.

Under conditions of the predominance of mass flow over diffusive one, the main contribution to the distribution of H_2 concentration in equation (1) will be given by fluidity, hence, this equation can be represented in the form (8) within the framework of the above approximations:

$$\frac{\mathrm{d}[H_2]}{\mathrm{dx}} = -\alpha \cdot [\mathrm{H_2}]\,\frac{3}{2}, \qquad (8)$$

where: α is the proportionality constant.

If all salt molecules entering the flame are converted into sodium atoms, the value of α can be determined. With the known value of sensitivity of the camera to the emission of Na* quanta, it can be determined the value of excited atoms of Na* quantities formed per unit volume per unit time in the extreme zone of flame H_2. From reactions (5) and (6) it turns out:

$$[\mathrm{H}]^2[\mathrm{Na}]\ \mathrm{k} = \mathrm{W_{Na}}*, \qquad (9)$$

where: (k = 8109 l^2/mol^2s), WNa* is the reaction rate (1) or, in other words, it can be said the amount of Na* formed per unit time per unit volume.

The channels of consumption of the formed excited sodium atoms are the emission stabilization channel, the stabilization channel due to impact with atmospheric gas, and various probable reaction channels. Hence, it can be written (10) for the number of quanta released from a unit volume per unit of time:

$$\mathrm{N_{hv}} = \frac{\mathrm{k_{r.s.}} \cdot \mathrm{W_{Na*}}}{\mathrm{K_{eff.}} + \mathrm{k_{r.s.}}}, \qquad (10)$$

where: $k_{r.s.}$ is the rate constant of the radiation stabilization channel, $K_{eff.}$ – is the effective rate constant of Na* consumption through other channels (besides the channel of stabilization by radiation).

And therefore, for the rate of formation of excited sodium, it turns out (11):

$$\mathrm{W_{Na*}} = \frac{\mathrm{N_{hv}}(\mathrm{K_{eff.}} + \mathrm{k_{r.s.}})}{\mathrm{k_{r.s.}}}. \qquad (11)$$

As in the dominant flux conditions, the inflow of sodium-containing molecules from outside allows us to always choose the conditions under which the requirement of a single participation of sodium atoms in the act of three-frequency recombination with hydrogen atoms is established. And so, from (9) and (11), it can be written (12):

$$[\mathrm{H}] = \sqrt{\frac{\mathrm{W_{Na*}}}{[\mathrm{Na}]\cdot \mathrm{k}}} = \sqrt{\frac{\mathrm{N_{hv}}(\mathrm{K_{eff.}} + \mathrm{k_{r.s.}})}{\mathrm{k_{r.s.}}\cdot[\mathrm{Na}]\cdot \mathrm{k}}}. \qquad (12)$$

And with the known sensitivity of the camera to the minimum number of photons from (7) it can be estimated the concentration of atoms H at the end of the luminous zone of the flame H_2. Since $k_{r.s} \gg K_{eff.}$ then the following is true (13):

$$[H] = \sqrt{\frac{N_{hv}}{[Na]\cdot k}}. \qquad (13)$$

It is known that light radiation is observable if the number of photons in 1 cm^3 is about 4·1014. Then the number of photons in the area 6 mm from the luminous flame torch of Figure 2, it can be suggested that ~4·1014 photons/cm^3, k=8·109 $l2/mol^2s$, according to M. Kajita [25] the partial pressure of saturated vapors of food salt and baking soda at temperatures above 1000K is approximately equal to 7 torr which corresponds to (14):

$$[Na] = 2.45 \cdot 10^{17}\,\frac{particles}{cm^3}. \qquad (14)$$

And accordingly obtained for the concentration of hydrogen atoms (15):

$$[H] \sim 4.28\ \cdot 10^{14}\,\frac{particles}{cm^3}. \qquad (15)$$

It is also of interest to obtain the dependence of the concentration of hydrogen molecules on the distance after the zone of the luminous flame torch by the formula (8). From formula (7) it can be determined the concentration of hydrogen molecules in the extreme zone of the glow flame $H_{2(l)}$, where l is the length at which the sodium atoms glow ends. Integration of equation (8) within the range from an arbitrary point x to the edge of the visible hydrogen flame zone will give (16):

$$\frac{2}{\sqrt{[\mathrm{H_2}]_l}} - \frac{2}{\sqrt{[\mathrm{H_2}]_x}} = \alpha \cdot (1 - \mathrm{x}), \qquad (16)$$

where: $[H_2]_l$ and $[H_2]_x$ are concentrations of hydrogen molecules at points x and l, respectively.

When x<l, the relation $[H_2]_x \gg [H_2]_l$ (17) holds:

$$\alpha = \frac{2}{\sqrt{[\mathrm{H_2}]_l \cdot 1}}. \qquad (17)$$

And thus, a formula is obtained for estimating the parameter T at known distance visually from the hydrogen flame zone and their concentration in this zone. From here, using formula (8), it can be estimated the contribution of the blowout to the flame propagation values (Fig. 5).

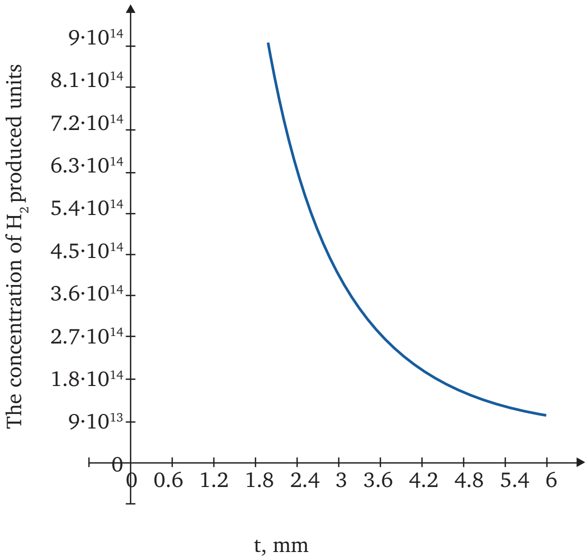

Figure 5. Distribution of the concentration of hydrogen molecules in the hydrogen afterburning zone in a diffusion propane flame in arbitrary units

Source: developed by the authors

Thus, visualization of the hydrogen flame by delivering alkali metal salts into the flame not only makes it possible to visualize this flame in the maximum possible size but also presents an opportunity to obtain a view of the distribution of the concentration of hydrogen molecules in this flame over its distribution distance and as a function of the flow rate and to estimate the growth rate of the hydrogen molecule concentration. As can be seen from Figure 4, the concentration of hydrogen molecules in the afterburning zone decreases 10 times in 6 mm.

Discussion

V. Mishra and S. Rashmi [26] considering methods for determining gas concentrations in general, argued that the use of methods related to optical absorption offers several advantages that alternative technologies cannot provide. Since measurements are based on a fundamental physical property of the molecule under study, there are ways to avoid some of the error mechanisms present in other technologies, including drift, lack of selectivity, and changes in sensitivity from experiment to experiment. Measuring the parameters of gases by optical means also opens several unique possibilities [27]. In particular, the adjustment of sensitivity, as well as the availability of feedback in the instrument, where one can monitor during operation whether they have failed (e.g., due to a faulty light source or failure to direct sufficient light to the photodetector). But the main advantage is the speed of signal transmission and the fact that measurements can be made in situ means that optical instruments can have a much higher response rate than alternative technologies.

The use of modern gas detection devices implies compliance with several requirements, such as high speed, minimum drift, and high gas selectivity, with zero sensitivity to other gases. Gas sensors with a carefully thought-out design using in their basis the phenomena of optical absorption can have time constants of less than 1 s, which provides them with high performance. Thus, the work by X. Liu and Y. Ma [28] shows an example of experimenting in real-time and situ without disturbing the gas sample, which is very important for process control. Such advantages of the approach are provided by the transduction method by directly measuring the physical absorption of the molecule at a certain wavelength. This leads to a reduction of drift in the system. In addition, it should be noted that the dependence on external factors drops significantly since it is possible to directly determine and control the intensity of the incident optical radiation. Considering all advantages, it can be stated that optical gas measurement is inherently very reliable, which allows it to take a place between inexpensive sensors with lower performance and high-quality laboratory equipment. The work by T. Strahl *et al.* [29] also shows a rather promising application of photoacoustic sensors for the calculation of gas concentrations. The described sensors differ in the approach used to detect absorbed light. Traditional sensors calculate the values of absorbed light to determine the transmittance, which can be obtained by comparing the light intensity at the photodetector with and without the presence of gas. Photoacoustic sensors, on the other hand, allow the absorbed light to be measured directly. Photoacoustic detection can be used in conjunction with the optical methods described above, including the method presented in this research.

In the quantitative study of gas concentrations, semiconductor gas sensors or electrochemical devices can compete with the traditionally dominant laboratory analytical equipment based on the effect of optical absorption by M. Kaloumenou *et al*. [30]. An example of such a device can be a pelistor, which, despite its relative cheapness, is a reliable device that responds to a change in gas concentration using a catalyst ball [31]. These devices have found widespread use in identifying flammable gases close to the lower explosive limit. The main disadvantage of pelistors compared to optical equipment is the zero drift at concentrations of fractions per million. In M.K. Nikolic's *et al*. [32] work, the efficiency and high sensitivity of other semiconductor gas sensors at low concentrations in the vicinity of ppm were shown. However, drift and low selectivity are present. In turn, electrochemical gas sensors can have high selectivity for individual gases at sensitivity in the region of particles per million or particles per billion [33], but they suffer from a limited lifetime as well as high humidity.

The mass spectrometric method described of C.P. Ruger's *et al*. [34], is based on the principle of separating ionized atoms and molecules according to the mass-to-charge ratio of the ion and the subsequent separate analysis. The amount of the desired component in the air is determined based on the proportional dependence of the spectral line intensity of each component on the partial pressure of the given component. It can provide a high sensitivity threshold of approximately 0.1 mg/m^3 and an error of up to 5%. However, the disadvantages of mass spectrometers compared to the presented solution are the high duration of analysis of the obtained data, the impossibility of creating compact devices, and the complexity of the ionization process [1; 2]. The biggest disadvantage of optical gas detection is its cost compared to material-based or electrochemical sensors. A second disadvantage is also reliability; in particular, the high degree of selectivity also means that several types of gas are difficult to detect simultaneously without a proportional increase in system complexity. Finally, using optical absorption, one must be guided by the information content available in the absorption spectrum. The second challenge is to be able to measure a wider range of gas compounds, particularly those composed of large molecules, including volatile organic compounds, which have a wider spectrum with less information content, requiring a wider wavelength coverage and greater accuracy and reliability of spectral fitting algorithms.

The use of the method of flame staining with sodium salts proposed in this work allowed us to significantly simplify the calculation of the concentration distribution of hydrogen molecules. In contrast to the absorption spectroscopy method widely used today [35], in method of this article the cost of operating the equipment is much lower. The sufficiently high accuracy and relative simplicity of the method make it promising for obtaining the hydrogen concentration distribution. In the future, the described approach can be applied to determine the concentrations of other gases in the combustion products, in particular, oxygen, methane, hydrogen sulfide, etc. The combination of experimental data and mathematical modeling makes it possible to visualize and qualitatively estimate the presence of hydrogen molecules along the entire combustion section. It should be noted that the calculations should take into account the sensitivity value of the charge-coupled device (CCD) matrix of the camera to the luminescence spectrum of alkali metal ions used for flame coloration. The use of sodium atoms in the experiment is explained by the fact that they have low electronic levels. This ensures their excitation with a small fraction of the heat released, which is another advantage of the method. The use of the semiempirical method to estimate the characteristics of gases is quite widely used today. Thus, in S. Muppala *et al*. [36], by applying an experimental and analytical model of two-component fuel mixtures of methane, propane, and hydrogen, the value of the turbulent flame combustion rate was obtained.

Ways of extending the capabilities of the method by using an additional hardware component are also considered. For example, the use of an infrared camera together with a conventional CCD camera is given in the article by B. Zhang *et al*. [24]. As a result of the proper selection of the temperature contour, it was possible to better determine the geometrical contour of the gas combustion flame. Such an approach can improve visibility and expand the possible applications of the method given in this work. When studying the properties of gases, the main parameters to be considered during the experiment are temperature and flow rate. The second parameter directly depends on the volumetric flow rate of the individual component of the gas flow, taking into account a set of chemical reactions and the effect of temperature. So, in O. Siryy [37], at a tube diameter of 75 mm the maximum combustion temperature of propane did not exceed 900K, and the reduction of the tube diameter to 0.5 mm resulted in a temperature increase in the molecular salt evaporation zone T>906K, which allowed a better evaluation of the flame coloration.

To summarize, despite the availability of several newer methods, the approach proposed in this work with the addition of alkali metal salts can be used to establish the concentration of hydrocarbon combustion products. The theoretical possibilities of extending the functionality may in the long term make its application effective at the level of modern optical methods for detecting gas molecules in the medium. The combination of a relatively simple setup with modern software solutions based on artificial intelligence will make it possible to build dependencies in real-time and conduct continuous data analysis.

Conclusions

From the theoretical data and results obtained in the course of the experiment in the presented work, the following conclusions can be drawn:

1. A semiempirical method for obtaining the distribution of hydrogen molecules in the flame during hydrocarbon combustion is presented. The experiment uses the delivery of alkali metal salt molecules, which can be used as an indication method for finding hydrogen ignition sources that cannot be visually detected.
2. As a result, a visualization of the hydrogen molecule concentration dependence over the entire combustion distance was obtained, which made it possible to obtain a view of the molecule distribution and estimate the rate of hydrogen concentration growth.
3. A series of studies on the shape, length, and experimental visualization of the structure of the diffuse hydrocarbon flame, carried out on the example of propane combustion, and the magnitude of the spread of the invisible flame combustion zone was established.
4. The intermediate product H_2, also allows to get the concentration of hydrogen atoms in the afterburning zone about 6 mm from the zone, the glowing flame of propane combustion.
5. The ways of future extending the functionality of the method based on modern approaches to detect and obtain gas concentrations are also analyzed. Namely, the use of photoacoustic methods or infrared cameras.
6. Based on the values of the parameters characterizing the experimental conditions, the value of hydrogen atoms at the end of the hydrogen-burning zone is calculated, which is also an important parameter of the diffusion flame and is the achievement of the method presented in the research.

In general, summarizing the results of the research, it can be stated that the combination of practical experiments with mathematical calculations has led to a new approach to determining the distribution of hydrogen molecules in the glow zone of the burning propane flame. Despite the relative simplicity of the proposed method, it was possible to determine the distribution of hydrogen concentration in the entire combustion zone very accurately. As a result, it is possible to talk about the prospects for developing new types of gas detectors or improving the capabilities of already known ones. The results obtained can be used in the laboratory for a better understanding of hydrocarbon combustion processes under diffuse flame conditions or in the industry for monitoring production processes under real-time conditions.

Conflict of Interest

The authors declare no conflict of interest.

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Дифузійне полум’я та напівемпіричний метод оцінки розподілу молекул водню в полум’ї пропану

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Анотація

Актуальність. Найбільша ефективність у визначенні основних характеристик спалювання газу була показана оптичними методами завдяки їх високій швидкості та точності. Незважаючи на всі переваги цих методів, їх головним недоліком є ціна та складання реалізації. Тому сьогодні необхідно вдосконалити підходи до вирішення цієї проблеми.

Мета. Дослідження присвячено вивченню полум’я дифузії напівемпіричним методом.

Методи. Дані експериментального дослідження дифузійного полум’я вуглеводнів представлені на прикладі пропану. Для візуалізації невидимої частини структури цього полум’я, а саме зони догоряння молекул водню, що утворюються в полум’ї у нерівноважних кількостях, у зоні полум’я випаровуються молекули, що містять атоми лужних металів (NaCl та Na_2CO_3).

Результати. Вперше застосовувався метод доставки молекул солей лужних металів ззовні, що дозволило більш ретельно дослідити це явище. На основі результатів досліджень, метод визначення концентрації атомів водню та відносного розподілу концентрації молекул водню вздовж осі поширення полум’я після запропонованої зони спалювання. Метод дослідження поєднує експерименти з математичним моделюванням. Застосування методу, описаного у статті, дозволяє визначити розподіл молекул водню над зоною світіння основного палива.

Висновки. Отримані результати допоможуть краще зрозуміти явища горіння вуглеводнів в умовах дифузійного полум’я, а також пошук нових способів отримання палива водню від домашніх відходів

Ключові слова: атом; паливо; сенсори; фізичні ефекти; газ