

# Measurement Algorithm for Determining Unknown Flammable Gas Concentration Based on Temperature Sensitivity of Catalytic Sensor

Alexey Karelin <sup>a</sup>, Alexander M. Baranov <sup>a</sup>, Saba Akbari<sup>a\*</sup>, Sergey Mironov <sup>b</sup> and Elena Karpova <sup>c</sup>

**Abstract**— The assessment of the explosion hazard of a combustible gas mixture is not a trivial task if the type of combustible gases is not known precisely. Typically, the concentration of combustible gas is defined as the response of a catalytic sensor to its presence in the air. It has been known that catalytic sensors have different sensitivities to different combustible gases. Usually gas analyzers are calibrated by methane and are not suitable for measuring other flammable gases without additional correction for each gas. In this paper we have investigated the dependency of catalytic sensor sensitivity on the sensor temperature for the binary mixture of methane, propane, butane, hexane and hydrogen with air in a wide temperature range. Based on the obtained dependencies, a measurement algorithm and an empirical equation were proposed that allow calculating the concentration of unknown combustible gas in % of LEL. The process of measuring and processing data can be automated using a digital processor. The experimental results have shown that the concentration measurement error is in the range 5-10% for binary mixture.

**Index Terms**— Catalytic sensors; flammable gases, temperature dependence of sensitivity, unknown gas concentration measurement.

## I. INTRODUCTION

Industrial processes of mining and quarrying, transporting and processing of minerals in different industry branches are associated with the real risk of generating explosive atmosphere in technological areas, warehouses and open spaces. Failure to comply with technology, results in equipment and gas pipelines explosions [1]. Natural gas explosions, periodically occurring in residential apartments, show the real danger of such risks. Accidents are severe, often lead to casualties and huge material damage.

Such incidents happen especially often during the heating season, sometimes as a consequence of non-professional

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Alexey Karelin, Alexander Baranov and Saba Akbari are with the Department of Radioelectronics, Telecommunications and Nanotechnology, Moscow Aviation Institute (National Research University), 125993, Moscow, Russia, Volokolamskoe shosse, 4 (email: alexey@karelin.site baranov\_64@mail.ru, akbarisaba@gmail.com).

Sergey Mironov is with LLC "NTC IGD", Lyubertsy, Moscow region, Russia (email: mironov.sergm@yandex.ru).

Elena Karpova is with STANKIN – Moscow State Technological University, Russia (email: ekarpova1@yandex.ru).

approach to the installation of heating devices, sometimes as a result of careless handling with the devices. Therefore, the control of explosion safety of the atmosphere in industrial and residential areas is one of the most significant tasks to provide life safety [2].

To implement such control tin oxide sensors [3], optical detectors [4] and catalytic sensors [5] are most widely used. Semiconductor gas sensors exhibit fast response as well as high sensitivity, however, their selectivity [6], power consumption and structural stability still need to be improved [7].

Many optical detection systems have been developed recently based on infrared absorption spectroscopy [8],[9], [10]. The known transmission windows in the optical range are following:

- Visible and very-near IR: from 0.4 to 1.4  $\mu\text{m}$
- Near IR: from 1.4 to 1.9  $\mu\text{m}$  and from 1.9 to 2.7  $\mu\text{m}$
- Mean IR: from 2.7 to 4.3  $\mu\text{m}$  and from 4.5 to 5.2  $\mu\text{m}$
- Far IR: from 8 to 14  $\mu\text{m}$ .

The absorption lines of many hydrocarbons such as methane, ethane, propane, butane, pentane, hexane and etc. lies in the wavelength range of 3.2–3.5  $\mu\text{m}$  [10]. Therefore, optical sensors of this particular range are most widely used for the monitoring of combustible gases. Optical detectors are characterized by having fast response time and being highly sensitive. On the other hand, they are more susceptible to spectral interference [11] and the change in ambient temperature: The optical detection systems have been developed using different light sources – mainly xenon lamps, LEDs and lasers. Xenon lamps and LEDs are used for non-dispersive infra-red measurements with rather broad light spectra with the width of the order of hundreds of nm, while laser diodes and lasers - for tunable spectroscopy with very narrow spectra with the width of tenth of a nm. But laser systems are rather expensive, while xenon lamps systems are rather high power consuming ones and besides need protecting shields, enlarging essentially the size of the constructions. So the best candidates for low cost and low power consuming systems are LED-based systems. However, the semiconductors in LED-based systems have a strong dependence of the forbidden zone on temperature and hence the radiation line shift. In order to exclude the dependence of the radiation wavelength on the ambient temperature, the diode temperature should be stabilized. In the past decade, NIR spectroscopy has been widely applied for monitoring pipeline, industrial plants and technological areas where explosive atmosphere could be formed [12],[13]. Based on NIR, different methods for

measuring the concentration of combustible gases in LEL, ppm and ppb ranges were developed; as examples of which absorption infrared sensors [14], open-path detectors [15], methods of hollow core fiber spectroscopy [16], [17] and wavelength modulation spectroscopy [18] can be mentioned. Nevertheless, NIR detectors have one fundamental flaw. It does not allow detecting hydrogen which can exist in the gas mixture containing hydrocarbons. The molecule of hydrogen does not have a dipole moment and cannot absorb IR radiation [19]. Moreover, NIR detectors are expensive.

The advantages of catalytic sensors compared to others are in low cost, sensitivity only to flammable gases and vapors, small size and weight. Small size with low power consumption allows catalytic sensors to be used in wireless sensor networks and Internet of Things application [20] in particular, for real-time leakage [21] and online pipeline inspection [22]. However, along with the benefits, there are some drawbacks, one of which is the existence of different sensor response to the same concentration of flammable gases [23], [24].

Therefore, gas analyzers are calibrated to methane as the most widespread flammable gas and the correction coefficients are introduced to define the concentration of other flammable gases [20]. If the type of flammable gas is unknown, the correction coefficient is also unknown and when determining the concentration of all gases except methane there will be a large error. However, it is not always known which gas or gas mixture is present in the atmosphere. Therefore, there have been a lot of attempts to develop methods for determining the concentration of combustible gases in the air if the type of combustible gas is not known [25], [26], [27]. In general, the main idea is about varying the temperature of the sensing element. Heavier gases start ignition earlier, than light gases. This effect is used to determine the composition of gas mixture. But the problem is that the temperature of initial oxidation is unstable and sensor works in kinetic zone, where the sensitivity depends on gas concentration.

Recently, a new method of estimation of a gas mixture explosion risk by measuring the oxidation heat within a catalytic sensor has been proposed [28]. This article presents an alternative way to measure the concentration of flammable gases in the air when the type of flammable gas is not known. The concentration of flammable gases is determined in percent of the LEL. The method is based on measuring the temperature dependency of the catalytic sensor sensitivity.

## II. EXPERIMENTAL DETAILS

### A. Catalytic Sensors

Pellistor type catalytic sensors produced by "NTC IGD" Ltd were chosen as flammable gas sensors. The sensor housing (which has a height of 9.5 mm and a diameter of 9 mm in diameter) contains working and comparative sensors. The power consumption is 150 mW in the continuous measurement mode. Sensors consist of a platinum coil of cast micro wire with quartz insulation. According to the research conducted by LLC "NTC IGD", this provides platinum with additional protection from environmental exposure and provides additional stability to its parameters for at least 1 year. A core

diameter is 10  $\mu\text{m}$  and insulation thickness is 2  $\mu\text{m}$ . The working sensor has a platinum micro wire covered by porous gamma alumina oxide material that is used as catalyst support for catalytically active metals (mixture of Pd and Pt). In order to impregnate the catalyst support by the catalytic metal, salts of palladium chloride ( $\text{PdCl}_2$ ) and platinum acid ( $\text{H}_2\text{PtCl}_6$ ) are used. After annealing at 500 C, noble metal clusters are formed in the catalyst support.

A principle of operation of such sensors is based on flameless burning (oxidation) of combustible gas on the catalytic active surface and measuring the amount of released heat, which is proportional to the concentration of combustible gas [29]. Fig. 1 shows the design of a catalytic sensor. To ensure the oxidation process, the platinum wire is heated to the temperature in the range 400 - 450  $^\circ\text{C}$  [30].

A signal proportional to the methane concentration is formed on the catalytically active element due to an increase in the temperature on the element surface due to methane combustion and a change in the wire resistance from the platinum wire having a rather high temperature coefficient of resistance (TCR). Thus, the increment of platinum wire resistance  $\Delta R$  is a measure of methane concentration.

When heat is released, the resistance  $R$  of the platinum wire changes by an amount  $\Delta R$ . The resistance of the spiral is determined by the formula:

$$R = R_0(1 + \alpha\Delta T) \quad (1)$$

where  $R_0$  is the resistance of the wire at  $T = 25^\circ\text{C}$ ;  $\alpha$  is the temperature coefficient of resistance (TCR) of the platinum wire,  $\Delta T$  is the change in the temperature of the wire.

A typical scheme for the sensors is the use of the Wheatstone bridge (Fig. 2). In one leg of the bridge, comparative and working sensors are connected. The comparative sensor is almost identical in its thermophysical properties to the working sensor, but no catalyst is deposited on its surface, so there is no oxidation reaction on it. Additional bridge resistors are included in the other leg of the bridge.

When flammable gases are applied to the sensor, oxidation of the combustible components takes place on the working element, which causes an increase of its temperature. Since platinum has a sufficiently large TCR, the induced oxidation of



Fig. 1. Pellistor consists of working (black) and comparative (white) sensors.

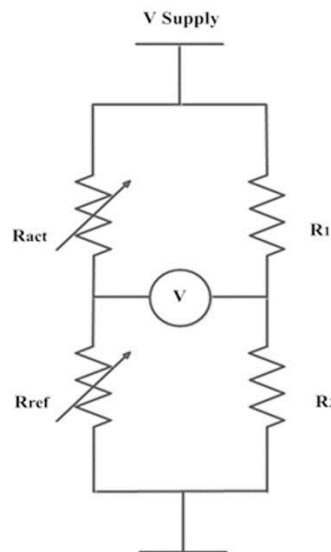


Fig. 2. Typical scheme for switching on a catalytic sensor. Rref is a comparative sensor, Ract is a working sensor.

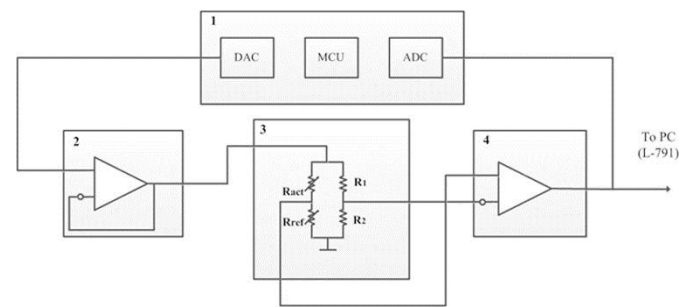


Fig.3. Test stand functional scheme.

the temperature increase causes a significant change in the resistance of the working element.

There is an imbalance of the bridge when the voltage drop on the working element changes by the magnitude of the imbalance, the concentration of the fuel component in the analyzed atmosphere is calculated.

Sensor sensitivity is usually expressed in [mV/ vol%CH<sub>4</sub>], that is the voltage of bridge imbalance with the sensors exposed to 1 vol% of methane (i.e., volume fraction of methane in the air).

Another convenient unit – [mV/ 25%LEL], that is the voltage of bridge imbalance with the sensors exposed to 25% of LEL concentration of any combustible gas.

For the experiments 3 sensors with sensitivity in range 35-50 mV/ vol%CH<sub>4</sub> were taken.

### B. Test Stand

Fig. 3 shows the scheme of test stand. The scheme consists of (1) AduC831 microcontroller that has two 12-bit DAC (Digital-to-Analog Converter) and 8-channel 12-bit ADC (Analog-to-Digital Converter). DAC is used to set sensor supply voltage. Supply power generator for sensor is based on (2) an operational amplifier AD8532 working as a current loop. (3) In measuring part, working and compensative sensitive elements are installed in a Wheatstone bridge. (4) Amplifying part is built on the AD8532 working as a differential amplifier. Scheme control is performed by the AduC831 microcontroller. Power to the circuit is supplied by a converter ADP3335. The resistance of sensing elements is about 10 Ohm at room

temperature. Output signal is amplified (4) tenfold. As for a data acquisition system, we used a universal input/output PCI-board L-791 produced by L-card. It has 32 analog input channels with 14-bit ADCs and the sample-rate 400 kHz. Fig. 4 shows the photo of the test stand.

### C. Combustible Gases

A number of different calibration gas mixtures with pre-explosive concentration of flammable gases was used for the experiment. Detailed description of binary mixtures is presented in Table 1. The table contains info both in vol% (volume fraction of a particular gas in the air) and in % LEL (concentration percentage from LEL). The calculations of the sensor sensitivity were made in [mV/ 25%LEL] as it is more convenient for all flammable gases. There is an assumption that the signal is linear and sensitivity does not depend on concentration. That is correct for catalytic sensor operating temperature (420-480 °C [29]). The choice of gases is caused by their wide use in household and industry. Methane – the main component of natural gas. Liquefied gases: butane, propane – are widely used in everyday life. Hexane – gas that has properties equal to petrol vapors, so its control is essential at the transport enterprises, organic synthesis factories. Hydrogen is used at chemical, food, aviation and other industries as fuel, chemical reagent or coolant.

### D. Methods of Measurement

To obtain the temperature dependence of catalytic sensor sensitivity to different flammable gases, a voltage ranging from 0.4 V to 3.1 V was applied to Wheatstone bridge. The output signal was registered with L-791. Each catalytic sensor was tested with every binary gas mixture presented in the Table 1.

To get sensor response at different temperatures the following method was chosen. At first, all the sensors were preheated during 1 hour at standard conditions. After pouring the chamber with the calibration gas mixture the stand was turned on. Bridge supply voltage was varied from 400 mV (200 mV for working element) to 3100 mV (1550 for working

TABLE I. CONCENTRATION OF THE ANALYZED COMPONENT IN BINARY MIXTURE (WITH AIR)

Gas type	Concentration in air, vol%	LEL, vol%	Concentration in % LEL
CH <sub>4</sub> (methane)	1.01 %	4.4 %	23 %
C <sub>3</sub> H <sub>8</sub> (propane)	1.01 %	1.7 %	59 %
C <sub>4</sub> H <sub>10</sub> (butane)	0.665 %	1.8 %	37 %
C <sub>6</sub> H <sub>14</sub> (hexane)	0.485 %	1.24 %	39 %
H <sub>2</sub> (hydrogen)	0.96 %	4 %	24 %



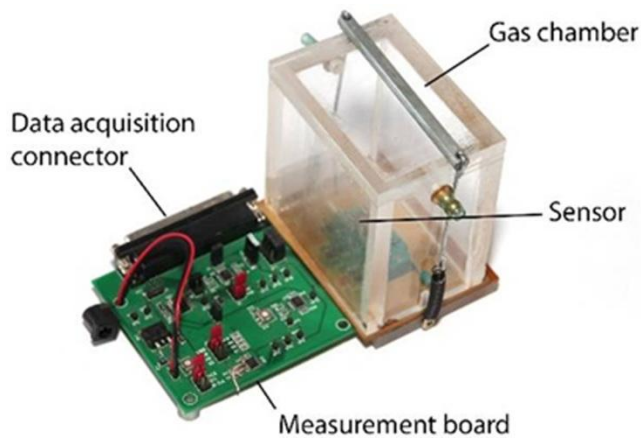


Fig. 4. Test stand photo.

element) in increments of 50 mV. An increase in the voltage above 3.1 V may cause the sensor to overheat and fail. Between measurements there was a 10 sec pause to complete transients.

The output was averaged for 5 sec with 500 total samples (100 Hz sample rate) after the pause and after that calculated value was written into memory.

As the sensors have different sensitivity to methane, readouts were normalized to the sensor sensitivity of the methane in order to align the output signal in one graph,

$$S_N = S_M / S_S \quad (2)$$

where  $S_N$  – normalized output of sensor sensitivity,  $S_M$  – output signal,  $S_S$  – sensitivity to methane at 2.8 V.

### III. RESULTS AND DISCUSSION

#### A. Sensitivity of the Sensors under Standard Conditions

Table 2 presents the sensor sensitivity to methane, propane, butane, hexane and hydrogen at 25% LEL in binary gas mixtures and 2.8 V applied to the Wheatstone bridge for three catalytic sensors.

As could be seen from the table, the obtained values of catalytic sensor sensitivity are varied in wide range. Therefore, if the type of flammable gas is unknown the error in the determination of gas concentration reaches up to 87% while measuring hydrogen relative to methane. It was noted that heavier gases, having less diffusion coefficient and high heat-generation ability, have low output signal (comparing to methane). While measuring such gases with devices calibrated to methane it is necessary to correct the measurement results. In other words, the smaller diffusion coefficient, the bigger correction coefficient must be applied to align measurement results. Some exceptions to this pattern exist for branched, unsaturated or oxygenated hydrocarbons, but arisen errors are minor, and moreover, such measurements are performed infrequently [31]. We set the task to develop a measurement method that will help reduce the measurement error in the determination of gas concentration if the gas is not known.

#### B. Sensor Response under Various Sensor Temperatures

Fig. 5 presents normalized sensor sensitivity to various gases. As a reference point the sensor response to the methane at 2.8V was chosen. Let us examine oxidation reactions with various temperatures (various voltages). As follows from Fig. 5,

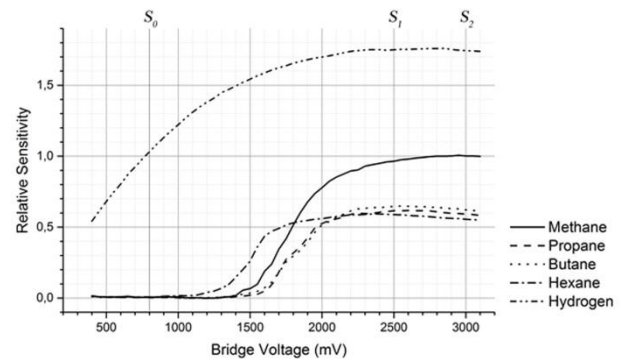


Fig. 5. Relative sensor sensitivity to methane, propane, butane and hydrogen depends on the voltage applied to the Wheatstone bridge. Sensitivity is normalized to 25% LEL.

almost all dependences have the character of S-shaped curves except for hydrogen that has a parabola-like curve. At the beginning, when temperature is not sufficient for catalytic reactions, sensitivity of catalytic sensor is zero. Then, after reaching the initial temperature of oxidation reaction, the sensitivity increases with sensor temperature. Oxidation in this zone has kinetic character, as a result the sensitivity is non-linear, that is it depends on gas concentration in the analyzed atmosphere. With increasing temperature, the oxidation becomes diffusive type, that is all amount of gas which can reach the surface of the catalyst is oxidized. Diffusion zone, a zone in which sensitivity does not depend on temperature change, is selected for the flammable gas measurement. It can be seen from Figure 5 that the diffusion zone starts at a voltage greater than 2.5 V. This temperature is the sensor working temperature. Further increase of temperature causes a slight drop of sensitivity associated with both the increase of heat transfer (e.g., by radiation) and the properties of particular reaction, the specific properties of the oxidizing gas (e.g. desorption energy of the fuel component from the surface of the active site of the catalyst).

Fig. 5 illustrates the relative sensor sensitivity normalized to 25% LEL depending on the voltage applied to the Wheatstone bridge. It is seen (Fig. 5) that each gas has its own onset oxidation temperature, temperatures of the diffusive oxidation zone and rate of reducing the sensitivity with a further increase of temperature. The kinetic zone of burning is characterized by instability of ongoing process of oxidation, and thus it is excluded from the analysis zone. Consequently the most interesting section in terms of measuring concentration of combustible gases and determining the ability of atmosphere to explode is the diffusion zone of flameless oxidation.

Then the approach to measuring the concentration of combustible gases of unknown type can be the following: We measure the sensitivity of the sensor in the diffusion zone at two different temperatures which are provided by supplying different voltages.

If we take the first operation temperature of the maximum of hydrocarbons diffusive oxidation 430-450°C (bridge voltage 2.5 V) as a basis, the sensitivity to methane slightly increases as the temperature rises, and the sensitivity to other gases starts to decrease.

The second voltage point is taken at 470-490°C (bridge voltage 3 V), because higher temperatures are dangerous for pellistor beads causing their degradation, and lower temperatures are not sufficient to catch the sensitivity decrease.

Methane has the highest temperature of beginning of the diffusion zone which is caused by high-energy decay of molecular bonds. Therefore, one can be sure that the diffusion zone for other gases begins at lower temperatures, and every gas has its own characteristic rate of sensitivity decrease depending on temperature. It has been established that the heavier the gas, the lower the temperature of the beginning of the gas desorption from the active centers of the catalyst surface, and the faster the sensitivity decreases with increase of the sensitive element temperature.

Based on the above logic, the following measurement algorithm based on the measurement of sensor sensitivity at different temperatures is proposed. The obtained results are presented in Table 3.

1. The measurements are carried out in pulse mode with multiple voltage supply levels. The sensor must be turned off when measurements start. In all cases the measuring signals  $S_i = (U_R - U_0)$  are calculated as the difference between measured voltages with the gas presented in chamber ( $U_R$ ) and voltages measured under the same conditions in clean air ( $U_0$ ).

2. Before the main measurement starts the voltage pulse  $U_P = 800$  mV is supplied to the sensor corresponding to a temperature 100-110°C, and maintained for 500 ms – the time required for evaporation of adsorbed water during the pause. At the end of the pulse an output signal  $S_0$  is measured – this signal is a reference (comparative) one. Since this temperature is not sufficient to start the combustion of hydrocarbons, the values obtained are zero, with the exception of hydrogen, which begins to burn at this temperature (column  $S_0$  in Tabl.3).

3. A voltage pulse corresponding to a working voltage of a sensitive element is supplied; In this case, the voltage value is 2.5 V which corresponds to the 430-450°C temperature range; this voltage level is maintained for 500 ms. After measuring output signal  $S_I$  as stated in paragraph 1, (the output signal  $S_I$  is the same as the values shown in Table 2) response signal  $S_M = S_I - S_0$  is calculated (column  $S_M$  in Table 3).

4. A voltage pulse 3.0 V (470-490°C), is supplied for 200 ms, a correction output signal  $S_2$  is measured. A correction factor  $K = S_I / S_2$ , characterizing the rate of sensitivity decrease on the analyzed gas during the temperature increase, is calculated (columns  $S_2$  and  $K$  in Table3).

5. Corrected response  $S_R$  is calculated using an empiric formula:

$$S_R = \frac{S_M e^{F \cdot K}}{C_S} \quad (3)$$

where  $F$  – the coefficient characterizing the rate of sensitivity decrease for a particular sensor,  $C_S$  – the correction coefficient to align the results of measurement.  $F$ ,  $C_S$  are calculated during sensor calibration by exposing it to calibration gas mixtures with air and must be included in MCU or other data processing means.

It is important to note that sensors have very high sensitivity to hydrogen because of high diffusion coefficient. At the same time hydrogen has very low ignition temperature, so reference  $S_0$ , taken at the temperature 100-110°C, does not equal 0, unlike other gases. As a result of subtracting  $S_0$  the sensitivity to hydrogen essentially approaches to sensitivity to other gases, and conducted correction gives satisfactory result. Fig. 6 shows such subtraction. Signal to hydrogen became noticeably closer to methane signal and thus it can be used for further calculations.

### C. Measurement Results after Recalculation

The results obtained using the proposed algorithm for the measured gases using three catalytic sensors are given in Table 3.

$\Delta c$  – measurement error for corrected results.

$\Delta$  – measurement error for source results.

Coefficients for sensors:

$F_1 = 3.4$ ,  $F_2 = 6.8$ ,  $F_3 = 5.5$ ;

$C_{S1} = 38.18$ ,  $C_{S2} = 1279.12$ ,  $C_{S3} = 389.27$ .

As could be seen from the table, corrected measurement results essentially narrowed the differences, thus decreased measurement errors.

The most noticeable difference is in the measurements of hydrogen. If the original measurement error ( $\Delta$ ) reaches up to 97% (Table III), the adjusted value alters from the true by less than 5%.

This difference is primarily due to the fact that there is one addition measurement at 100-110°C followed by a subtraction.

An error was also decreased for hydrocarbons. The error for hydrocarbons is less than 10% instead of 30-40%. The only significant error is in measurement propane with sensor #3, which is 11%, what exceeds 10% range; nevertheless it is much better than error before the correction.

TABLE II. SENSORS SENSITIVITY TO VARIOUS BINARY GAS MIXTURES

Sensor #	Sensitivity, mV/25% LEL				
	CH <sub>4</sub> +Air	C <sub>3</sub> H <sub>8</sub> +Air	C <sub>4</sub> H <sub>10</sub> +Air	C <sub>6</sub> H <sub>14</sub> +Air	H <sub>2</sub> +Air
1	44.4	27.8	30.4	29.1	83.2
2	50.7	29.2	30.4	25.9	78.3
3	37.9	23.7	24.0	20.4	70.9

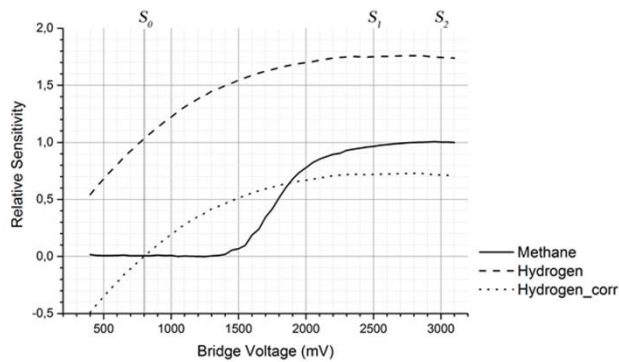


Fig. 6. Subtracted signal for hydrogen.

In general, the use of this method allowed us to reduce the error to acceptable values. In the future, an investigation of the effects of influence of combustible gas mixtures appears to be interesting and valuable.

#### IV. CONCLUSIONS

In this article we have proposed a measurement method of concentration of flammable gases of unknown type. The method based on the correction of measurement results of catalytic sensors using correction factor  $K$  characterizing the rate of sensitivity decreasing during the temperature increase in diffusion zone was described.

Suggested measurement algorithm allows aligning of measurement results for different flammable gases. Measurement error decreases from 90% to less than 10% while measuring hydrogen. For hydrocarbons the error decreases from 30-40% to 0-10%. The only error misses 10% range – 10.9%, during measurement propane on sensor #3.

The use of this algorithm requires changing the mode of pre-calibration of the catalytic sensor. Usually, the calibration is carried out as follows. The sensor is heated to operating temperature and placed in a chamber with known hydrocarbon concentration. The obtained values are stored in the gas analyzer memory. With this algorithm, it is necessary to measure several hydrocarbon responses at two different temperatures and calculate the coefficients  $K$  and  $F$ , which are

recorded in the memory of the gas analyzer. The calculation of the gas concentration or  $S_R$  is carried out according to equation 3.

The frequency of calibration depends on the operating conditions. The regular calibration is essential to the safe use of combustible sensors of all types.

The main difference is in further measurements. The proposed algorithm makes it possible to determine the concentration of a gas in percent of LEL, i.e. how explosive the concentration of combustible gas is. This is more convenient than in volume percent, because the flammability range varies widely between individual gases and vapors, most regulatory standards express hazardous condition thresholds for combustible gas in air in percent LEL concentrations.

It is important to note that the temperature of platinum heater can change over time when supplied by the same heating voltage. However, we present a catalytic sensor of a certain type in this paper. The sensor consists of a platinum coil of cast micro wire with quartz insulation. This provides platinum with additional protection from environmental exposure and brings additional stability to its parameters including pulse mode. Therefore, the change in platinum resistance is only a few percent during one year operation of sensor. Nevertheless, the temperature of platinum will change in the long term. It is necessary to note that measurements in the diffusion zone, where the sensitivity of the catalytic sensor does not depend on temperature, minimize this effect.

Recommended application – gas-filling stations, organic synthesis companies working with natural gas and propane-butane mixtures. The potentials of catalytic sensors along with the implementation of the proposed algorithm onboard nodes can make these sensors appropriate candidates for a wide spectrum of industrial and urban applications.

As mentioned earlier, catalytic gas sensors can be used in wireless sensor networks due to their small size and low power consumption. Moreover, energy harvesting techniques can improve the autonomous operation time of catalytic sensors and consequently reinforce their integration with WSN networks and generally Internet of Things applications [32].

TABLE III. CORRECTED RESULTS OF MEASUREMENTS ALIGNED TO 25% LEL

Gas	Sensor#	$S_0$ , mV	$S_1$ , mV	$S_2$ , mV	$S_M = S_1 - S_0$ , mV	$K = S_1/S_2$	$S_R = \frac{S_M e^{F \cdot K_{II}}}{C_S}$	$\Delta c$	$\Delta$
H <sub>2</sub>	1	46.26	81.80	83.38	35.54	0.9811	26.15	4.6%	97.0%
	2	39.68	77.34	78.64	37.66	0.9835	23.62	-5.5%	57.3%
	3	42.52	71.40	68.43	28.88	1.0434	23.05	-7.8%	90.2%
CH <sub>4</sub>	1	0.00	41.52	45.03	41.52	0.9221	25.00	-	-
	2	0.00	49.18	51.63	49.18	0.9525	25.00	-	-
	3	0.00	37.54	37.15	37.54	1.0105	25.00	-	-
C <sub>3</sub> H <sub>8</sub>	1	0.00	28.15	27.10	28.15	1.0397	25.20	0.8%	-32.2%
	2	0.00	28.95	28.45	28.95	1.0176	22.90	-8.4%	-41.1%
	3	0.00	24.19	22.62	24.19	1.0694	22.27	-10.9%	-35.6%
C <sub>4</sub> H <sub>10</sub>	1	0.00	30.09	29.88	30.09	1.0070	24.19	-3.3%	-27.5%
	2	0.00	30.59	29.82	30.59	1.0258	25.59	2.4%	-37.8%
	3	0.00	24.96	22.87	24.96	1.0914	25.94	3.7%	-33.5%
C <sub>6</sub> H <sub>14</sub>	1	0.00	29.21	28.86	29.21	1.0121	23.89	-4.4%	-29.6%
	2	0.00	26.98	25.60	26.98	1.0539	27.32	9.3%	-45.1%
	3	0.00	21.85	19.43	21.85	1.1245	27.25	9.0%	-41.8%



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