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IDENTIFICATION OF GASES BY NOISE SPECTRUM PARAMETERS BASED ON THE EINSTEIN-SMOLUCHOWSKI EQUATION

In this work, a mathematical model based on the Einstein–Smoluchowski stochastic equation describing the output voltage of gas sensors is presented. The Ornstein–Uhlenbeck stochastic process was used to analyze the noise spectrum of laser gas sensors, as a result of which it was proved that the output signal has the form of a Lorentz spectrum. The model allows us to determine the frequency spectrum of the output voltage, taking into account the diffusion and relaxation processes of the gas. Experimental studies have shown changes in time series and correlation parameters for various gases (air, methane, ethanol, ammonia). The proposed model can serve as a basis for creating digital twins of sensors and developing self-calibration systems. The analytical approach establishes a relationship between stochastic fluctuations caused by molecular diffusion and the measurable spectral characteristics of the sensor output. Characteristic parameters of the Lorentzian spectrum, including spectral density, relaxation time, and correlation properties, were evaluated for different gaseous media. Comparative analysis demonstrates that each gas exhibits distinct noise signatures determined by its physical and diffusion properties, enabling reliable discrimination without introducing additional sensing elements. The proposed methodology improves the understanding of fluctuation-induced processes in laser gas sensors and provides a theoretical framework for noise-based gas identification. The obtained results may contribute to the development of intelligent gas sensing systems, real-time signal processing algorithms, and adaptive monitoring platforms for environmental, industrial, and safety applications.

Keywords: gas sensor, Einstein-Smoluchovsky equation, Lorentz spectrum, stochastic model, diffusion, relaxation.

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Эйнштейн-Смолуховский теңдеуі негізінде шуыл спектрінің параметрлері бойынша газдың түрлерін анықтау

Бұл жұмыста газ сенсорларының шығыс кернеуін сипаттайтын Эйнштейн-Смолуховскийдің стохастикалық теңдеуіне негізделген математикалық модель ұсынылған. Лазерлік газ сенсорларының шуыл спектрін талдау үшін Орнштейн-Уленбек стохастикалық процесі қолданылып, нәтижесінде шығыс сигналының Лоренц спектрі түрінде болатыны дәлелденді. Әзірленген модель газ ортасында жүретін диффузиялық және релаксациялық процестерді ескере отырып, шығыс кернеуінің жиіліктік спектрін анықтауға мүмкіндік береді. Эксперименттік зерттеулер әртүрлі газдар (ауа, метан, этанол және аммиак) үшін уақыттық қатарлар мен корреляциялық параметрлердің өзгеретінін көрсетті. Ұсынылған модель газ сенсорларының цифрлық егіздерін құруға және оларды өзін-өзі калибрлеу жүйелерін әзірлеуге негіз бола алады. Ұсынылған аналитикалық тәсіл молекулалық диффузиядан туындайтын стохастикалық флуктуациялар мен сенсордың шығыс сигналының өлшенетін спектрлік сипаттамалары арасындағы өзара байланысты анықтайды. Әртүрлі газ

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орталары үшін Лоренц спектрінің негізгі параметрлері, оның ішінде спектрлік тығыздық, релаксация уақыты және корреляциялық сипаттамалар анықталды. Салыстырмалы талдау зерттелген әрбір газдың өзінің физикалық және диффузиялық қасиеттерімен анықталатын бірегей шуыл сипаттамаларына ие екенін көрсетті, бұл қосымша сезімтал элементтерді қолданбай-ақ оларды сенімді сәйкестендіруге мүмкіндік береді. Ұсынылған әдіснама лазерлік газ сенсорларындағы флуктуациялық процестер туралы түсінікті кеңейтіп, газдарды шуыл сипаттамалары бойынша сәйкестендірудің теориялық негізін қалыптастырады. Алынған нәтижелер интеллектуалды газ талдау жүйелерін, нақты уақыт режимінде сигналдарды өңдеу алгоритмдерін, сондай-ақ экологиялық, өндірістік және технологиялық мониторингке арналған бейімделетін платформаларды әзірлеуде қолданылуы мүмкін.

Түйін сөздер: газ сенсоры, Эйнштейн-Смолуховский теңдеуі, Лоренц спектрі, стохасты модель, диффузия, релаксация.

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Идентификация газов на основе параметров шумового спектра с использованием уравнения Эйнштейна-Смолуховского

В настоящей работе представлена математическая модель, основанная на стохастическом уравнении Эйнштейна-Смолуховского, описывающем выходное напряжение газовых сенсоров. Для анализа шумового спектра лазерных газовых сенсоров использован стохастический процесс Орнштейна-Уленбека, в результате чего показано, что выходной сигнал имеет вид лоренцевского спектра. Разработанная модель позволяет определить частотный спектр выходного напряжения с учетом диффузионных и релаксационных процессов, протекающих в газовой среде. Экспериментальные исследования показали изменения временных рядов и корреляционных параметров для различных газов (воздуха, метана, этанола и аммиака). Предложенная модель может служить основой для создания цифровых двойников газовых сенсоров и разработки систем их самокалибровки. Предлагаемый аналитический подход устанавливает взаимосвязь между стохастическими флуктуациями, обусловленными молекулярной диффузией, и измеряемыми спектральными характеристиками выходного сигнала сенсора. Для различных газовых сред были определены характерные параметры лоренцевского спектра, включая спектральную плотность, время релаксации и корреляционные характеристики. Сравнительный анализ показал, что каждый исследуемый газ обладает уникальными шумовыми признаками, определяемыми его физическими и диффузионными свойствами, что обеспечивает возможность их надежной идентификации без применения дополнительных чувствительных элементов. Предложенная методология расширяет представления о флуктуационных процессах в лазерных газовых сенсорах и формирует теоретическую основу для идентификации газов по шумовым характеристикам. Полученные результаты могут быть использованы при разработке интеллектуальных систем газового анализа, алгоритмов обработки сигналов в реальном времени, а также адаптивных платформ мониторинга для экологических, промышленных и технологических применений.

Ключевые слова: сенсор газа, формула Эйнштейна-Смолуховского, спектр Лоренца, стохастический модель, диффузия, релаксация.

Introduction

Gas sensors are an integral component of modern environmental monitoring systems, industrial safety, medical diagnostics, and smart technologies. The need to detect and quantify a wide range of gases – from toxic (NO_x, CO, H_2S) and greenhouse gases (CO_2, CH_4) to metabolic disease markers in exhaled

air – drives the constant improvement of sensor technologies [1]. In the context of the fourth industrial revolution and the development of the Internet of Things (IoT), sensors are subject to stringent requirements: they must provide high sensitivity and selectivity, operate for many years without calibration and with minimal power consumption, and be integrated into wireless networks [2].

Recent years have seen intensive development of both sensor materials and designs, as well as mathematical methods for signal processing. Review papers devoted to modern gas sensors emphasize the need for an interdisciplinary approach integrating physics, materials science, electronics, and mathematical modeling [3]. Increasing attention is being paid not only to the steady-state response of the sensor, but also to its dynamic characteristics, as well as signal fluctuations, which have traditionally been viewed as interference [4].

Noise is a key factor limiting the sensitivity of gas sensors. However, in recent years, the so-called Fluctuation-Enhanced Sensing (FES) approach has been actively developing. In this approach, noise fluctuations in the signal are considered not as unwanted interference, but as an additional source of information about the type and concentration of gas [5]. As noted by Scandurra et al. [6], FES is a very powerful technique for detecting odors and gases and can play a fundamental role in environmental monitoring and the detection of hazardous gases. Research shows that the analysis of low-frequency noise caused by the adsorption and desorption of gas molecules on the surface of the sensing element can significantly improve the selectivity of sensors, in particular, the discrimination between structurally related compounds [7]. For example, the analysis of noise spectra allows one to distinguish between gases that produce a similar static response, which is critical for the creation of electronic noses and multisensor systems [8].

In parallel with experimental advances, a theoretical framework for describing sensor systems is being developed. Cheremisina et al. [9] describe the formation of an "image" of a substance based on measurements by multisensor systems using stochastic transformations and the calculation of correlation and fractal dimensions of reconstruction attractors. This approach emphasizes the importance of mathematical modeling for recognizing complex images of multicomponent gaseous media, which is particularly relevant for the creation of "electronic nose" devices [10].

Optical methods of gas analysis based on laser spectroscopy occupy a special place due to their high sensitivity and selectivity. In a review by Zhu et al. [11], advances in photothermal spectroscopy (PTS) are discussed, which is characterized by high sensitivity, a large dynamic range, and a virtually complete absence of background signal. PTS is based on recording changes in the refractive index or temperature of a gas caused by the absorption of laser radiation [12]. Of particular interest are methods of quartz-enhanced photoacoustic spectroscopy (QEPAS), which use a high-Q quartz tuning fork as a sensitive element, ensuring the recording of acoustic waves generated during the relaxation of excited gas molecules [13].

The physical basis of most laser gas sensors is the effect of radiation absorption by gas molecules. When a laser beam passes through a gas medium, its intensity is attenuated in accordance with the Beer-Lambert law, with the degree of attenuation depending on the concentration of absorbing molecules and the optical path length [14]. The gas absorption spectrum is a set of lines whose shape (Lorentzian, Gaussian, or Voigt) is determined by broadening mechanisms, including Doppler and impact broadening [15]. By recording the change in the intensity of transmitted or scattered radiation using a photodetector, it is possible to obtain an electrical signal proportional to the gas concentration. However, this signal is always accompanied by noise of various natures: shot noise of the detector, excess 1/f noise of the laser and electronic components, as well as specific noise associated with fluctuations in the density and composition of the gas in the measuring cell [16]. It is these noise components, superimposed on the useful signal, that limit the detection threshold and can be used in the FES approach [5].

In this paper, we consider a mathematical model of the output voltage of a gas sensor based on the stochastic Einstein-Smoluchowski equation. This equation describes the relationship between diffusion and relaxation processes and, in the context of sensorics, allows us to understand how the statistics of random forces affecting the signal change [17]. The analytical solution of this equation is a process characterized by an exponentially decaying autocorrelation function and a Lorentzian power spectrum [18]. This description adequately reflects the physics of fluctuations that occur when laser radiation passes through a gas medium, where random changes in concentration, pressure, and temperature lead to absorption fluctuations and, consequently, to noise at the output of the photodetector [19].

The aim of this work is to experimentally verify a method for identifying various gases (air, methane, ethanol, ammonia) based on noise spectrum parameters (correlation time τ and relaxation coefficient γ) using the Einstein-Smoluchowski

equation. The proposed approach can serve as the basis for creating digital twins of sensors that enable self-diagnostics, compensate for zero drift, and extend calibration intervals, which meets modern Industry 4.0 requirements[20].

Mathematical model of a noise signal

The output voltage of the laser gas sensor $U(t)$ is considered as the realization of a stochastic process, which is affected by a random force $\xi(t)$ [21]. The dynamics of stress is described by the Einstein-Smoluchowski equation [22]:

$$\frac{dU(t)}{dt} + \gamma U(t) = \xi(t), \qquad (1)$$

$$\langle \xi(t) \rangle = 0, \ \langle \xi(t)\xi(t') \rangle = 2D\delta(t - t').$$

where γ is the relaxation coefficient or the inverse correlation time $\tau_c=1/\gamma$, depending on the gas parameters and the sensor structure, $\xi(t)$ is the white noise, and D is the noise intensity. The Einstein-Smoluchowski equation gives the relationship between diffusion and relaxation. This helps the electronics learn and compensate for zero-point drift by understanding how the statistics of random forces in the sensor change. The dynamics of the output voltage $U(t)$ of the laser sensor can be viewed as a stochastic process. This model adequately describes signal fluctuations arising as a result of adsorption-desorption processes on the surface of the sensitive element and random changes in gas density in the measuring system.

The stationary solution of equation (1) is an Ornstein-Uhlenbeck process characterized by an exponential autocorrelation function [21]

$$K(\tau) = \langle U(t)U(t+\tau) \rangle:$$

$$K(\tau) = D/\gamma \ exp(-\gamma|\tau|\,). \qquad (2)$$

The memory of this system, i.e. the signal at time $t=\tau$ is related to the signal in the future, is larger the weaker the relaxation coefficient. After the Fourier transform, the exponential decay over time leads to the Lorentz spectrum [23]:

$$S(\omega) = 2D/(\gamma^2 + \omega^2\,). \qquad (3)$$

In sensorics, this expression means that the voltage fluctuations at the output of a laser detector have a maximum intensity at low frequencies and decrease according to the law $(1/\omega)^2$ at high frequencies.

Gas sensors rely on narrow spectral absorption lines, a linear relationship between concentration, absorption coefficient, and measured signal. The full width at half maximum is equal to 2γ. It is directly related to gas pressure and collision frequency (Lorentz broadening). Without the Lorentz spectrum, accurate gas leak detectors, medical diagnostic lasers, and precision instruments for monitoring gas leak systems in manufacturing would not exist. Mathematical models based on the Einstein-Smoluchowski equation allow the creation of digital twins of sensors. This helps the electronics to self-learn and compensate for zero-point drift by understanding how the statistics of random forces in the sensor change.

Experimental setup and data processing methods

A laboratory setup for analyzing a laser gas sensor (Figure 1) was used for experimental studies. The setup includes a laser source (wavelength λ = 532 nm, power 60 mA), a 20 ml gas cuvette, a photodetector, and a data acquisition system based on the NI ELVIS II+. Laser radiation passes through the gas medium, where it is absorbed according to the Beer-Lambert-Bouguer law [24]. Changes in the intensity of the transmitted radiation are recorded using a photodetector, the output signal of which is recorded by a high-temporal-resolution data acquisition system. The photodiode bias voltage was U = -2.3 V, which corresponds to the stability region of the PIN characteristic.

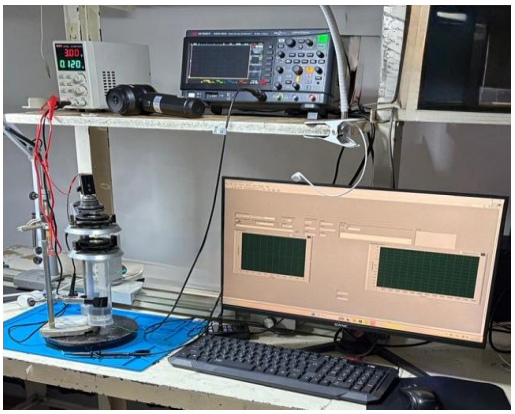


Figure 1 – External view of the setup for analyzing a laser gas sensor

The following gases were used for the study: atmospheric air, methane (CH_4), ethanol (C_2H_5OH), and ammonia (NH_3). These gases were chosen due to their widespread use in environmental monitoring and industrial safety. Methane is the main component of natural gas and a significant greenhouse gas, ethanol is used as a biofuel and solvent, and ammonia is used in agriculture and refrigeration, and is also a marker for a number of pathological conditions when analyzed in exhaled breath [5].

A laser beam is directed through a gas cell containing the gas being studied. As it passes through the gas, the radiation intensity is attenuated due to molecular absorption [24]. A photodetector converts the optical signal into an electrical voltage, which is continuously recorded over a specified time interval.

The output voltage time series $U(t)$ were recorded at a sampling rate sufficient for analyzing noise spectra in the frequency range of up to several kilohertz. For each gas type, time sequences were recorded with a duration sufficient to ensure the stationarity of the measured process and sufficient frequency resolution for subsequent spectral analysis [25]. The output voltage $U(t)$ time series were recorded at a sampling rate sufficient for analyzing noise spectra in the frequency range of up to several kilohertz. For each gas type, time series of 120 seconds were recorded, ensuring the stationarity of the measured process and sufficient frequency resolution for subsequent spectral analysis.

For each registered time series $U(t)$ the autocorrelation function estimate was calculated:

$$\hat{K}(\tau) = \frac{1}{N-\tau}\sum_{t=1}^{N-\tau}(U_t - \overline{U})(U_{t+\tau} - \overline{U}), \qquad (4)$$

where N is the number of samples, $\overline{U}$ is the average signal value. The resulting autocorrelation function was approximated by an exponential function (2) using the least squares method, which allowed us to determine the relaxation coefficient γ and the correlation time $\tau_c = 1/\gamma$.

The power spectral density $S(\omega)$ was estimated using the periodogram method with segment averaging (Welch's method). The resulting spectrum were approximated by a Lorentzian function (3), which allowed for independent estimation of the γ parameter and comparison with the value obtained from autocorrelation analysis. A logarithmic scale was used to plot the spectra to clearly display the frequency dependence of $1/\omega^2$ in the high-frequency region. For each gas type, the mean value $\overline{U}$ and standard deviation σ were calculated. These characteristics allow us to quantitatively describe the amplitude of noise fluctuations and their dependence on the type of gas. Gas identification was based on noise spectrum parameters (γ, τ_c) and statistical characteristics ($\overline{U}$, σ). Each gas is characterized by a unique set of these parameters, allowing them to be used as identification features. This approach is consistent with the Fluctuation-Enhanced Sensing (FES) methodology, which considers the noise signal as an additional source of information about the gas type and concentration.

Results and discussion

Figure 2 shows the output voltage time series $U(t)$, recorded as the laser beam passed through various gaseous media: air, methane, ethanol, and ammonia. The recording duration was 120 seconds. A clear difference in the amplitude and nature of the fluctuations is observed for the different gases: for air (minimum absorption), the voltage is maximum, while for the other gases, the average value is lower due to the absorption of laser radiation by the gas molecules.

To quantitatively describe the fluctuations, statistical characteristics of the time series were calculated and presented in Table 1.

The standard deviation characterizes the amplitude of noise fluctuations, which depends on the gas type. The highest standard deviation is observed for methane, which may be due to more intense adsorption-desorption processes on the surface of the sensing element. The correlation time τ_c, determined from the autocorrelation function, is also a gas-specific parameter.

Table 1. Parameters of gases

Gas type	Mean value $\overline{U}$	Standart deviation, σ	τ_c, ms
Air	0.4611	0.0325	8.44
Methane	0.7609	0.0482	16.39
Ethanol	0.7510	0.0373	13.62
Ammonia	0.7612	0.0404	15.54

Figure 3 shows the autocorrelation functions K(τ) calculated for the voltage time series. The autocorrelation functions exhibit exponential decay for all the gases studied. Air exhibits the fastest decay of correlations, corresponding to the short process memory time (τ = 8.44 ms). For gases with higher molecular weights and more complex structures (methane, ammonia), the correlations decay more slowly, resulting in longer correlation times (τ > 15 ms). The obtained experimental curves are approximated by the function (2), which confirms the adequacy of the proposed mathematical model.

Figure 4 shows the power spectra S(f), obtained by Fourier transforming the autocorrelation functions. The spectra have a Lorentzian shape, which is consistent with theoretical predictions.

All spectra are characterized by a maximum intensity at zero frequency and a $1/\omega^2$ decay in the high-frequency region. Spectral intensity depends on the gas type: methane exhibits the highest spectral power density, consistent with a large standard deviation.

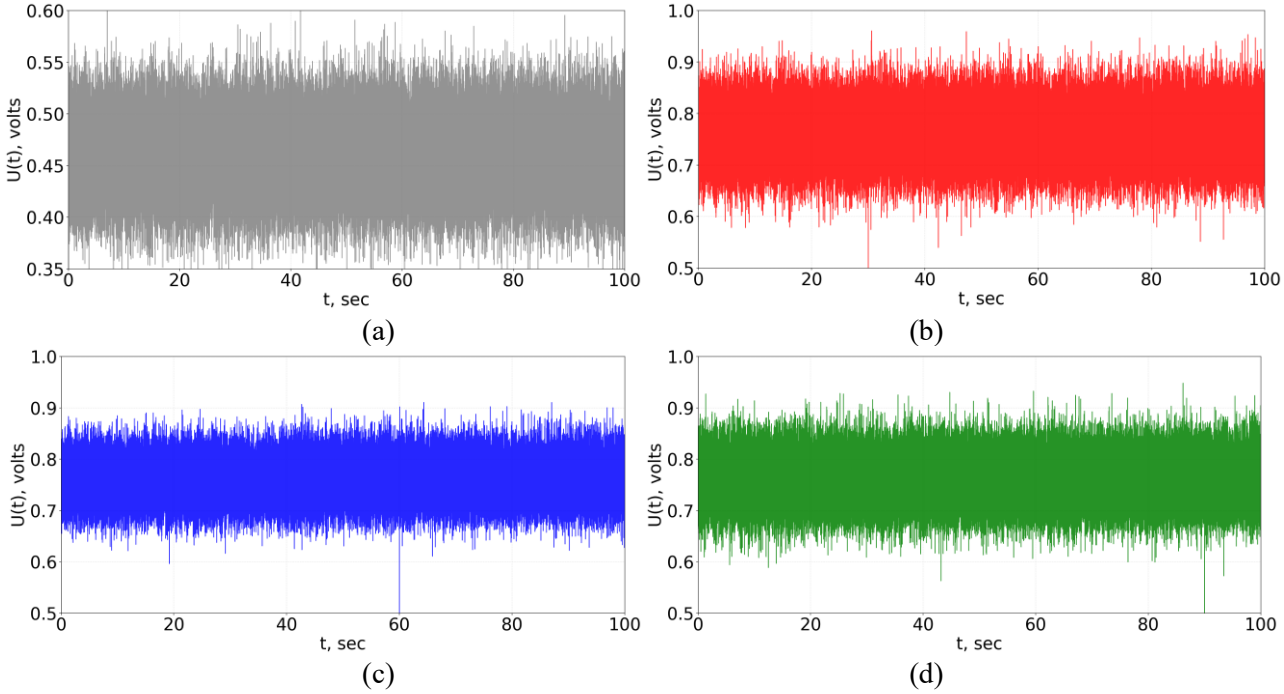


Figure 2 – Time series (a) – air, (b) – methane, (c) – ethanol, (d) – ammonia

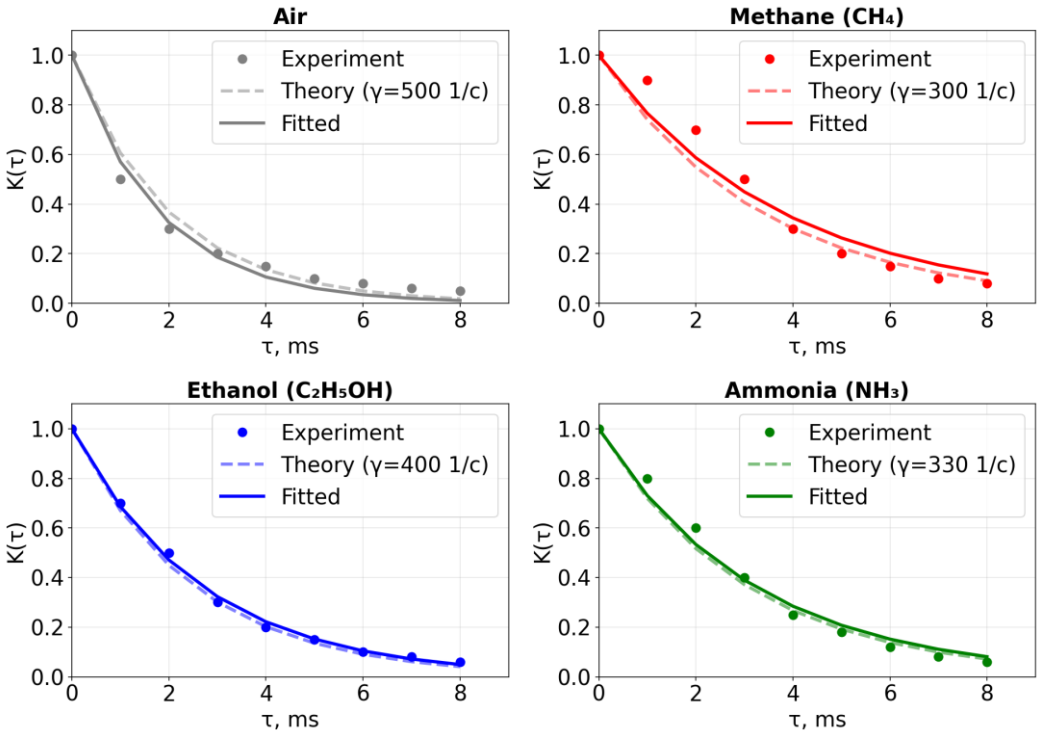


Figure 3 – Autocorrelation functions $K(\tau)$ calculated for time series of voltage of different gases.

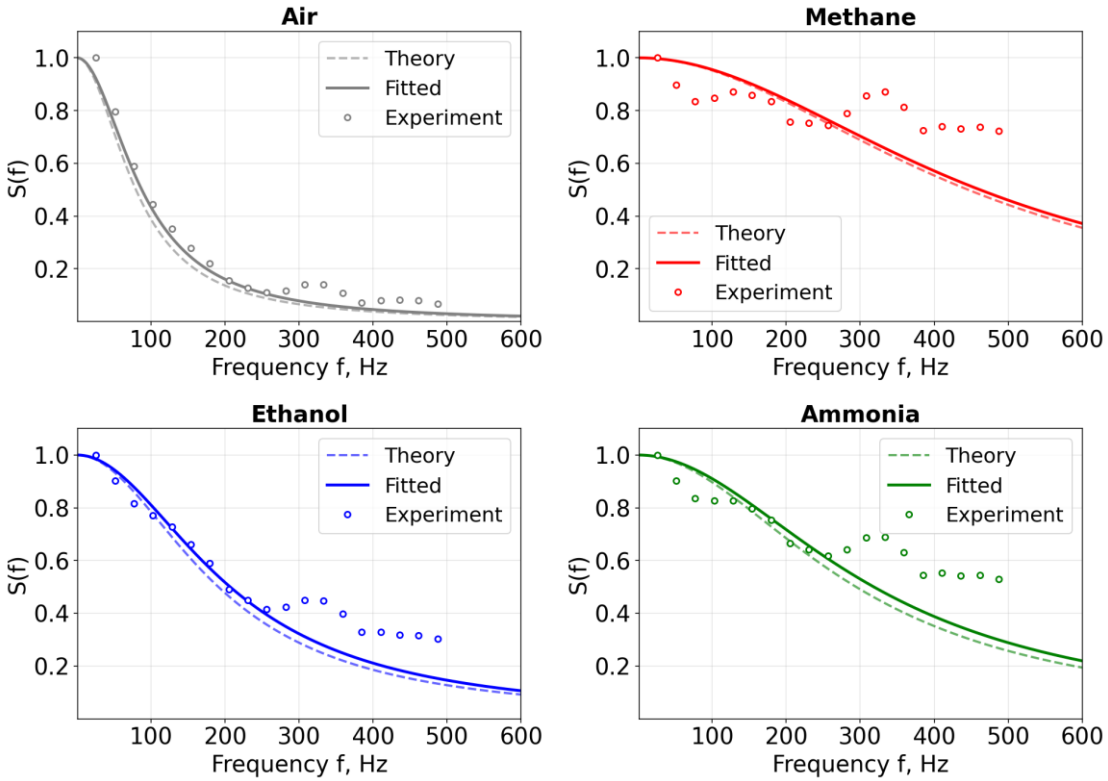


Figure 4 – Power spectra S(f) of various gases

The obtained results confirm the effectiveness of the proposed gas identification method based on the Einstein-Smoluchowski equation. The correlation time τ and standard deviation values are gas-specific and can serve as identification indicators. Methane has the longest correlation time (16.39 ms) and standard deviation (0.0482 V) among the gases studied, which is explained by its more complex molecular structure and the specific adsorption interactions with the sensor material.

The exponential nature of the autocorrelation functions and the Lorentzian shape of the power spectra confirm that the process of changing the output voltage of a laser gas sensor is described by the Einstein-Smoluchowski equation. This is consistent with studies showing that noise fluctuations in gas sensors have a Lorentzian spectrum.

The observed decrease in the intensity of spectral lines with increasing gas concentration indicates a saturation effect in the gas sensor response. This phenomenon is described within the framework of fluctuation-dissipation theory, where the critical concentration is determined by the equality of the quantum and thermal factors.

Conclusion

In this paper, a method for identifying gases (air, methane, ethanol, ammonia) is proposed and experimentally verified based on the analysis of the parameters of the noise spectrum of the output voltage of a laser gas sensor within the framework of the Einstein-Smoluchowski stochastic model.

It has been experimentally confirmed that the output voltage time series of a laser gas sensor for various gases are described by the Ornstein-Uhlenbeck process. The autocorrelation functions are exponential, and the power spectra are Lorentzian, which fully corresponds to the theoretical predictions of the Einstein-Smoluchowski equation.

Statistical parameters of time series and noise spectra were determined for four gases. The correlation time τ was found to be gas-specific: 8.44 ms for air, 13.62 ms for ethanol, 15.54 ms for ammonia, and 16.39 ms for methane. The largest standard deviation (0.0482 V) was observed for methane, indicating more intense adsorption-desorption processes.

The proposed method for gas identification based on the analysis of low-frequency noise fluctuations (200-400 Hz) is simple and cost-effective, as it does not require expensive spectral equipment. It can be implemented in compact and inexpensive sensor systems for industrial monitoring and environmental control.

The developed approach provides the basis for creating digital twins of sensors that enable self-

diagnostics, zero-drift compensation, and extended calibration intervals, all in line with modern Industry 4.0 requirements. Promising areas for further research include expanding the range of identifiable gases, studying multicomponent mixtures, and developing machine learning algorithms for automatic gas classification based on noise spectrum parameters.

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