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Development of a combined model for analyzing gas mixtures using machine learning methods

Yurii Yu. Bilak
ORCID: https://orcid.org/0000-0001-5989-1643; yuriy.bilak@uzhnu.edu.ua. Scopus Author ID: 57213689747
Uzhgorod National University, 3, Narodnaya Square. Uzhgorod, 88000, Ukraine

ABSTRACT

Analysis of gas mixtures is an important task in spectroscopy, environmental monitoring, industrial control and scientific research. Accurate determination of component concentrations in complex gas environments requires advanced approaches that combine physical modeling and artificial intelligence methods. The use of neural networks in spectral analysis allows increasing the accuracy and stability of calculations under variable experimental conditions, which indicates the relevance of the work. The aim of the research is to develop a combined model for spectral light flux analysis that combines physical modeling of spectral absorption of gases with machine learning methods. This provides increased accuracy in determining the concentration of components in multicomponent gas mixtures and allows adaptive adjustment of analysis parameters depending on the measurement conditions. An integrated methodology is proposed, which includes modeling of spectral light flux based on Gaussian and Lorentzian absorption profiles, the use of the Bouguer-Lambert-Beer equations to determine gas concentrations, and training a neural network to predict the light flux. To assess the performance of the developed model, a series of numerical experiments were conducted with varying network parameters and optimizing the configuration. The results obtained confirmed the high efficiency of the model, which is reflected in the high value of the coefficient of determination and low values of the mean square error. The model was tested when changing gas concentrations and the length of the optical path, which confirmed its stability and adaptability. The study showed that the optimal configuration of the neural network includes three hidden layers with an optimal number of neurons, which provides a balance between accuracy and efficiency. A rectified linear activation function was used for stable convergence, and for weight optimization - an adaptive stochastic gradient descent method, which improves performance. The proposed method of combining physical modeling and machine learning provides high accuracy of gas mixture analysis and resistance to variations in external conditions. The scientific novelty of the study lies in the use of a combined approach, which allows adapting the model to a wide range of spectral characteristics. The practical significance of the work lies in the possibility of applying the developed methodology for industrial control, environmental monitoring, and laboratory research, providing a reliable tool for the analysis of complex gas mixtures.

Keywords: Spectral analysis; gas mixtures; complex models; neural networks; optimization methods; machine learning

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INTRODUCTION

The development of methods for analyzing multicomponent gas mixtures is a key task in many fields, such as environmental monitoring, industrial safety, and scientific research. The use of infrared spectral analysis allows for the accurate determination of gas component concentrations based on their unique spectral characteristics. The integration of modern approaches, in particular machine learning and mathematical modeling, significantly increases the accuracy and efficiency of such methods. This is especially important for working with complex mixtures or under conditions of limited experimental data. Traditional analysis methods, such as chromatography or mass spectrometry, are highly accurate, but often require sophisticated equipment and expensive consumables. Infrared (IR) spectral analysis is afaster and more affordable method that can be implemented in the form of compact gas analyzers. However, to increase accuracy, adaptive data processing algorithms, cross-effects correction, and the use of machine learning methods to improve results are required.

The proposed model combines classical physical approaches with neural network algorithms, which allows increasing the accuracy of gas mixture analysis, reducing the influence of noise and adapting to variable experimental conditions. Variable conditions in the context of gas mixture analysis can include temperature fluctuations that affect the spectral characteristics of gases, as well as changes in pressure and humidity, which can change the intensity and spectral lines. In addition, the composition of gas mixtures can vary depending on

the emission source or processing process, which requires adaptive approaches for accurate analysis.

Also, environmental factors, such as the presence of dust or pollutants in the air, can affect the spectra, complicating their interpretation. Traditional approaches have limitations in sensitivity and selectivity, therefore, the use of neural networks is proposed to optimize the model, increase the accuracy of spectral light flux prediction and automate data processing. This makes it promising for wide application in various fields of science, technology and industry.

In general, spectral analysis and numerical modeling form an effective synergy aimed at studying complex processes, which emphasizes the relevance of this work.

1. ANALYSIS OF LITERARY DATA AND PROBLEM STATEMENT

The effectiveness of air quality monitoring and pollutant gas detection systems depends on two key aspects, namely the development of sensor technologies and the improvement of data processing methods. Modern μGC (micro gas chromatography) systems [1] provide high selectivity for target gases, but the integration of accurate sensors, in particular based on IDE structures, still requires further research [2]. Data processing systems include smoothing methods, such as moving average and Kalman filter [3], which allow reducing the noise of sensor signals. At the same time, the Kalman filter provides noise suppression without losing important information.

In datasets, the removal of uninformative outliers and the reduction of data dimensionality are usually achieved using principal component analysis (PCA) [4]. Nonlinear real-time data obtained from sensors are effectively converted into meaningful information and used in networks with back propagation algorithms (BPNN), recursive neural networks (RNN) and deep convolutional neural networks (DCNN) [5, 6]. All these machine learning algorithms are based on various mathematical models of neural networks. ANN algorithms are widely used in monitoring weather phenomena and environmental impacts [7], diagnosing diseases in humans and animals [8], camera surveillance, distance measurement and object detection in robots [9], and for successful classification of gas mixtures using various gas sensors [10].

Recently, modern spectral analysis methods have gained considerable interest, especially due to the integration of machine learning, which contributes to increasing the accuracy and automation of data processing. Deep learning (DL) is a powerful tool for spectral classification and modeling [11, 12], but it requires large amounts of data and has problems with the interpretation of results [13]. Support vector methods (SVM) are effective for analyzing NIR spectra, although their accuracy depends on the choice of kernel function and regularization parameters [14]. The article [15] provides selected references discussing the application of artificial intelligence (AI) in analytical chemistry and molecular spectroscopy, as well as examples of its use for various vibrational spectroscopy methods, such as Raman, infrared (FT-IR), near-infrared (NIR) and ultraviolet-visible (UV-vis) spectroscopy.

Convolutional neural networks (CNNs) are widely used for automatic processing of spectra without prior training [16, 17], although their effectiveness in dynamic spectral analysis is limited. Combining CNNs with dimensionality reduction methods improves the accuracy of classification of complex spectral data, in particular for the detection of illegal substances [18]. CNNs are also effective in parallel processing and optimization of spectral algorithms, which contributes to improving the accuracy of calculations and diagnostics [19]. The use of CNN spectral analysis via the Laplacian graph allows for improved image segmentation. Neural networks are also successfully used to assess the quality of alpha spectra, which is important for the detection of contaminants in the working environment [20]. One-dimensional CNNs are used in LWIR spectroscopy and Raman spectroscopy, providing noise immunity [21], and optimized hybrid models (CNN+LSTM) can improve the accuracy and adaptability of spectroscopic studies [22]. Creating a universal synthetic dataset for testing machine learning models is key to evaluating their effectiveness [21]. Studies have confirmed that nonlinear activation functions, in particular ReLU, play an important role in classification, while additional architectural complications, such as residual blocks, do not always improve the result. Despite the high accuracy (>98 %), peak overlap and intensity variations remain problematic, which requires further research. Also interesting is the approach to numerical modeling of electron kinetics in plasma based on the Boltzmann equation [23], where plasma parameters are calculated at different E/N, which is key for the optimization of plasma chemical reactors and controlled synthesis of zinc nanostructures.

Literature analysis has shown that the use of neural networks in spectral analysis significantly improves the capabilities of data processing and

interpretation. However, there are still a number of unresolved problems in spectroscopic analysis. The development of universal models that can adapt to changing measurement conditions without loss of accuracy is relevant [21]. An important task remains to improve the interpretability of deep neural networks, which complicates their use in scientific and industrial applications [24]. Optimization of CNN architecture for spectral data analysis, especially at low signal intensity or significant noise levels, requires further research [25]. In addition, the combination of neural networks, interferometric methods and adaptive spectral models can significantly improve the analysis of complex multicomponent mixtures [22]. The possibility of using graph methods to optimize the topology of neural networks, which could increase the speed and accuracy of calculations, has not been sufficiently explored [19]. Further research should focus on improving machine learning algorithms for spectroscopic analysis, which will increase their robustness to noise and experimental artifacts [26].

For data analysis, [27] was used, which covers methods for processing, cleaning, and analysis using Python, in particular the Pandas, NumPy, and IPython libraries. In [28] investigated the effectiveness of visualization libraries, comparing them in terms of functionality and convenience. The most popular are Matplotlib, Seaborn, and Plotly, which provide a wide range of capabilities for creating static and interactive graphs.

GOAL AND RESEARCH OBJECTIVES

The main task is to develop a model for analyzing multicomponent gas mixtures based on their spectral characteristics in the infrared range.

The aim of the research is to develop a combined model for spectral light flux analysis that combines physical modeling of spectral absorption of gases with machine learning methods. This provides increased accuracy in determining the concentration of components in multicomponent gas mixtures and allows adaptive adjustment of analysis parameters depending on the measurement conditions.

The main objectives include:

• development of a combined spectral model based on Gaussian and Lorentzian profiles for modeling the spectral light flux in multicomponent mixtures;

• implementation and training of neural networks for predicting the parameters of gas mixtures;

• implementation of the model algorithm and the corresponding software implementation;

• testing the system to assess its stability under various conditions.

2. MAIN RESEARCH RESULTS

2.1. Overview of mathematical models

There are several mathematical models [29, 30] that can be used for modeling and optimization in gas analysis. First of all, this is a *model for infrared analysis (IR analysis)* [31]. This model describes the ratio of light fluxes in the working and reference channels for analyzing the concentration of components of a gas mixture.

The basic equation for the ratio of light fluxes has the form:

$$\frac{\Phi_i^{\varpi}}{\Phi_i^{r}} = K\,, \tag{1}$$

where Φ_i^{ϖ} is luminous flux in the working channel; Φ_i^{r} is the luminous flux in the reference channel; K is a constant that ensures the same sensitivity for all components.

Next, we determine the flux through the optical path, according to the formula:

$$\Phi_i(\lambda) = \Phi_0(\lambda)\exp(-X_i K_i L)\,, \tag{2}$$

where $\Phi_0(\lambda)$ is intensity of the radiation source; X_i is concentration of the i-th gas in the optical channel; K_i is absorption coefficient of the i-th gas; L is optical path length.

Finally, we determine the concentration through the ratio of the fluxes:

$$X_i = \frac{1}{K_i L}\ln\left(\frac{\Phi_i^{r}}{\Phi_i^{\varpi}}\right). \tag{3}$$

The next approach is a *model for interferometric analysis* [32]. This model describes the shift of the interference fringe as a function of the refractive index of the gas.

The formula for the optical path of the interferometer is:

$$\Delta = \frac{2d}{\lambda}(n_g - n_0)\,, \tag{4}$$

where Δ is interference band shift; d is the thickness of the working cell; λ is the wavelength; n_g is the refractive index of the gas; n_0 is the refractive index in the air.

Next, we determine the refractive index due to the gas concentration by the formula:

$$n_g = n_0 + \alpha X_i \tag{5}$$

where α is proportionality coefficient for the *i*-th gas; X_i is the concentration of the *i*-th gas.

There is considerable interest *in improving the sensitivity of the IR analyzer*. To achieve the same sensitivity for all components, the method of negative gas filtration is used.

The optimal concentration in the filter is determined by the formula:

$$X_f = \frac{1}{K_i L_f \ln\left(\frac{\Phi_i^r}{\Phi_i^{\varpi}}\right)} \quad (6)$$

where X_f is concentration of the *i*-th gas in the filter; L_f is the length of the filter cell.

Another approach is to solve the *sensitivity equation for multicomponent mixtures*.

In this case, the basic formula has the form:

$$S = \frac{\partial \Phi}{\partial X_i} = \Phi_0 K_i L \exp(-K_i X_i L) \quad (7)$$

where *S* is sensitivity of the device to changes in the concentration of the *i*-th gas.

Finally, we will consider an approach based on the *optimization of the spectral filter for IR analysis*.

In this approach, the basic formula is:

$$\int_{\lambda_1}^{\lambda_2} A_i(\lambda)\tau(\lambda)d\lambda = \int_{\lambda_1}^{\lambda_2} A_j(\lambda)\tau(\lambda)d\lambda \quad (8)$$

where $A_i(\lambda)$, $A_j(\lambda)$ are absorption functions of the *i*-th and *j*-th gases; $\tau(\lambda)$ is spectral filter pass function; $[\lambda_1, \lambda_2]$ are limits of the working spectral range.

All the models considered above can be adapted depending on the specific experimental conditions and instrument parameters.

2.2. Mathematical description of the model

In this work, a system was developed for complex theoretical modeling of gas mixture analysis. It includes calculation of the light flux through the optical channel, the ratio of light fluxes for different components, and also optimization of filter concentration for sensitivity equalization. The developed theoretical model belongs to IR-analysis, since its main goal is to study the spectral absorption of gases depending on the wavelength λ. The model uses Gaussian and Lorentzian profiles to describe the resonant absorption peaks, which are characteristic of gas molecules in the infrared range. It reflects the behavior of the light flux after passing through the gas mixture, taking into account the intensity inversion to match the experimental data. Prediction using neural networks is also implemented.

It should be noted that interferometric analysis is not suitable for describing this model, since it does not take into account changes in the phases of light waves. Also, the model is not an example of sensitivity optimization, since it is not aimed at increasing the accuracy of sensors. It does not apply to spectral filtering, since it does not deal with the selection or optimization of the transmission of certain wavelengths. Thus, the model is a classic example of infrared spectral analysis, which is based on the physical principles of light absorption by gas molecules. Let us dwell in more detail on the implementation of the model.

As the main component, a *model of the spectral absorption coefficient of gases* is used, which allows us to evaluate how different components of the mixture absorb light at different wavelengths.

It is implemented according to the formula for the absorption coefficient and is based on a combination of Gaussian and Lorentzian profiles:

$$K(\lambda) = 0.5\left(A_g \exp\left(-\frac{(\lambda-\lambda_0)^2}{\sigma^2}\right) + \frac{A_l}{1+\left(\frac{(\lambda-\lambda_0)}{\sigma}\right)^2}\right) \quad (9)$$

where A_g and A_l are the amplitudes of the Gaussian and Lorentzian components; λ is the central wavelength; σ is the width of the spectral peak.

Next, the *spectral light flux model* is combined, which is used to calculate the spectral light flux passing through the gas mixture. The main function of this part is to show how the concentration of gases and their absorption coefficient affect the spectral distribution of the light flux.

The intensity of the light flux through the gas mixture is defined as:

$$\Phi(\lambda) = \Phi 0 \cdot \exp(-X \cdot K(\lambda) \cdot L), \quad (10)$$

where Φ_0 is the initial light intensity; *X* is the gas concentration; $K(\lambda)$ is the absorption coefficient; *L* is the optical path length.

The next step is to add a *model of the light flux ratio*, which is used to assess the effect of gas absorption in the working channel, compared to clean air in the reference channel and is determined by the formula:

$$R(\lambda) = \frac{\Phi_{working}(\lambda)}{\Phi_{reference}(\lambda)} \quad (11)$$

Next, the *filter optimization for sensitivity equalization* is added, which uses the above formula for determining the gas concentration in the filter and provides the same sensitivity for different components. The use of a gas filter in the model is confirmed by formula (6). The main function of this filter is to equalize the sensitivity of the analysis, minimizing the difference in absorption for different components of the gas mixture.

The formula for determining the optimal gas concentration in the filter is:

$$X_{filter} = \frac{1}{K \cdot L \cdot \ln(R_{target})} \quad (12)$$

where R_{target} is the target ratio of light fluxes.

Finally, prediction using neural networks is implemented. The neural network uses the wavelength λ and the spectral absorption coefficient $K(\lambda)$ as input features for training. The output is the predicted intensity of the light flux.

2.3. Algorithm of the model operation

The algorithm of the operation is shown in Fig. 1.

The model operation begins with the input parameters, which include λ, X, L and spectral absorption parameters A_g, A_l, λ_0, σ for each component. Next, the absorption coefficient $K(\lambda)$ is calculated, which is modeled as a combination of Gaussian and Lorentzian profiles according to formula (9). The program is implemented by the functions *gaussian_profile(lambda_range, lambda_0, amplitude, width); lorentzian_profile(lambda_range, lambda_0, amplitude, width); combined_profile(lambda_range, lambda_0, amplitude, width)*. This allows us to accurately describe the spectral features of the gas mixture and take into account real experimental dependencies.

Based on the calculated absorption coefficient, the spectral light flux through the gas mixture is calculated according to the Bouguer-Lambert-Beer law according to formula (10), which takes into account the influence of the gas concentration and the optical path length on the total signal intensity. Software implemented by the function *light_flux_spectral(X, K_func, L, lambda_range)*. After that, the ratio of light fluxes in the working and reference channels is calculated according to formula (11), which allows estimating the influence of the gas mixture on the total intensity.

Software not implemented by a separate function, but the ratio is calculated as:

K_ratio = Phi_working / Phi_reference

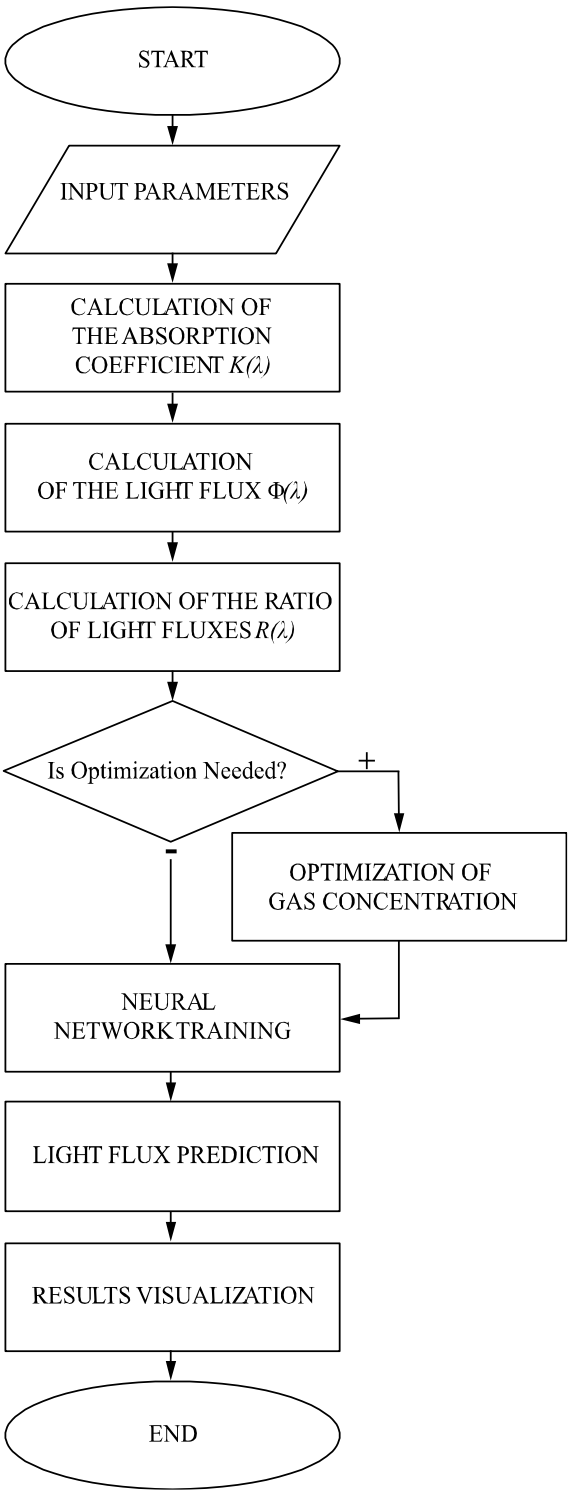

Fig. 1. **Model operation algorithm**
Source: **compiled by the author**

If the flux ratio does not correspond to the specified parameters, the gas concentration in the filter is optimized according to formula (12), which

allows ensuring uniform sensitivity of the analysis. Software implemented by the function in the code *optimize_filter_concentration(K, L, target_ratio)*. The optimized parameters are passed to the next stage of the algorithm, which consists in training a neural network to predict the spectral light flux.

The input data is $X_{train}=[\lambda,K(\lambda)]$, and the output data is $y_{train}=\Phi(\lambda)$.

The MLPRegressor neural network performs training:

$$L=\frac{1}{N}\sum_{i=1}^{N}(y_i-\hat{y}_i)^2. \quad (13)$$

We see that the training is carried out by minimizing the mean square error between the calculated and real values, which allows the model to adapt to changing spectral parameters. After training, the network is used to predict the spectral light flux, which allows us to obtain an estimate of the parameters of the gas mixture even in the case of incomplete or noisy data.

Programmatically implemented by functions in the *MLPRegressor* code from the *sklearn library* (a neural network that is trained on data to model predicted values). For training – *nn_model.fit(X_train, Y_train)*, and for prediction – *nn_model.predict(X_train)*. The results are limited by realistic limits *np.clip()*.

Finally, the prediction results are analyzed and visualized for comparison with experimental and theoretical data. In case of significant discrepancies between the predicted and experimental values, the model can be retrained by adjusting the input parameters or updating the training sample.

2.4. Description of the neural network

The final stage of the combined model is the use of a multilayer perceptron (MLP) to solve the regression problem. The choice of MLP as the basic architecture is justified by the fact that this network is well suited for regression problems and can approximate complex nonlinear dependencies between input parameters and spectral light flux.

The neural network receives model data as input, calculated using physical formulas (9)-(11). This allows the network to be trained to find dependencies between gas mixture parameters and spectral light flux. The use of model data at the training stage is justified by the fact that they provide a wide range of parameters, including limiting cases that may be difficult to access in real experiments. However, in the end, the neural network works with real data, so during testing it is intended to use both model and experimental values. This makes it possible to adjust the model and adapt it to the features of real measurements.

2.5. Neural network training and optimization

The neural network training process included preparing a dataset containing experimental spectral characteristics of gases, normalizing input parameters, and dividing the sample into training and test. For training, the Adam optimizer with adaptive learning rate selection was used, as well as a loss function to minimize the deviation between predicted and actual values. The cross-validation provided generalization of the model and prevented overtraining.

To optimize the model, a series of numerical experiments were conducted with different neural network configurations, which are presented in Table 1. The selected range of neural network parameters is justified by the specifics of spectral analysis of gas mixtures and the need to achieve a balance between accuracy, performance, and model stability. The number of hidden layers and neurons in the layers varies between 2-4 layers and 64-256 neurons, which allows finding a compromise between the generalization ability of the model and its computational complexity. A smaller number of layers speeds up training, but may not be sufficient for accurate recognition of spectral patterns, while a larger number of layers and neurons improve the representation of complex spectral dependencies, but increases the risk of overtraining.

The activation functions ReLU, Tanh, and Sigmoid are chosen to take into account different features of spectral data. ReLU is effective for deep networks, Tanh works well with normalized data, and Sigmoid provides a nonlinear transformation with probabilistic interpretation. Adam was used for optimization.

The number of epochs in the range of 1000-2500 was determined experimentally, since a sufficient number of iterations is required for accurate learning, but too large a value can cause overtraining. The batch size of 32-128 provides an optimal balance between the learning speed and the quality of gradient updates, where smaller batches allow better adaptation to local data features, and larger ones ensure the stability of the learning process.

Table 1. **Tested neural network configurations**

N.	Number of layers	Number of neurons per layer	Activation function	Optimizer	Number of epochs	Model accuracy (%)
1	2	64	ReLU	Adam	1000	92.5
2	3	128	ReLU	Adam	2000	94.3
3	3	256	Tanh	Adam	2000	91.7
4	4	128	ReLU	SGD	2500	88.2
5	2	256	ReLU	Adam	1500	95.1
6	3	128	Sigmoid	Adam	2000	89.8
7	2	64	ReLU	RMSprop	1500	90.6

***Source*: compiled by the authors**

Thus, the selected parameters allow achieving the optimal ratio between performance, accuracy and speed of the model in the spectral analysis of gas mixtures. Based on the results obtained, the optimal parameters were determined that provide the best balance between accuracy and performance. The optimal option is a model with three hidden layers and 128 neurons in each, the ReLU activation function and the Adam optimizer, which provides high accuracy (94.3 %). Increasing the number of neurons and layers after this level does not provide significant improvement, and the use of alternative activation functions, such as Tanh or Sigmoid, slightly reduces accuracy.

In the proposed model, the problem of limited data is solved by using synthetic data for initial training of the neural network. The physical model of spectral absorption allows generating a large set of training data covering different gas concentrations, wavelengths and optical parameters. This allows providing the necessary variety of input characteristics and compensating for the lack of real experimental measurements. Synthetic data are generated based on physical equations describing the spectral absorption of gases, according to formulas (2) and (9). The expansion of synthetic data for the neural network is carried out by varying the gas concentration, optical path length and temperature shifts within the limits of real experimental conditions. Adding random noise simulates experimental errors, increasing the stability of the model. Generation of mixed spectra by linear combination of components allows better recognition of the contribution of each gas. After training on synthetic data, the model is retrained on real spectra, which adapts it to the characteristics of the sensors and experimental conditions. This approach ensures high accuracy and stability of the neural network even with a limited amount of experimental data.

DISCUSSION OF RESULTS

A significant part of scientific works is devoted to obtaining experimental data that require theoretical modeling and optimization [33, 34], [35, 36], [37]. In [33], it is proposed to improve interferometric methods of gas analysis by switching to measuring frequency shifts, which increases accuracy and sensitivity. Work [34] describes optical correlation methods for analyzing gas mixtures, in particular, the use of a Fabry-Perot interferometer as a correlation mask, which is discussed in detail in [35]. In [36], infrared and interferometric methods of gas analysis are investigated, device schemes and methods for increasing selectivity with an error of up to 10 %. Article [37] is devoted to the metrological support of gas analyzers with an open cell, in particular, calibration methods that minimize measurement errors.

Work [36] was chosen to test the system on experimental data. The validation of the research results was carried out by comparing theoretical, experimental and predicted data for the analysis of spectral light flux through multicomponent gas mixtures. Theoretical models built on the basis of Gaussian and Lorentzian profiles were checked for compliance with experimental absorption spectra for CH_4 and C_3H_8. The combined model demonstrated the ability to accurately reflect the position and width of the absorption peaks, which confirms its effectiveness for modeling real physical processes.

Prediction using neural networks was tested by training on theoretical and experimental data, after which the models were used to predict the spectral light flux. The predicted results were consistent with the experimental data, demonstrating the ability of neural networks to take into account key characteristics of spectral absorption.

The developed system can be used for the analysis of gas mixtures in laboratory and industrial conditions. Testing at different gas concentrations and optical path lengths showed that the model

remains stable and adaptive to changes in external parameters. This indicates its versatility and practical value in the tasks of environmental monitoring, industrial control and scientific research. The graph of the dependence of the normalized light flux of CH_4 on the gas concentration and optical path length is shown in Fig. 2. It shows how changing this parameter affects the measurement results.

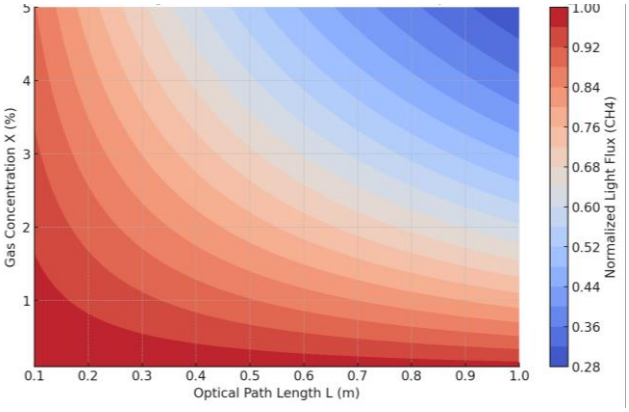

Fig. 2. **Dependence of CH_4 light flux on concentration and optical path length**
Source: **compiled by the author**

Regarding the accuracy of the simulation, a graph of the model accuracy versus gas concentration and optical path length was plotted, which is shown in Fig. 3. The graph shows that at low concentrations (X<1 %) the model demonstrates high accuracy of over 90 %, since weak absorption provides a stable signal. With increasing concentration to X>3 %, the accuracy decreases due to saturation effects, which makes it difficult to distinguish gas components. Similarly, at short optical path lengths (L<0.3 m), the accuracy remains high, since absorption is insufficient for significant signal losses, while at long optical paths (L>0.7 m) the model loses accuracy due to excessive absorption, which leads to a decrease in the intensity of the light flux and loss of information. Optimal conditions for the model operation are observed at gas concentrations within X≈1-2 % and a length L≈0.3-0.6 m, which provides a balance between sensitivity and measurement accuracy.

To assess the accuracy of the regression model, two main metrics were chosen, namely RMSE (root mean square error) and R^2 (coefficient of determination). RMSE shows the average deviation of the predicted values from the actual ones in the same units as the input data, and R^2 demonstrates how well the model explains the variability of the data. A value close to 1 means a high correspondence between the model predictions and the experimental data. The evaluation results showed a high efficiency of the neural network in reproducing the experimental data. The obtained value of the coefficient of determination R^2=0.9957 indicates a high correspondence of the model to the experimental data, which confirms its accuracy in predicting the spectral luminous flux. Low values of RMSE=0.01997 demonstrate minimal errors between the predicted and actual values, which makes the proposed model suitable for the analysis of multicomponent gas mixtures. Thus, the results confirm that the developed neural network can be effectively used for spectroscopic analysis, providing high accuracy and stability when changing the parameters of the gas mixture.

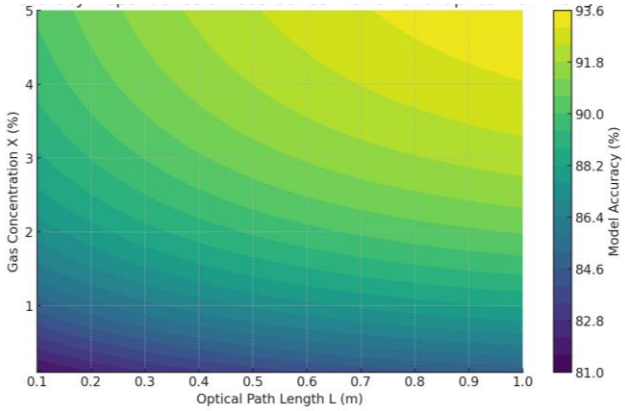

Fig. 3. **Model accuracy on gas concentration and optical path length**
Source: **compiled by the author**

Regarding the validation of the accuracy of the model on experimental data, the concentration of methane and propane was calculated using the Bouguer-Lambert-Beer equation (Table 2). From the table, we see that the concentration of CH_4 varies within 100-475 %. This indicates the need to correct the absorption coefficients or take into account additional factors (for example, intermolecular interactions). The concentration of C_3H_8 in some cases exceeds the physically possible values (>900%), which may indicate an error in determining the absorption coefficients or the influence of other gases in the mixture. For a more accurate analysis, it is necessary to take into account calibration coefficients, take into account nonlinearities in spectral absorption, or apply corrective functions of the neural network.

The main results of the model are displayed in a graph showing the values of the spectral luminous flux. Fig. 4 presents the experimental data, combined calculated and predicted spectral luminous flux for comparison of their values.

Table 2. **Results of gas mixture analysis and concentration calculation**

Wavelength (м)	$\Phi_{measured,\ CH_4}$	K_{CH_4}	X_{CH_4} (%)	$\Phi_{measured,\ C_3H}$	$K_{C_3H_8}$	$X_{C_3H_8}$ (%)
$3.1*10^{-6}$	0.95	0.20	102.59	0.85	0.15	433.38
$3.2*10^{-6}$	0.80	0.25	357.03	0.65	0.20	861.57
$3.3*10^{-6}$	0.70	0.30	475.57	0.50	0.28	990.21
$3.4*10^{-6}$	0.85	0.22	295.49	0.70	0.23	620.30
$3.5*10^{-6}$	0.90	0.18	234.13	0.80	0.19	469.78

***Source*: compiled by the authors.**

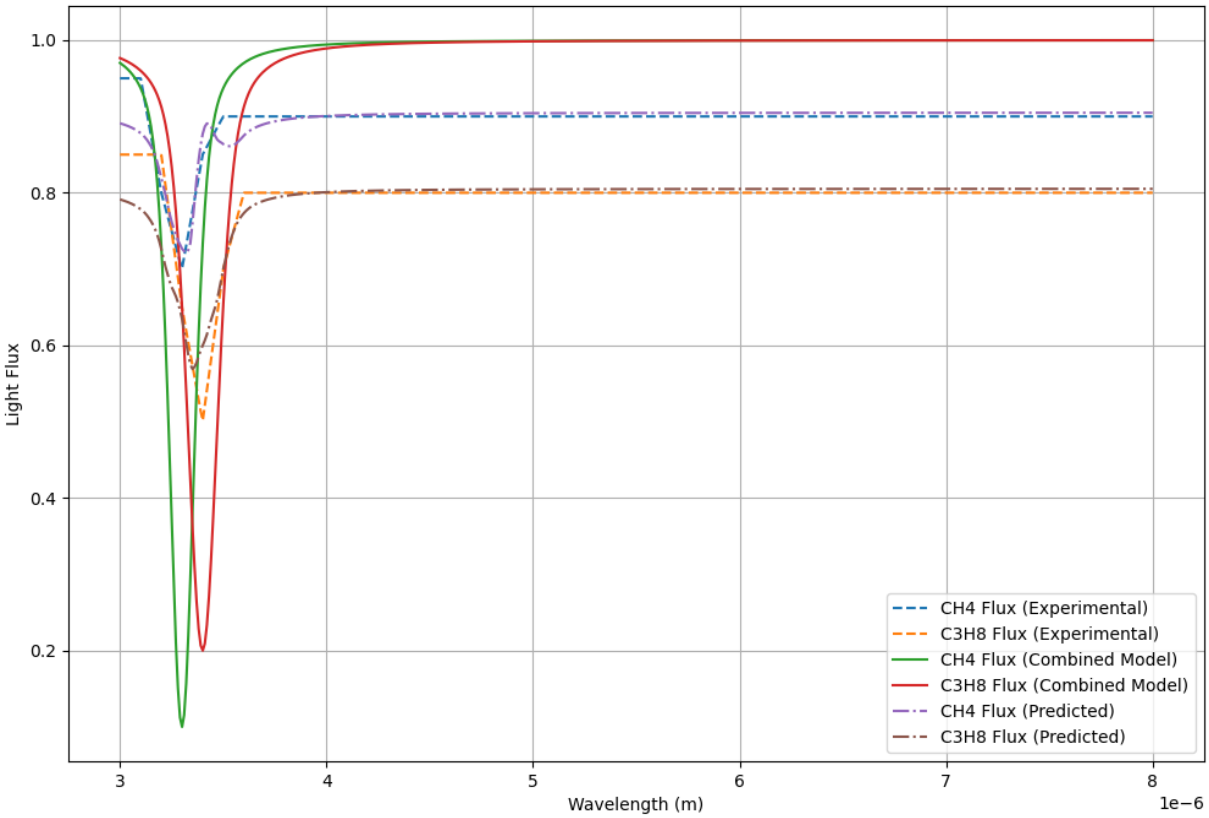

Fig.4. **Experimental vs combined model vs predicted spectral light flux**

***Source:* compiled by the author**

In graph 4, the series of curves Combined Model is the result of physical and mathematical modeling of the luminous flux, which takes into account the spectral absorption of gases according to the corresponding equation (9) taking into account the combination of Gaussian and Lorentzian profiles; and Predicted is the output of the MLP regression algorithm, which, based on model or experimental data, predicts the value of the luminous flux.

Thus, the graph displays three main series of data for each of the gases CH_4 and C_3H_8 depending on the wavelength λ. The experimental data are represented by dashed lines and show the decrease in the intensity of the luminous flux in the corresponding spectral regions. This indicates the absorption of light by gases in the wavelength ranges of 3.3 μm for CH_4 and 3.4 μm for C_3H_8.

The data have smooth declines, reflecting the physical properties of gas molecules. The combined model, shown in solid lines, combines Gaussian and Lorentzian profiles. It allows for both narrow peaks (characteristic of a Lorentzian profile) and broader spectral features (corresponding to a Gaussian profile). This provides a better agreement with the real physical characteristics of spectral absorption. The profiles are inverted to reflect the decrease in light intensity due to absorption, and they generally agree well with the experimental data. The predicted data, shown in dotted lines, were obtained using a neural network. The input data for the network were the wavelength and the combined model. The predicted values generally reproduce the main trends of the experimental data, including the position and width of the peaks. This indicates that the model has successfully learned to capture the key features of

the dependence of the luminous flux on wavelength. Overall, the graph demonstrates the consistency of the combined model and predicted data with experimental data [36], confirming their effectiveness in describing and predicting the behaviors of the luminous flux in the spectral absorption regions.

Overall, the experimental data show an accurate distribution of absorption in gases, the theoretical model helped to better understand the physical basis of the experiment, and the neural network successfully reproduced the main trends, which indicates its effectiveness in predicting the behavior of the luminous flux under similar conditions. The graph demonstrates how different approaches – experimental, theoretical, and machine learning – complement each other to better analyze the absorption process.

CONCLUSIONS

The developed model for the analysis of gas mixtures using neural networks and combined spectral models demonstrates an effective combination of machine learning methods and classical physical models. The use of artificial intelligence algorithms allowed to increase the accuracy of determining the concentrations of components in spectral analysis, which is confirmed by low RMSE values and a high coefficient of determination R^2= 0.9957.

Additionally, the neural network configuration was optimized to achieve the best balance between prediction accuracy and calculation speed. Analysis of different architectures allowed determining effective parameters, such as the number of hidden layers, the dimension of neurons and regularization methods. This allows increasing the performance of the model while maintaining high accuracy, which is critically important for its use in large data analysis systems.

The use of deep neural networks in spectral analysis of gas mixtures opens up new opportunities for automation, processing of large data sets and increasing the adaptability of algorithms to changing environmental conditions. The developed system integrates signal processing methods and optimization approaches to improve spectral identification, which makes it promising in the field of information technology, in particular in environmental monitoring, industrial automation and intelligent sensor systems.

The practical significance of the work lies in the possibility of implementing the presented methodology in intelligent data analysis systems used for air quality control, monitoring of production processes and ensuring safety in industry. Further research can be focused on optimizing the architecture of neural networks, expanding the set of input parameters and is integrating the developed technology with distributed computing systems to increase the performance of real-time analysis.

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Розробка комбінованої моделі аналізу газових сумішей з використанням методів машинного навчання

Білак Юрій Юрійович
ORCID: https://orcid.org/0000-0001-5989-1643; yuriy.bilak@uzhnu.edu.ua. Scopus Author ID: 57213689747
Ужгородський національний університет, площа Народна, 3. Ужгород, 88000, Україна

АНОТАЦІЯ

Аналіз газових сумішей є важливим завданням у спектроскопії, екологічному моніторингу, промисловому контролі та наукових дослідженнях. Точне визначення концентрацій компонентів у складних газових середовищах потребує

вдосконалених підходів, що поєднують фізичне моделювання та методи штучного інтелекту. Використання нейронних мереж у спектральному аналізі дозволяє підвищити точність та стійкість розрахунків за змінних умов експерименту, що вказує на актуальність роботи. **Метою дослідження** є розробка комбінованої моделі аналізу спектрального світлового потоку, яка поєднує фізичне моделювання спектрального поглинання газів із методами машинного навчання. Це забезпечує підвищену точність визначення концентрації компонентів у багатокомпонентних газових сумішах та дозволяє адаптивно коригувати параметри аналізу залежно від умов вимірювання. Запропоновано інтегровану методику, що включає моделювання спектрального світлового потоку на основі гаусових та лоренцівських профілів поглинання, використання рівнянь Бугера-Ламберта-Бера для визначення концентрації газів, а також навчання нейронної мережі для прогнозування світлового потоку. Для оцінки продуктивності розробленої моделі проведено серію чисельних експериментів з варіюванням параметрів мережі та оптимізацією конфігурації. **Отримані результати** підтвердили високу ефективність моделі, що відображено у високому значенні коефіцієнта детермінації та низьких значеннях середньоквадратичної помилки. Проведено тестування моделі при зміні концентрацій газів та довжини оптичного шляху, що підтвердило її стабільність і здатність до адаптації. Дослідження показало, що оптимальна конфігурація нейромережі включає три приховані шари з оптимальною кількістю нейронів, що забезпечує баланс між точністю та ефективністю. Використано випрямлену лінійну активаційну функцію для стабільної збіжності, а для оптимізації ваг – адаптивний метод стохастичного градієнтного спуску, що покращує продуктивність. **Запропонована методика** поєднання фізичного моделювання та машинного навчання забезпечує високу точність аналізу газових сумішей та стійкість до варіацій зовнішніх умов. **Наукова новизна** дослідження полягає у застосуванні комбінованого підходу, що дозволяє адаптувати модель до широкого діапазону спектральних характеристик. Практична значущість роботи полягає у можливості застосування розробленої методики для промислового контролю, екологічного моніторингу та лабораторних досліджень, забезпечуючи надійний інструмент для аналізу складних газових сумішей.

Ключові слова: спектральний аналіз; газові суміші; комплексне моделювання; нейронна мережа; методи оптимізації; машинне навчання

ABOUT THE AUTHOR

Yurii Yu. Bilak – PhD (Physical and Mathematical Sciences), Associate Professor, Head of the Department of Software systems Uzhhorod National University, 3, Narodnaya Square. Uzhgorod, 88000, Ukraine
ORCID: https://orcid.org/0000-0001-5989-1643; yuriy.bilak@uzhnu.edu.ua. Scopus Author ID: 57213689747
Research field: Intelligent information technology, comprehensive analysis and optimization methods, physics, neural networks and artificial intelligence

Білак Юрій Юрійович - кандидат фізико-математичних наук, доцент, завідувач кафедри Програмного забезпечення ситем. Державний вищий навчальний заклад «Ужгородський національний університет», пл. Народна, 3. Ужгород, 88000, Україна