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Application of Artificial Neural Networks for Determining the Temperature and Partial Pressures of the Components of High-Temperature Gaseous Media

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***Abstract*—The paper deals with the development of methods for solving the inverse problem of gaseous media optics by determining the parameters of high-temperature gaseous media from its spectral characteristics. It is proposed to use artificial neural networks to determine the temperature and partial pressures of water vapor, carbon dioxide, carbon oxide and nitrogen oxide from its transmissivities.**

***Keywords*—artificial neural network, gas, transmissivity, temperature, pressure.**

I. Introduction

The optical methods are actively applied to remote analysis of gaseous media of different origins. Contactless study of gaseous mixture is the main advantage of optical measuring [1]. These methods are irreplaceable for the study of very distant objects such as space objects or objects dangerous to human life, for example, emissions from volcanoes and industries or jet engines exhaust [1–3].

In [4], it was proposed to use artificial neural networks (ANN) to find the temperature and partial pressure of one gas. This paper discusses the case of solving the inverse problem of the optics of gaseous media in the case of a four-component gaseous medium.

II. Method of Transmissivity Calculation

To calculate the transmissivity of the gaseous medium the following formula was used:

$$\tau(v) = \frac{1}{\Delta v}\int e^{-k(v,T,P)l}\,, \qquad (1)$$

where v is the wavenumber; Δv is the spectral resolution; $k(v, T, P)$ is the absorption coefficient; T and P are temperature and total pressure of gas mixture; l = 55 cm is optical path.

The absorption coefficients were calculated by the line-by-line method:

$$k(v,T,P) = \sum_i p_i \sum_j S_{ij}(T)\, f(v - v_{ij})\,, \qquad (2)$$

where p_i is the partial pressure of the i-gas; v_{ij} is the wavenumber of j-line of the i-gas with the shift coefficient of δ_{ij}; $S_{ij}(T)$ is the intensity of the j-line of the i-gas at temperature T:

$$S_{ij}(T) = S_{ij}(T_0)\cdot\frac{Q(T_0)}{Q(T)}\cdot\frac{e^{-hcE/k_BT}}{e^{-hcE/k_BT_0}}\cdot\frac{1-\mathrm{e}^{-hcv_{ij}/k_BT}}{1-e^{-hcv_{ij}/k_BT_0}}\,, \qquad (3)$$

where $Q(T)$ is the statistical sum; E is the energy of the low state of transition; h, c , and k_B are the fundamental physical constants; T_0 = 296 K.

To calculate the spectral line profile, the Lorentz lineshape was used:

$$f(v - v_{ij}) = \frac{1}{\pi}\cdot\frac{\Delta_{ij}}{\Delta_{ij}^2 + (v - v_{ij})^2}\,, \qquad (4)$$

In the case under consideration, the main reason for the broadening of spectral lines is collisions of the components of the gaseous medium. Half-width of the j-spectral line of the i-gas for required temperature and total pressure was calculated as:

$$\Delta_{ij}(P, p_i, T) = P\cdot(\,p_i\Delta_{ij}^{self} + (1-p_i)\Delta_{ij}^{air}\,)\cdot\left(\frac{T_0}{T}\right)^{n_{ij}}, \qquad (5)$$

where Δ_{ij}^{self} and Δ_{ij}^{air} are the self- and air-broadening half-width of the j-line of the i-gas at temperature T_0, n_{ij} is temperature-dependence exponent of half-width of the j-line of the i-gas which were taken from HITEMP2010 [5].

III. Selecting the Spectral Centers

To determine the unknown parameters of a gaseous medium, it is sufficient that the number of spectral centers is equal to the number of these parameters. For the case

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considered in this article, it is necessary to determine the partial pressures of four gases (H_2O, CO_2, CO and NO) and the temperature of the gaseous medium, therefore the number of spectral centers should be equal to five. However, as it has been shown previously [6], the use of a larger number of spectral centers leads to an increase in the accuracy of solving the inverse problem. This is due to the fact that at different combinations of temperature and partial pressures, the same amount of absorption by the gaseous medium can be observed. Therefore, the spectral centers should be chosen in such a way as to provide different temperature dependences of absorption.

Another criterion for the choice of spectral centers is that for each spectral center there should be a predominance of the absorption of a certain gas over the absorption of other components of the gaseous medium.

The spectral centers suitable for solving the inverse problem under consideration were chosen from the spectral interval 1000–2500 cm^{-1} in which the absorption bands of water vapor, carbon dioxide, carbon oxide and nitrogen oxide are located (Table I).

TABLE I. THE APPLIED SPECTRAL CENTERS

No.	Spectral center (cm^{-1})			
	H_2O	CO_2	CO	NO
1	1136	1023	2004	1853
2	1152	1049	2009	1900
3	1173	2070	2021	1926
4	1186	2084	2025	1940
5	1198	2398	2033	1960

There are many spectral lines of water vapor that meet the given criteria. The best suited spectral lines falling within the range 1100–1200 cm^{-1}, where there is practically no overlap of spectral lines of water vapor with spectral lines of other components of the gaseous medium.

The intersection of the carbon oxide absorption band with the carbon dioxide one complicates the selection of spectral centers in the case of CO_2. At $T = 800$ K on the spectral centers 2070 cm^{-1} and 2084 cm^{-1}, the absorption of CO is greater than CO_2 one. However, the situation changes with increasing temperature. At $T = 1800$ K the absorption of CO is many times less than the absorption of CO_2. In the case of the spectral centers 1023 cm^{-1} and 1049 cm^{-1} at $T > 1000$ K, water vapor absorption dominates.

The spectral centers with the dominant absorption of carbon oxide were selected from the spectral range 2000–2050 cm^{-1}. The greatest influence of absorption of the main interfering gas H_2O is observed at spectral centers 2004 cm^{-1}, 2021 cm^{-1} and 2025 cm^{-1} of CO, reaching 25% at a temperature of 1800 K. It should be noted that nitric oxide is another interfering gas, which has a similar effect on the absorption value as water vapor only at spectral centers 2004 cm^{-1} and 2009 cm^{-1} of CO.

In the case of nitric oxide, the spectral centers were selected from the spectral interval 1850–2000 cm^{-1}. Lines from the absorption band of water vapor also fall into this spectral interval, and at a temperature of 1800 K at spectral centers 1853 cm^{-1} and 1926 cm^{-1}, they contribute 30% to the total absorption of the gaseous medium. The spectral center 1960 cm^{-1} of NO has an overlap with lines of CO absorption band that contribute less than 25% to absorption.

Thus, 20 spectral centers were selected (five for each of the gases under consideration), which are suitable for determining the partial pressures of water vapor, carbon dioxide, carbon oxide and nitrogen oxide entering the gaseous medium and temperature when changing them in the ranges from 0.1 atm to 0.7 atm and from 800 K to 1800 K respectively.

IV. ARTIFICIAL NEURAL NETWORK

For solving the problem under consideration a feed-forward neural network (Fig. 1) was used [7]. The number of spectral centers specifies the number of inputs of the input layer of the ANN. The desired parameters (temperature and partial pressure of gases) were obtained at output neurons of the ANN.

The output signal y_k of the kth neuron (Fig. 2) is defined as follows

$$y_k = \varphi(\upsilon_k), \tag{6}$$

$$\upsilon_k = u_k + b_k = \sum_{i=1}^{m} \omega_{ki} x_i + b_k, \tag{7}$$

where $\varphi(\upsilon_k)$ is the activation function; υ_k is the activation potential; u_k is a linear combination of input signals; b_k is shift; x_i are input signals; ω_{ki} are synaptic weights of the kth neuron. Logistical function with the slope parameter a was used as the activation function

$$\varphi(\upsilon) = \frac{1}{1 + \exp(-a\upsilon)}, \tag{8}$$

Software implementation of the ANN was realized in the Python language using the open neural network library Keras. The TensorFlow library was as a backend.

For training the ANN, the Adam optimization algorithm was used. The values of the transmissivity were used as input data for training the ANN, and the values of the gas temperature and partial pressures at which they were calculated were output data.

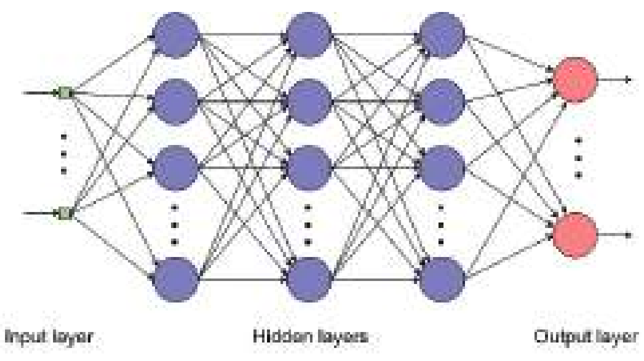

Fig. 1. Feed-forward neural network.

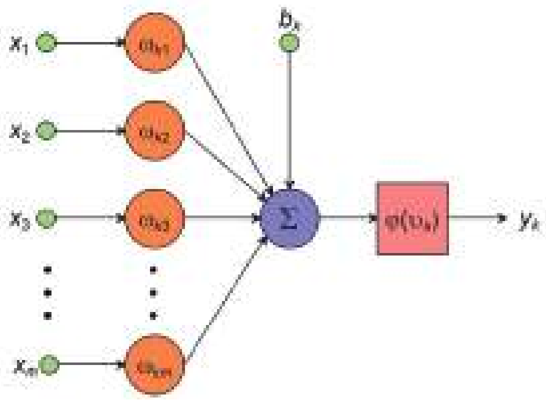

Fig. 2. Model of the *k*th neuron.

V. RESULTS AND DISCUSSION

The transmittance was calculated for a mixture of H_2O, CO_2, CO, NO gases in the temperature range from 800 K to 1800 K in increments of 100 K and in the range of partial pressures from 0.1 atm to 0.7 atm with increments of 0.1 atm.

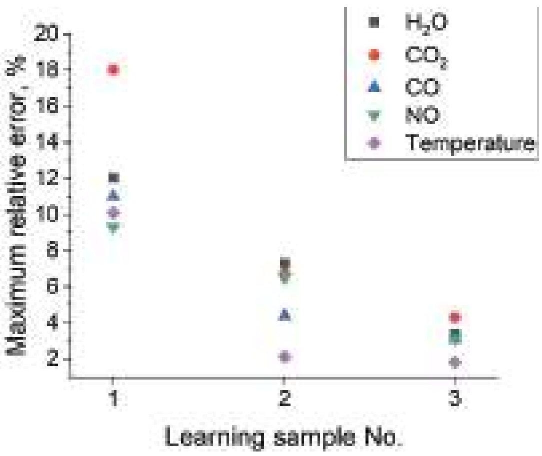

Fig. 3. Dependenses of the maximum relative error of determining temperature and partial pressure of gases on the learning sample size in the case of ANN with three hidden layers of fifteen neurons.

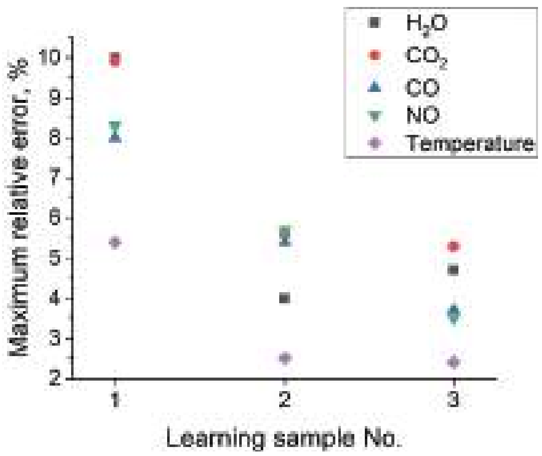

Fig. 4. Dependenses of the maximum relative error of determining temperature and partial pressure of gases on the learning sample size in the case of ANN with three hidden layers of twenty neurons.

Training the ANN was carried out on three learning samples (LS) differing in the number of examples in them. The size of the learning sample No. 1, No. 2, No. 3 was respectively 10%, 20%, 30% of the total number of samples. ANN with a different number of hidden layers and neurons in them were considered.

Figs. 3–4 and Table II show the results of solving the inverse problem of the optics of gaseous media.

TABLE II. MAXIMUM RELATIVE ERRORS IN DETERMINING TEMPERATURE AND PARTIAL PRESSURES OF GASES (ANN WITH THREE HIDDEN LAYERS OF TWENTY NEURONS)

LS No.	Maximum relative errors (%)				
	Partial pressure				*T*
	H_2O	CO_2	CO	NO	
1	4.0	5.6	5.4	5.7	2.5
2	7.3	6.7	4.4	6.5	2.1
3	3.4	4.3	3.1	3.1	1.8

As the size of the learning sample increases, the relative error decreases. An increase in the number of neurons from 15 to 20 in the hidden layers also reduced the relative error.

The relative error in determining the partial pressures is approximately three times greater than the relative error in determining the temperature.

VI. CONCLUSION

Thus, as a result of this research, ANN was obtained that allows to determine the temperature and partial pressures of water vapor, carbon dioxide, carbon oxide and nitrogen oxide in the interval 800–1800 K and 0.1–0.7 atm, respectively, with a relative error of less than 5%.

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