Determining temperature and partial pressures of the components of a high-temperature gas mixture using artificial neural networks

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Abstract. The article deals with solving the inverse problem of gaseous media optics by determining the parameters of high-temperature gaseous media from its transmittances using the artificial neural networks. The study of the dependence of the maximum relative error in determining the desired parameters on the size of the training set and the artificial neural network configuration is carried out. The possibility of solving the inverse problem in the case of a four-component gas mixture (water vapor, carbon dioxide, carbon oxide and nitrogen oxide) is shown.

1. Introduction

Optical measurements are actively used to determine the concentrations of components of gaseous media of natural and anthropogenic origin [1-4]. Each gas has an individual absorption spectrum, which makes it possible to identify the gas in the gas mixture. The main advantage of optical methods is the ability to remotely analyze the gas composition.

Earlier in [5], the case of determining temperature and partial pressure of one gas using artificial neural networks (ANN) was considered. Unlike [5], this work generalizes the approach to the case of multicomponent gaseous media, namely, the inverse problem of the optics of gaseous media is solved for the case of a four-component (H₂O, CO₂, CO, and NO) gaseous medium.

2. Transmittance calculation

The transmittances of the gaseous media were calculated as follows

\[ \tau(v_0) = \frac{1}{\Delta v} \int_{v_0-\Delta v}^{v_0+\Delta v} e^{-k(v,T,P)v} dv, \]

where \( v_0 \) is the spectral center; \( \Delta v \) is the spectral resolution; \( k(v,T,P) \) is the absorption coefficient; \( T \) and \( P \) are temperature and total pressure of gas mixture; \( l \) is optical path, which was 55 cm.

To calculate the absorption coefficients the line-by-line method was used

\[ k(v,T,P) = \sum_i P_i \sum_j S_j(T) f(v-v_j), \]
where $p_i$ is the partial pressure of the $i$-gas; $v_j$ is the center of $j$-line of the $i$-gas with the shift coefficient of $\delta_j$; $S_j(T)$ is the intensity of the $j$-line of the $i$-gas at temperature $T$ calculated as follows

$$S_j(T) = S_j(T_0) \cdot \frac{Q(T_0)}{Q(T)} \cdot \frac{\exp\left(-\frac{hcE}{k_BT}\right)}{1 - \exp\left(-\frac{hc\nu_j}{k_BT_0}\right)} \cdot \frac{1 - \exp\left(-\frac{hc\nu_j}{k_BT}\right)}{1 - \exp\left(-\frac{hc\nu_j}{k_BT_0}\right)}$$

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:

$$f(v - v_j) = \frac{1}{\pi} \frac{\Delta_j}{\Delta_j^2 + (v - v_j)^2}.$$

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 can be calculated as

$$\Delta_j(P, p_i, T) = P \cdot (p_i \Delta_j^{\text{eff}} + (1 - p_i) \Delta_j^{\text{air}}) \cdot \left(\frac{T}{T_0}\right)^{n_j},$$

where $\Delta_j^{\text{eff}}$ and $\Delta_j^{\text{air}}$ are the self- and air-broadening half-width of the $j$-line of the $i$-gas at temperature $T_0$, $n_j$ is temperature-dependence exponent of half-width of the $j$-line of the $i$-gas.

All spectral line parameters necessary for calculating the transmittances were taken from HITEMP2010 [6].

### 3. 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 considered in this article, it is necessary to determine the partial pressures of four gases (H$_2$O, 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 [7], 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 twenty spectral centers (five for each of the gases under consideration) were chosen from the spectral interval 1000–2500 cm$^{-1}$ (table 1). They 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, at which the transmission spectra of H$_2$O and CO$_2$ were measured in [8].

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.

**Table 1. The used spectral centers.**

| No. | H$_2$O | 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 |

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$_2$O 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, 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.

4. **Artificial neural network**

To solve the problem under consideration a feed-forward neural network (figure 1), more specifically a multilayer perceptron, was used [9]. The number of inputs of the ANN input layer is determined by the number of spectral centers used to solve the inverse problem. The desired parameters (temperature and partial pressure of gases) are obtained at output neurons of the ANN.

![Feed-forward neural network](image)

**Figure 1.** Feed-forward neural network.

The output signal $y_k$ of the $k$th neuron (figure 2) is defined as follows
\[ y_k = \varphi(\nu_k), \]

\[ \nu_k = u_k + b_k = \sum_{i=1}^{m} \omega_{ik} x_i + b_k, \]

where \( \varphi(\nu_k) \) is the activation function; \( \nu_k \) is the activation potential; \( u_k \) is a linear combination of input signals \( x_i \); \( b_k \) is shift; \( \omega_{ik} \) are synaptic weights of the \( k \)th neuron. Logistical function with the slope parameter \( a \) was used as the activation function

\[ \varphi(\nu) = \frac{1}{1 + \exp(-a\nu)}. \]

Figure 2. Model of the \( k \)th neuron.

Software implementation of the ANN was realized in the Python language using the open neural network library Keras [10]. The TensorFlow [11] library was as a backend.

For training the ANN, the Adam [12] 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. To solve the problem under consideration when training the ANN, it is necessary to minimize the maximum relative error among the relative errors for all samples in a training set. This is not provided by the standard methods of the Keras. Therefore, the own loss function for training the ANN was implemented.

5. Results and discussion

The transmittance was calculated for a mixture of H\(_2\)O, 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. On the basis of these data, training, validation and test sets were formed.

Training the ANN was carried out on the three training sets differing in the number of samples in them. The size of the training set 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.

Figure 3 and figure 4 show the results of solving the inverse problem of the optics of gaseous media. As the size of the training set 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 greater than the relative error in determining the temperature.
6. 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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