Simulating the determination of component content of thermodynamically inhomogeneous gaseous media

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A method for estimating total content of a component of a gas mixture having inhomogeneous temperature and concentration distribution is proposed. The approach assumes selection of a spectral region with minimum temperature dependence of the absolute absorption coefficient. Variation of the shape and width of the spectrometer's instrumental function allowed us to reveal optimal parameters providing for the smallest error in determination of the gas concentration from transmission measurements. Measurements of carbon monoxide have been numerically simulated, and it has been shown that in a practically important case (temperature distribution of a forest fire) the error in concentration restoration does not exceed 10%.

Introduction

Due to the wide variety of spectral distributions of absorption coefficients (AC) for different gases, they can be used for analysis of gaseous media. In our recent paper[1] we have simulated determination of the path-averaged temperature of an inhomogeneous medium by pyrometric measurements in spectral regions with the minimum and maximum temperature dependence of AC.

In this paper, we consider the possibility of finding the total content of an absorbing gas along a path with high temperature and concentration gradients and estimate the corresponding error. In this case, the spectral region with the minimum variation of the absorption coefficient in the entire temperature range seems to be optimal as a working interval for solution of the problem considered. This rather obvious idea was studied in Ref. 2 as applied to the actual atmosphere and more recently discussed in Ref. 3 for continuum absorption spectra, but the temperature range considered was small. Such regions were experimentally recorded by Moskalenko with colleagues[4] and are illustrated by our calculations (Fig. 1) for the temperature range of 300–1200 K. As the initial data for AC calculations, we used the parameters of carbon dioxide, carbon monoxide, and water vapor spectral lines generated for a wide temperature range (300–3000 K) by the HOTGAS 2.0 information system.[5]

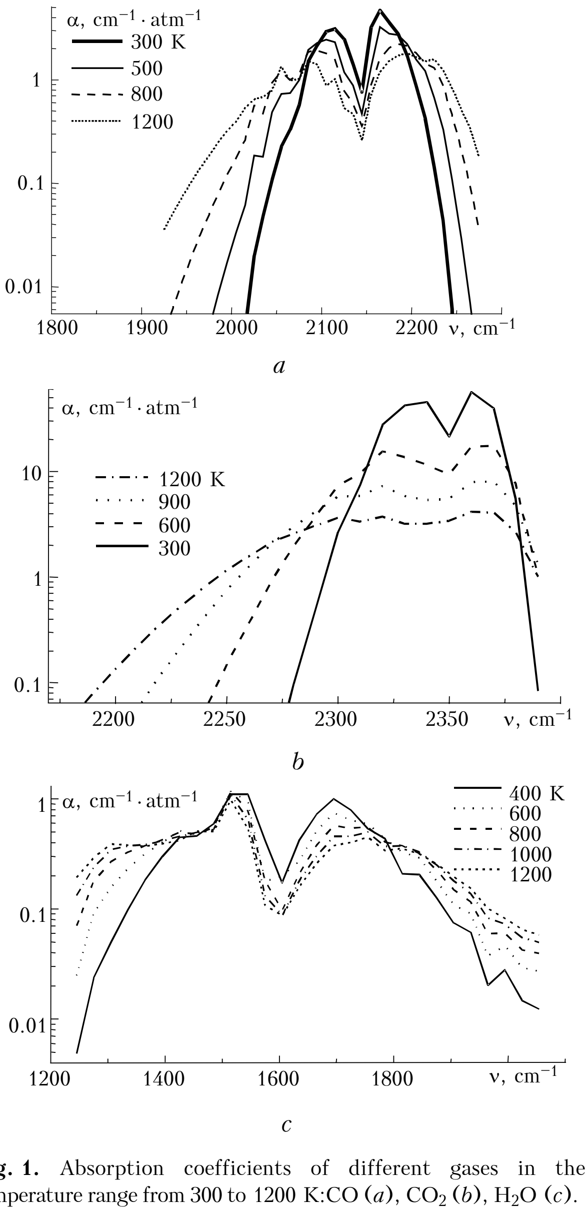

Fig. 1. Absorption coefficients of different gases in the temperature range from 300 to 1200 K:CO (*a*), CO_2 (*b*), H_2O (*c*).

Formal basis for determination of the total content of components of inhomogeneous gaseous media

The amount of optical radiation energy absorbed, as recorded with a receiving system, is significantly affected by the instrumental function determined by the source spectrum and the receiver's spectral sensitivity curve as a product of the corresponding instrumental functions.

Assume that we can select such an instrumental function $A(\nu, \nu')$ that, in some spectral region $[\nu_1, \nu_2]$, reduces the absorption coefficient in the entire temperature range occurring along the optical path approximately to a constant

$$\int A(\nu, \nu')\, \alpha(\nu')\, d\nu' \cong \alpha_0(\theta, l) = \text{const}, \quad (1)$$

where $\alpha(\nu')$ is the spectral absorption coefficient; θ is the kinetic temperature; l is the spatial coordinate along the optical path; ν is the central frequency of the instrumental function in the interval $[\nu_1, \nu_2]$ formed by the spectral points of intersection of the AC temperature dependences in the chosen temperature range. Since in reality the interval $[\nu_1, \nu_2]$ determined by accurate calculations of the transmission function is rather small, we can take $\nu = [\nu_1, \nu_2]/2$. The integration limits are determined by the width of the instrumental function $\Delta\nu$ defined as usually (full width at half maximum). The shape of the instrumental function and the width can vary corresponding to different types of receivers or optical filters used in the experiments.

Assume also that radiation extinction in the thermally inhomogeneous medium is caused by the presence of a gas studied and other gases and aerosols, and the absorption coefficient of the latter $\tilde{\alpha}(l)$ is known and nonselective within the instrumental function, as well as weakly depending on temperature. This assumption is justified for continuum absorption, aerosol extinction, and the sum of far wings of spectral lines of other gases. Then, when measuring the medium transmission with a spectrometer having the instrumental function $A(\nu, \nu')$, we obtain

$$T(\nu) = \int A(\nu, \nu') \times$$

$$\times \exp\left\{-\int_L [\tilde{\alpha}(l) + \alpha(\nu', l)\, n(l)]\, dl\right\} d\nu' \neq$$

$$\neq \exp(-\alpha_0 N)\, \tilde{T}, \quad (2)$$

where L is the optical path length; $\tilde{T}$ is the transmission of the medium in the absence of the absorbing gas; $N = \int_L n(l)\, dl$ is the total gas content along the path.

Consider the case that

$$\int_L \alpha(\nu, l)\, n(l)\, dl \ll 1 \quad (3)$$

for all ν belonging to the range of nonzero values of the instrumental function, that is, the optically thin layer of the gas studied. In this case, we can expand the exponent in Eq. (2) into a series and restrict our consideration to the first terms:

$$T(\nu) \cong \tilde{T}\left[1 - \int A(\nu, \nu') \int_L \alpha(\nu', l)\, n(l)\, dl\, d\nu'\right]. \quad (4)$$

Changing the integration order and taking into account Eq. (1), we have

$$T(\nu) \cong \tilde{T}\left[1 - \alpha_0 \int_L n(l)\, dl\right] =$$

$$= \tilde{T}\, [1 - \alpha_0 N] \approx \tilde{T} \exp(-\alpha_0 N). \quad (5)$$

Thus, with the optically thin layer and the information available on the radiation extinction by other factors, the selection of the instrumental function for the temperature range on the optical path allows us to estimate (with a certain error) the total content of the gas studied directly from the Bouguer law.

Let us discuss the effect of possible experimental errors on the estimated total content of the components of a thermally inhomogeneous gaseous medium at fulfillment of the conditions (1) and (3) and the relative measurement error $\Delta = \Delta T/T$. Since the total content of the gas sought can be found from the equation

$$N = \frac{1}{\alpha_0}\left(1 - \frac{T}{\tilde{T}}\right) \quad (6)$$

at $\alpha_0 N \ll 1$, the accuracy of the result depends on $\tilde{T}$ and can be determined as

$$\frac{\Delta N}{N} = \frac{T}{(\tilde{T} - T) - \Delta T}\Delta\, . \quad (7)$$

At unknown $\tilde{T}$, the error of an actual experiment can hardly be predicted. The smallest error in the measurement results can be obtained under conditions of maximum transparency caused by background factors.

Computer experiment on restoration of the total content of carbon monoxide in thermally inhomogeneous media

Below we present some results of numerical simulation on the determination of carbon monoxide (CO) concentration for the conditions typical of forest fires[6] (high temperature (300–1400 K) and concentration (0.05–50 atm · cm) gradients). In this situation, the total pressure keeps constant, because of the open space, in which burning occurs. Estimation of the role of pressure variations requires other prototype connected with the closed space for simulation and, consequently, additional investigations, which are beyond the scope of this paper.

Carbon monoxide was selected as a gas to be estimated due to the availability of the most accurately calculated parameters of rovibrational spectral lines (the error in calculation of line intensities is less than 3% in the entire temperature range) and a relatively small array of line parameters. Besides, carbon monoxide is one of the main products of underburning and it is available for actual experiments.

The schematic of the model experiment was rather simple: a source, a medium consisting of plane-parallel layers, and a receiver oriented normally to the layers. The parameters varied were the number of layers and the temperature and concentration distribution. Some examples of the media are tabulated below.

The spectral dependence of the CO absorption coefficients at different temperature shown in Fig. 2 demonstrates the presence of characteristic ranges near 2170 and 2210 cm^{-1} with the minimum temperature dependence of the absorption coefficient. It should be noted that this plot was drawn using a more accurate line-by-line method.[7]

For these conditions, we determined, by simple fitting, a suitable instrumental function centered at 2189 cm^{-1} with the dispersion profile and the halfwidth of 12 cm^{-1}, at which the CO absorption coefficient is almost temperature independent.

The integral concentration of CO along the optical path can be measured accurate to several percent if using a spectrometer with such an instrumental function. In actual measurements, the accuracy will be determined by the error in transparency measurements.

Results of computer experiment on restoration of the total CO content in thermally inhomogeneous media

Studied medium		Temperature, K	CO content, atm · cm (STP)	Medium transparency	Initial total CO content, atm · cm (STP)	Restored total CO content, atm · cm (STP)	Discrepancy, %
medium #	layer #						
1	1	400	0.5	0.433	2.5	2.605	4.2
	2	800	2				
2	1	600	0.1	0.792	0.3	0.307	2.33
	2	800	0.1				
	3	1200	0.1				
3	1	600	0.1	0.647	0.8	0.876	9.5
	2	1400	0.5				
	3	800	0.2				
4	1	400	0.1	0.106	11.1	11.71	5.5
	2	1000	1				
	3	600	10				
5	1	400	0.1	0.535	1.5	1.601	6.73
	2	600	0.2				
	3	800	0.3				
	4	1000	0.4				
	5	1200	0.5				
6	1	1400	0.2	0.576	1.2	1.306	8.83
	2	1200	0.2				
	3	1000	0.2				
	4	800	0.2				
	5	600	0.2				
	6	400	0.2				

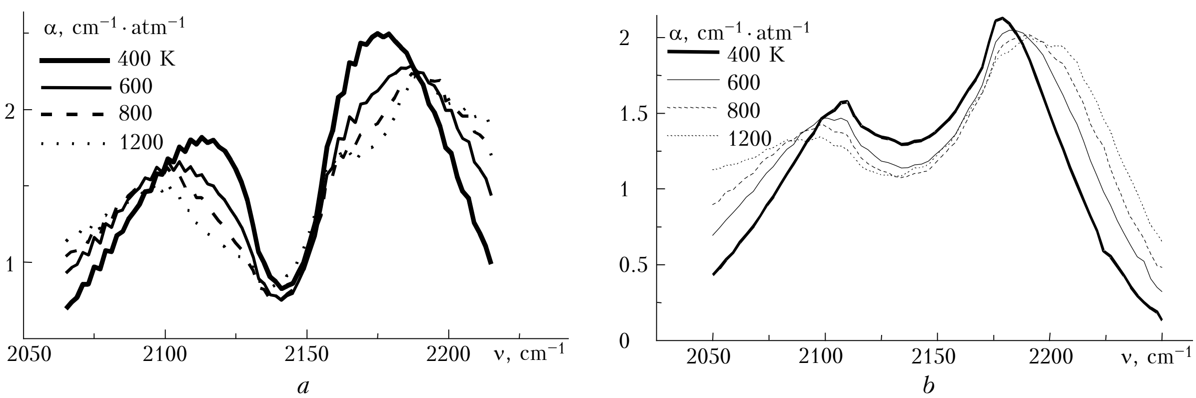

Fig. 2. Spectral dependence of the CO absorption coefficient at different temperature as calculated by the line-by-line method with the dispersion instrumental function and the halfwidth of 12 (*a*) and 30 cm^{-1} (*b*).

Unfortunately, the capabilities of optimizing the instrumental function are restricted by the available set of filters and sources. In this case, it is proposed to use, as a source, a thermal source with the characteristic close to the black body, that is, a Nernst pin or globar. In this case, the instrumental function is fully determined by the spectral characteristic of a filter. Reference 8 presents the data on 700 narrowband filters with centers in the range from 1.36 to 5.52 μm and FWHM of 0.05–0.1 μm corresponding to 25–50 cm^{-1} in the region under consideration, that is, much larger than the optimal one. Calculation with FWHM of 30 cm^{-1} showed that the narrowband filter centered at 2180–2184 cm^{-1} allows the CO concentration to be determined from the transmission measurements with the accuracy of 15–30%, which is good enough for the current level of investigations in this field.

It should be noted that the correct selection of the filter transmission maximum plays more significant role in determination of the total content than the selection of the profile.

Let us analyze the concentration dependence of $K_{eff} = \ln(T)/N$, which will be called the effective absorption coefficient of the medium, determining it from the total transmission function calculated with the selected dispersion instrumental function having the halfwidth of 12 cm^{-1}. The principal attention was paid to the search for the boundaries of the dynamic range of optical depths, in which the use of this instrumental function leads to minimization of the temperature dependence of the effective absorption coefficient.

The temperature dependence of the effective absorption coefficient shown in Fig. 3 suggests that measurement of the medium transmission with this instrumental function allows the total CO content to be determined accurate to 10% at the medium temperature varying from 400 to 1400 K and the total content of the absorbing gas along the optical path from 0.05 to 20 atm · cm (STP).

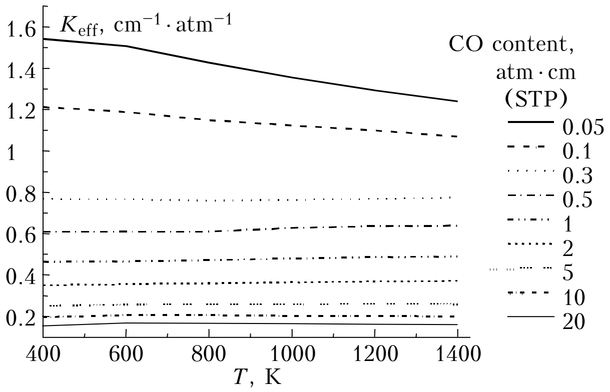

Fig. 3. Temperature dependence of the effective absorption coefficient calculated with the dispersion instrumental function with the halfwidth of 12 cm^{-1} at different total CO content.

The dependence of the log transparency (Fig. 4) on the total content is a nomogram for determination of the latter from measurements of the transmission of gaseous medium under study for radiation with this instrumental function. To plot this dependence, we used the temperature-averaged values of the effective absorption coefficient.

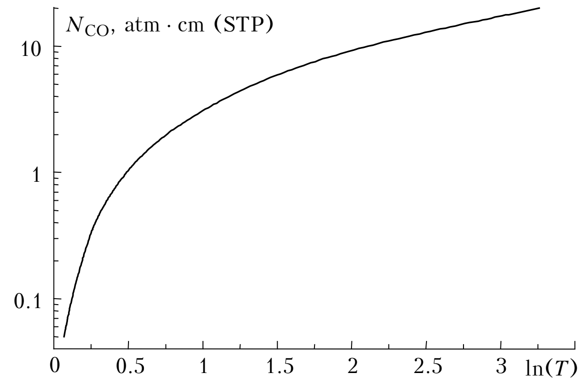

Fig. 4. Log transparency measured by a spectrometer with the dispersion instrumental function with the halfwidth of 12 cm^{-1} as a function on the total CO content.

To test the proposed method for estimation of the total gas content in thermally inhomogeneous media, we have conducted a computer experiment with the single-component (carbon monoxide) gaseous medium. The transmission of the stratified inhomogeneous medium was calculated by the line-by-line method, and the calculated values of the transmission function were used as the initial data for determination of the total CO content along the optical path (Fig. 4). The simulated and reconstructed results are given in the Table. As expected, the growth of the temperature gradient and the increase of the gas content lead to the increase of the error in determination of the total content of the gas under study, but suggest the conclusion about the possibility of applying this approach to analysis of the total gas content in a significantly inhomogeneous, thermodynamically, medium.

At the same time, calculations show that the condition (3) is not rigorous, and its fulfillment only minimizes the error in determination for the concentration. Thus, for example, the error is less than 3% for the second version of the medium.

Conclusion

This paper is devoted to the search for approaches to solution of inverse problems in optics of inhomogeneous gas media with high temperature and component concentration gradients in order to find the spatial distribution of gas concentrations. In spite of difficulties, this subject attracts attention of investigators in recent time, because the level achieved in processing of remote measurements of optical characteristics of fires, volcanic eruptions, and emissions of industrial plants requires improvement of the accuracy in determination of the medium characteristics and development of the corresponding mathematical apparatus.

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