Methodical principles of processing the data of laser open-path gas analysis

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Principal methodical problems associated with reconstruction of gas composition of the atmosphere from the data of laser open-path gas analysis by the differential absorption lidar (DIAL) method are considered. Main factors affecting the accuracy of the gas concentration reconstruction, such as inadequate knowledge of absorption coefficients, aerosol extinction coefficients, continuum absorption models, etc., are determined. The problems of selection of optimal spectral sensing channels and detection of gases are examined as well. The methods of taking into account the finite width of a laser radiation line and its effect on the accuracy of reconstruction of gas concentration are demonstrated. Specialized software for solution of these problems is described.

Introduction

To monitor the gas composition of the atmosphere with optical absorption gas analyzers, it is necessary to have the devices highly sensitive to absorption and capable of measuring gas concentrations in multicomponent gas mixtures in a wide dynamic range. One of such devices is an open-path gas analyzer with various laser sources (CO_2 and CO lasers, parametric light oscillators, etc.). To analyze the content of gases under study, these devices use radiation passing along atmospheric paths from a laser source to a reflector (mirror or topographic target) and backward. In the general case, the problem of gas concentration determination from measured signals is reduced to solution of a system of linear algebraic equations. The accuracy of solution depends both on accidental experimental errors and numerous systematic factors (aerosol, gas absorption, etc.). In this paper, we consider main stages in processing the data obtained with a laser open-path gas analyzer.

1. Differential absorption lidar (DIAL) method

The essence of the DIAL method[1–8] consists in emitting laser radiation at two wavelengths, one falling on the absorption line of a gas under study (λ_{on}) and another lying off it (λ_{off}), where the gas absorptance is low (Fig. 1). The measured signals for the selected wavelengths are described by the equation

$$I(\lambda_i) = I_0(\lambda_i)\, S_{app}(\lambda_i)\, \eta(\lambda_i) \times$$
$$\times \exp\{-\, 2LK_0(\lambda_i)\, x_0 - 2L\alpha_\Sigma(\lambda_i)\}, \qquad (1)$$
$$i = \text{on, off},$$

where L is the length of the sensing path from the source to the reflector; S_{app} is the apparatus constant; I_0 is laser radiation at a selected laser transition; K_0 and x_0 are the absorption coefficient and the concentration of the gas under study; $\alpha_\Sigma(\lambda)$ is the total extinction by interfering factors:

$$\alpha_\Sigma(\lambda) = \alpha_a(\lambda) + \alpha_c(\lambda) + \alpha_g(\lambda). \qquad (2)$$

In Eq. (2), $\alpha_a(\lambda)$ is the extinction due to aerosol; $\alpha_c(\lambda)$ is the extinction due to the water vapor continuum absorption; $\alpha_g(\lambda) = \sum\limits_{j=1}^{N_g} K_j(\lambda)x_j$ is the absorption by interfering gases, and N_g is the number of interfering gases; $\alpha_0(\lambda_i) = K_0(\lambda)x_0$ is the volume coefficient of absorption by the gas under study; $S_{app} = q$ when using a mirror reflector and $S_{app} = \rho/\pi$ when using a topographic target (building, tree, etc.) as a reflector; q is the coefficient of efficiency of the receiving antenna; ρ is the reflection coefficient.

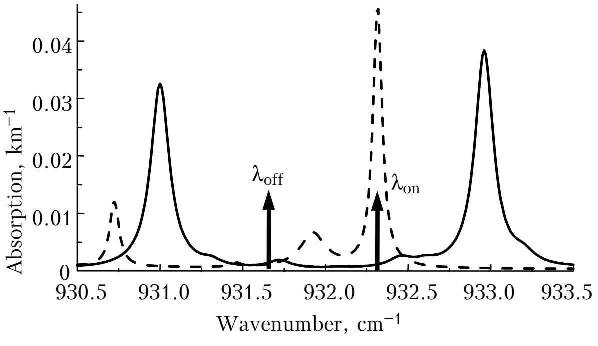

Fig. 1. Selection of sensing wavelengths λ_{on} and λ_{off} of the gas under study (absorption spectrum is shown by a dashed line) against the background of interfering absorption (solid line) in DIAL method.

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The calibration constant $\eta(\lambda)$ is determined by transmission of the transmitting q_t and receiving q_r optics, as well as the receiver's sensitivity χ:

$$\eta(\lambda) = q_t(\lambda)\, q_r(\lambda)\, \chi\, (1 - q_l),$$

where q_l are other losses in the transmitting-receiving system.

In the DIAL method, the path-average concentration of the sought gas is determined by the equation

$$x = \frac{1}{2\Delta K L} \ln \left[C \frac{I(\lambda_{\text{off}})\, I_0(\lambda_{\text{on}})}{I(\lambda_{\text{on}})\, I_0(\lambda_{\text{off}})} \right] - \frac{\Delta\alpha_\Sigma}{2\Delta K}, \quad (3)$$

where $\Delta\alpha_\Sigma = \alpha_\Sigma^{\text{on}} - \alpha_\Sigma^{\text{off}}$; $\Delta K = K_0^{\text{on}} - K_0^{\text{off}}$.

The error in determination of the gas concentration can be estimated as[2]:

$$\sigma_x = \frac{1}{2L\Delta K} \left\{ \sum_{i=1}^{2} \left[\left(\frac{\sigma_i}{I_i} \right)^2 + \left(\frac{\sigma_{0i}}{I_{0i}} \right)^2 \right] + \left(\frac{\sigma_C}{C} \right)^2 \right\}^{1/2}; \quad i = \{1 - \text{on},\ 2 - \text{off}\}, \quad (4)$$

where σ_i, σ_{0i}, and σ_C are errors in the signals measured at the wavelengths λ_{on} and λ_{off} and the error of determination of the calibration constant $C = \eta(\lambda_{\text{off}})\, S_{\text{app}}(\lambda_{\text{off}}) / [\eta(\lambda_{\text{on}})\, S_{\text{app}}(\lambda_{\text{on}})]$.

2. Multiwave open-path method

In the multiwave open-path DIAL method, the measured signals are connected with the concentration of the sought gases x_j by the equation

$$\tilde{y}_i = f[I(\lambda_i)] = \sum_{j=1}^{N_g} K_{ij}\, x_j,\ i = 1, \ldots, N_\lambda, \quad (5)$$

where $\tilde{y}_i = \tilde{y}(\lambda_i)$ is the volume extinction coefficient obtained from the measured signals ($\tilde{y}_i = y_i + \varepsilon_i$, ε is the measurement error); $f(*)$ is some function of measured signals:

$$f_i = \frac{1}{2L} \left\{ \ln \left[C_i \frac{I(\lambda_i)}{I_0(\lambda_i)} \right] \right\} - z_i; \quad (6)$$

$K_{ij} = K_j(\lambda_i)$ is the absorption coefficient of the jth gas at the ith wavelength; N_g and N_λ are the number of gases in a mixture and the number of sensing wavelengths; z_i is a nonselective component of absorption caused by the aerosol extinction, water vapor continuum absorption, and absorption by interfering gases.

After the system of equations (5) is solved at $N_g = N_\lambda = N$, the concentrations of the sought gases are determined as

$$\mathbf{x} = \mathbf{K}^{-1}\, \tilde{\mathbf{y}}, \quad (7)$$

where $\mathbf{x} = \{x_1, x_2, \ldots, x_{N_g}\}$ is the vector of the sought gases concentrations; $\mathbf{K}$ is the matrix of absorption coefficients of gases; the value of $\tilde{\mathbf{y}}$ is determined by Eq. (5).

The error in determination of the gas concentrations by Eq. (7) can be estimated as[9]:

$$\sigma_{x_j}^2 = \sum_{i=1}^{N_\lambda} K_{ij}^{-2}\, \sigma_y^2(\lambda_i),$$

$$\sigma_y^2(\lambda_i) = \frac{1}{NL} \sqrt{ \left(\frac{\sigma_{0i}}{I_{0i}} \right)^2 (1 + e^{2\bar{\alpha}(\lambda_i)}) + \left(\frac{\sigma_{C_i}}{C_i} \right)^2 },$$

where $\sigma_y(\lambda_i)$ is the error in $\tilde{\mathbf{y}}$ at the wavelength λ_i; $\bar{\alpha}$ is the measured extinction coefficient averaged over N realizations.

When the number of the used sensing wavelengths is larger than the number of gases to be determined $N_g < N_\lambda$, the gas concentrations are found by the least square method (LSM) using one of the formulae:

$$\mathbf{x} = (\mathbf{K}^{\mathrm{T}}\, \mathbf{K})^{-1}\, \mathbf{K}^{\mathrm{T}}\, \tilde{\mathbf{y}} \text{ or } \mathbf{x} = (\mathbf{K}^{\mathrm{T}}\, \mathbf{W}\mathbf{K})^{-1}\, \mathbf{K}^{\mathrm{T}}\, \mathbf{W}\, \tilde{\mathbf{y}}. \quad (8)$$

Here $\mathbf{W}$ are weighting coefficients ($\mathbf{W} = 1/\sigma_y^2$); T denotes a transposition. The errors of gas concentration reconstruction are determined by the equations:

$$\sigma_x^2 = [(\mathbf{K}^{\mathrm{T}}\, \mathbf{K})^{-1}]_{ii}\, \sigma_y^{-2}, \text{ or } \sigma_x^2 = [(\mathbf{K}^{\mathrm{T}}\, \mathbf{W}\mathbf{K})^{-1}]_{ii}\, \sigma_y^{-2},$$

$$\sigma_y^2 = \frac{1}{N_\lambda} \sum_{j=1}^{N_\lambda} \sigma_{yj}^2.$$

The systems of equations (7) and (8) are ill-posed. A difficulty in solution of ill-posed problems is that minor measurement errors can lead to large errors in solution. One of the methods to solve such problems is known as the Tikhonov method.[10] In this case, the solution for the vector of sought gas concentrations is written in the form

$$\mathbf{x} = (\mathbf{K}^{\mathrm{T}}\, \mathbf{K} + \gamma \mathbf{E})^{-1}\, \mathbf{K}^{\mathrm{T}}\, \tilde{\mathbf{y}} \text{ or}$$

$$\mathbf{x} = (\mathbf{K}^{\mathrm{T}}\, \mathbf{W}\mathbf{K} + \gamma \mathbf{G})^{-1}\, \mathbf{K}^{\mathrm{T}}\, \mathbf{W}\tilde{\mathbf{y}}, \quad (9)$$

where γ is the regularization parameter; $\mathbf{E}$ is the unit matrix; $\mathbf{G}$ is the matrix-stabilizer.

However, in the case of strong distortion of measurement data by noise or weak absorptance of a gas under study, neither LSM (8) nor the Tikhonov method (9) guarantee some acceptable solution corresponding to physical concepts (solution must be positive). In this case, methods of linear programming

$$C\mathbf{x} \to \min;\ \mathbf{K}\mathbf{x} = \tilde{\mathbf{y}};\ x > 0;\ C = \sum_i K_i$$

or nonlinear programming

$$\{\mathbf{x}^{\mathrm{T}}\, \mathbf{K}^{\mathrm{T}}\, \mathbf{W}\mathbf{K}\mathbf{x} - 2\mathbf{x}^{\mathrm{T}}\, \mathbf{K}^{\mathrm{T}}\, \mathbf{W}\mathbf{y}\} \to \min$$

at the restrictions $x_1 \le x \le x_2$; $x \ge 0$ are used. These methods allow the solution to be obtained in the presence of physically determined restrictions (known range of variability of the gas concentration under study).

Figure 2 shows the results of modeling an inverse problem on reconstruction of the gas concentrations in the region 9–11 μm from the sensing data on six gases (H_2O, CO_2, O_3, NH_3, C_2H_4, C_6H_6) by the multiwave open-path method with a CO_2 laser. The figure demonstrates the total errors for the gas concentrations δx reconstruction by the methods listed above: least squares method (LSM), method of linear programming (MLP), method of nonlinear programming (MNP), and Tikhonov regularization method (TRM). The errors are shown as functions of the measurement error δy. One can see that the error provided by the LSM depends strongly on the measurement error. The reconstruction error is the smallest for the MNP and TRM. In our opinion, the MNP is the most convenient for practical application, because it compares well with the TRM in the accuracy of reconstruction up to the measurement error of 15%, and there is no need to calculate the regularization parameter (it is important for automation of measurements allowing an unattended processing of the data). However, at measurement errors higher than 15%, the TRM is preferable.

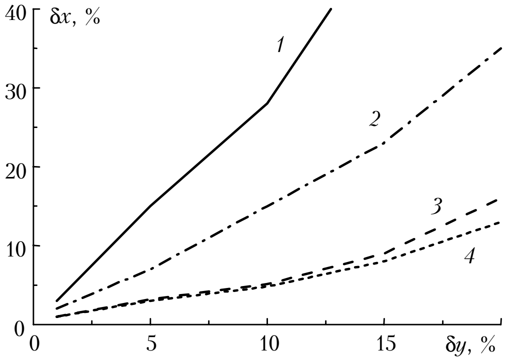

Fig. 2. Comparison of the errors summed up for all measured gases provided by different methods of solution of the inverse problem: LSM (*1*), MLP (*2*), MNP (*3*), and TRM (*4*).

3. Accuracy of solution of the inverse problem

A search for optimal spectral channels is an important stage prior to measurements. Thus, for example, if the sensing wavelengths λ_{on} and λ_{off} are very close, interfering factors are minimum, but the value of ΔK may be very small, thus leading to low concentration sensitivity. On the other hand, increase of separation between λ_{on} and λ_{off} leads to increase of the sensitivity, but $\Delta\alpha_\Sigma$ increases too, thus decreasing the efficiency.

At the stage of signal pre-processing, measurement errors are determined by some chosen method of rejection, accumulation, and calibration. Measurement errors are random. Systematic errors depend on inexact knowledge of the mixture composition, spectral behavior of the aerosol extinction coefficient, the atmospheric temperature, etc.[11–14] The effect of the temperature factor can be diminished by measuring the temperature during experiments. The atmospheric composition at the time of measurement can be found from independent measurements or by numerical simulation.

The accuracy of solution of the inverse problem depends also on the error in setting the absorption coefficients of the gas under study and interfering gases. Table 1 gives the absorption coefficients calculated based on the HITRAN–92 atlas and the measured coefficients available in the literature. It is seen that the calculated and measured coefficients differ significantly in most cases. As a result, the gas concentration depends on which value of the absorption coefficient is taken. The relative error in the gas concentration reconstruction due to the error in the system matrix and the measurement error can be found from the following equation[15]:

$$\delta_x \le \frac{\text{cond}(K)}{1 - \delta_K} \{\delta_K + \delta_y\},\ \delta_K < 1,$$

where cond(K) is the conditionality number of the system matrix; δ_K and δ_y are the relative error of the system matrix and the relative measurement error. The less pronounced is the selective structure of reference absorption spectra and the larger is the number of gases in a mixture, the larger is the conditionality number.

We can conclude herefrom that the problem of choice of absorption coefficients should be solved properly in advance of the experiment.

Consider now what errors in solution of the inverse problem can be caused by improper knowledge of the continuum absorption model. Table 2 gives the calculated coefficients of water vapor continuum absorption as functions of water vapor content for different models.[19] It is seen from Table 2 that the values of continuum absorption differ widely. Naturally, this can lead to errors in solution of both qualitative and quantitative problems.

Table 1. Comparison of calculated and measured absorption coefficients, in $\text{cm}^{-1} \cdot \text{atm}^{-1}$

Transition	CO_2 laser frequency, cm^{-1}	H_2O		CO_2		O_3	
		Calc.	Ref. 16	Calc.	Ref. 17	Calc.	Ref. 18
9*P*24	1043.163	0.124e-5	0.820e-4	0.311e-2	0.270e-2	0.621e-0	0.830e-0
9*P*14	1052.196	0.149e-5	0.930e-4	0.332e-2	0.320e-2	0.119e+2	0.124e+2
9*R*30	1084.635	0.301e-3	0.130e-3	0.235e-2	0.170e-2	0.832e-1	0.173e-0
10*P*20	944.194	0.189e-5	0.910e-4	0.251e-2	0.220e-2	0.765e-3	0.270e-3
10*P*14	949.479	0.134e-5	0.850e-4	0.235e-2	0.180e-2	0.173e-2	0.290e-2
10*R*20	975.930	0.742e-3	0.800e-3	0.270e-2	0.210e-2	0.106e-0	0.148e-0

Table 2. Coefficients of water vapor continuum absorption, in km^{-1} (λ = 10.591 μm, T = 293 K, P = 1 atm)

ρ_{H_2O}, g/m^3	Ref. 20	Ref. 21	Ref. 22	Ref. 23
1	5.05e-3	4.20e-3	3.91e-3	1.70e-3
5	4.65e-2	3.99e-2	3.48e-2	2.71e-2
10	1.46e-1	1.27e-1	1.07e-1	9.80e-1
15	2.99e-1	2.62e-1	2.18e-1	2.19e-1

Thus, the data presented in Ref. 24 demonstrate the effect of the continuum absorption on the results of solution of the inverse problem of reconstructing concentrations of some gases in atmospheric air. It is shown that the reconstructed values of gas concentrations differ significantly depending on the used model of continuum absorption (for example, 60 to 120 ppm for CO_2).

The aerosol extinction should be also taken into account when processing measurements, because the value and spectral behavior of the aerosol extinction may be additional sources of errors. The use of model representations on the aerosol extinction spectral behavior often can decrease the effect of this factor, but not always. Measurements, conducted in different regions and under various weather conditions may strongly differ from model values of the aerosol extinction. In this case, we can apply the technique of simultaneous reconstruction of both gas concentrations and continuum extinction coefficients.[15] We assume that continuum absorption by each gas is not changed within the spectral region between on- and off-lines. Then the system matrix (5) can be presented as

$$\breve{K} = \left|\begin{array}{cc} & 1\;0\;0\;0\;0 \\ & 1\;0\;0\;0\;0 \\ K & .\;.\;.\;.\;. \\ & 0\;0\;0\;0\;1 \\ & 0\;0\;0\;0\;1 \end{array}\right|.$$

It is necessary in this case to use $N_\lambda + N_\lambda/2$ sensing wavelengths.

4. Detection problem

In some problems of gas analysis, there is no need to measure directly the gas concentration, it is sufficient to detect only the presence of a gas in a mixture. To do this, let us use the algorithm described in Refs. 25 and 26. Consider some gas mixture, in which only one gas is under study, and all other gases are thought interfering. Rewrite Eq. (1) in the form[26]:

$$y = y_0\, C \exp\{-\,2L\Delta Kx\} \exp\{-\,2L\Delta\alpha_\Sigma\}, \qquad (10)$$

where $y = I_{\rm on}$ and $y_0 = I_{\rm off}$.

The problem of some gas detection is reduced to testing the statistical hypothesis H_1: from the measured parameters y, y_0, and C, the decision is made that x belongs to a class of states X_1 ($x \in X_1$) against the alternative $x \in X_2$ (hypothesis H_2).

Let the classes of states X_1 and X_2 be specified by conditional probability densities $f(y|H_i) \equiv f(y|x \in X_i)$, and the parameters y_0, C, and $\Delta\alpha_\Sigma$ be described by densities $f_1(y_0)$, $f_2(C)$, and $f_3(\Delta\alpha_\Sigma)$. To test the hypotheses H_1 and H_2, let us use the Neumann–Pearson criterion. The decision rule has the form[27]:

$$h(y) = \frac{1}{2\sigma_1^2}(y - M_1)^2 - \frac{1}{2\sigma_2^2}(y - M_2)^2 - \ln\frac{\sigma_2}{\sigma_1};$$

$$M_1 = M_0\, C\, {\rm e}^{-2L\Delta\alpha_\Sigma};\ \sigma_1^2 = \sigma_y^2 + \sigma_{y_0}^2\, C^2\, {\rm e}^{-4L\Delta\alpha_\Sigma},$$

$$M_2 = M_0\, C\, {\rm e}^{-2L\Delta\alpha_\Sigma}\, {\rm e}^{-2L\Delta Kx};$$

$$\sigma_2^2 = \sigma_y^2 + \sigma_{y_0}^2\, C^2\, {\rm e}^{-4L\Delta\alpha_\Sigma}\, {\rm e}^{-2L\Delta Kx}.$$

For the detection limit we have

$$\Lambda = -\,d - \{|\tilde{M}_1| - \sqrt{2}\,\tilde{\sigma}_1^2\,\Phi^{-1}\,(1 - 2\varepsilon_0)\}^2.$$

The correct detection probability is calculated by the equation

$$P = \frac{1}{2}\,[1 + \Phi(g_2)];$$

$$g_2 = -\,\frac{1}{\tilde{\sigma}_2\sqrt{2}}\,\big[\,|\tilde{M}_2| - |\tilde{M}_1| + \sqrt{2}\,\tilde{\sigma}_1\,\Phi^{-1}\,(1 - 2\varepsilon_0)\big],$$

where $\Phi(g)$ is the error function; $\Phi^{-1}(*)$ is the inverse error function; the values of other parameters are determined by the following equations:

$$\tilde{M}_1 = \frac{1}{\sqrt{2}}\,\frac{M_2 - M_1}{\sqrt{|\sigma_2^2 - \sigma_1^2|}}\,\frac{\sigma_1}{\sigma_2},\ \tilde{M}_2 = \frac{1}{\sqrt{2}}\,\frac{M_2 - M_1}{\sqrt{|\sigma_2^2 - \sigma_1^2|}}\,\frac{\sigma_2}{\sigma_1},$$

$$\tilde{\sigma}_1^2 = \frac{|\sigma_2^2 - \sigma_1^2|}{2\sigma_2^2},\ \tilde{\sigma}_2^2 = \frac{|\sigma_2^2 - \sigma_1^2|}{2\sigma_1^2}.$$

The above algorithm allows the gases whose concentrations exceed a preset value to be detected automatically.

5. Sensing by radiation of finite spectral width

Consider an open-path gas analyzer, using the DIAL method, for the case of laser radiation of a finite spectral width $\Delta\lambda$ (for the parametric light oscillator $\Delta\lambda \approx 0.1$–$0.3$ cm^{-1} (Refs. 28 and 29)). The character of the inverse problem solution is determined by the nonlinear dependence of the measured parameter and the gas concentration under analysis. This is due to the fact that absorption spectra of atmospheric gases have a selective structure and therefore are distorted in the receiving system providing the linewidth $\Delta\lambda$ of the used laser source is comparable with the absorption linewidth under near-surface conditions. In this case, the measured signals are connected with the gas concentration under study averaged over the path through the equation

$$y(\lambda) = y(\lambda_0)\, S_{\text{app}}(\lambda)\, \eta(\lambda)\, \mathrm{e}^{-2L\Delta\alpha_{\text{a.c}}(\lambda)} \times$$
$$\times \int\limits_{\Delta\lambda} g(\lambda - \lambda')\, \mathrm{e}^{-2L\sum\limits_{j=1}^{N_g} K_j(\lambda) x_j}\, \mathrm{d}\lambda, \qquad (11)$$

where $\alpha_{\text{a.c}}$ is the coefficient of extinction due to aerosol and continuum absorption; $g(*)$ is the normalized profile of the laser band.

For the finite laser radiation linewidth, the coefficient of volume absorption by gases is determined not by Eq. (5), but by a nonlinear equation of the following form[30]:

$$\alpha_i^{\text{ef}} = -\frac{1}{2L} \ln \left\{ \int\limits_{\Delta\lambda} g(\lambda - \lambda') \exp\left[-2L \sum_{j=1}^{N_g} K_j(\lambda')\, x_j \right] \mathrm{d}\lambda' \right\},$$
$$i = \text{on, off.}$$

The effect of the finite laser radiation linewidth manifests itself in a decrease of the reconstructed concentration of the gas under analysis. It should be noted that the effect of the apparatus function is minimal when studying substances with smooth spectra (hydrocarbons). For atmospheric gases, this effect can be taken into account in the following ways.

First, by minimizing the functional:

$$\Phi(x) = \sum_{i=1}^{N} [\tilde{y}_i - y(\lambda_i, x_1, \ldots, x_{N_g}, g, \Delta\lambda)]^2 \to \min_x. \qquad (12)$$

Functional (12) can be minimized by different methods (Newton, Levenberg–Marquardt, etc.).

Another way is to use the method proposed in Ref. 31, which consists in application of the deconvolution methods to the recorded spectra. Many deconvolution methods are now available. The classic method is based on the ideas of the Tikhonov regularization method.[32] The method of maximum likelihood is most widely used in practice.[33]

Deconvolution by the method of maximum likelihood is made with the use of the following iteration equation[31]:

$$y_k^{l+1} = y_k^l + \gamma\, y_k^l \sum_{i=1}^{N} G_{ik} \left(\frac{\tilde{y}_i}{\sum\limits_{j=1}^{M} G_{ij}\, y_j^l} - 1 \right)^{\tau},$$

where G is the algebraized analog of the apparatus function (laser radiation line); γ and τ are the parameters determining convergence of the iteration process; l is the number of an iteration step.

Table 3 gives the results of solution of the inverse problem on methane concentration reconstruction in the region of 3.3 μm with a parametric- light oscillator-based gas analyzer for the case of a signal distortion by the apparatus function (widths of 0.1 and 0.3 cm^{-1}) and after application of the method of maximum likelihood. It is seen that application of deconvolution reduces the error of concentration reconstruction, but not to zero.

Table 3. Comparison of methods for solution of inverse problem

x_{CH_4}, ppm	x_{CH_4} after convolution	δ_x, %	x_{CH_4} after deconvolution	δ_x, %	$\Delta\nu$, cm^{-1}
1.7	1.598	5.8	1.636	3.5	0.1
1.7	1.521	10.5	1.582	7.1	0.3

In any case, the laser line profile and its variation in the spectral region under study must be known for proper account for the effect of the apparatus function.

6. Software for the experiment

Software now becomes one of the important components of any experiment, and its quality often determines the quality of the obtained experimental results. This is connected with the fact that amounts of experimental and archive information have extended significantly, and the problems to be solved, physical models, and processing methods have become much more complicated. The problem of selection of informative wavelengths is rather important in gas analysis.

As an example, we can mention two software packages LPM and TRAG, which allow simulation and processing of measurements made by open-path gas analyzers of various types. The LPM dialog software[34] serves for simulation of laser sensing of gases (H_2O, CO_2, O_3, NH_3, C_2H_4) by the open-path method with a gas analyzer based on two tunable CO_2 lasers. In the simulation mode, the LPM determines optimal pairs of wavelengths and the error of reconstruction of gas concentrations caused by the measurement and systematic errors (the latter is due to the errors in spectroscopic data, the effect of interfering gases, etc.).

Optimal experimental conditions can be chosen using our algorithms and programs based on application of the theory of testing statistical hypotheses. The Bayes criterion of detection is put in the foundation.

The TRAG software[30] serves the same functions as the LPM but for the open-path gas analyzer based on a parametric light oscillator. The TRAG allows one to find optimal sensing wavelengths, make deconvolution of the measured spectrum, and then solve the inverse problem.

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