**Numerical Study of Solving the Problem of Identifying the Gas Composition of the Atmosphere**

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**Abstract.** This article proposes a local regularizing algorithm that replaces a single regularization parameter with a set of parameters, enabling a solution with reduced error. A method is presented for constructing stable solutions of linear algebraic equations by incorporating qualitative or quantitative a priori information about the desired solution. The study shows that even trivial a priori information can significantly lower the error of the regularized solution. By leveraging prior knowledge and distributing regularization across multiple parameters, the approach improves solution accuracy and stability, offering an effective framework for addressing ill-posed problems in various applications.

**Keywords**: algorithm, noise signal, singular, equations, operator, identity matrix, covariance, decomposition matrix.

**INTRODUCTION**

Every year, human industrial activity increasingly aggravates the problem of environmental protection. Among the diverse human impacts on nature, air pollution occupies a special place. Every year, up to 500 thousand various pollutants are emitted into the atmosphere [1].

In this regard, the task of monitoring the composition of the atmosphere is very relevant [2]. When developing means of monitoring the state of the environment, special attention is paid to methods that could provide prompt quantitative and qualitative information about the sources of air pollution and identify the dynamics of the spread of polluting components [3,4,5] These requirements are best met by methods of remote laser analysis of the atmosphere based on the phenomena of absorption, fluorescence or Raman scattering of radiation by gas molecules [8]. The most sensitive laser method, absorption, is based on the principle of resonant absorption, which occurs when laser radiation has the same wavelength as the main transition in absorption for the molecules to be detected [6;7]. This method served as the basis for the creation of devices for monitoring the state of air using the absorption method on long (up to several kilometers) routes [9,10].

Practical implementation of parametrically adaptive estimation algorithms in the present case meets considerable difficulties of a computational nature, connected with the fact that in their formation it is necessary to consider problems, solutions of which are unstable to small changes of initial data. They are characterized by the fact that any small changes in the source data can lead to arbitrarily large changes in solutions. In this regard, it is advantageous to use regularization techniques to increase the accuracy of estimating the state of dynamic systems under conditions of correlation of input noise of an object [11-14].

**METHODS**

The volumetric attenuation coefficient of a medium for radiation with a wavelength is understood as the proportionality coefficient in Bouguer’s law, which characterizes the properties of a medium to transmit radiation. In the case of a homogeneous medium, Bouguer's law transforms into an expression of the exponential decay law.

 (1)

where and *(W/cm2)* are the radiation intensity, respectively, at the beginning and at the end of an atmospheric channel of length ; the exponent is called the optical thickness of the layer [10].

On the other hand, the measured volumetric attenuation coefficient of the medium for an isolated absorption line is related to the concentration of the target gas by the relation [10]:

(2)

where is the concentration of the desired gas, averaged along the propagation path of the laser beam,  is the mass absorption coefficient of the desired gas at wavelength .

If at a given wavelength the study is absorbed by several gases, then expression (2) will take the form:

(3)

where is the number of gases that absorb radiation at wavelength .

With the creation of tunable lasers, it has become possible to scan the spectral absorption lines of molecules, which makes it possible to select wavelengths where the probability of their overlap is minimal. In our case, we use a molecular gas is the laser with a fixed wavelength and the possibility of its discrete tuning. Then, if the measurements were carried out at lengths, equation (3) can be rewritten as a system of linear algebraic equations

(4)

in which is a matrix of the size of the mass absorption coefficients of the desired gases at measurement wavelengths, - a dimensional vector of concentrations; -dimensional vector of the volumetric absorption coefficient of the medium with projections [10]. Based on the measurement results, taking into account (1), these projections can be calculated as follows:

(5)

It is assumed that the vector of the right side of system (4) contains a vector of measurement noise with zero mean and a covariance matrix , which has a diagonal structure . To estimate the dispersion of the -measurement, the following formula was proposed in [12], [10]:

(6)

where is the number of measurements at a wavelength ; - average value calculated from sales ; -relative error of the optics-electronic path; - relative error in measuring the radiation intensity at the entrance to the atmosphere; - length of the route. The values of and do not exceed 1% for the equipment used by the authors of [10].

In the general case, in the presence of aerosols and vapors , equation (4) takes the form:

(7)

Where  is the continuous attenuation coefficient due to the presence of aerosol particles in the air. The value  varies slightly depending on the wavelength.

Systems (4) and (7) are ill-conditioned, which causes instability of their solutions with respect to errors  on the right side and therefore the use of regularizing algorithms is necessary.

An additional circumstance that complicates the solution of these systems is the large scatter in the concentrations of the gases under study. Thus, according to data from [3], the concentration in mid-latitudes in winter is and - in summer. At the same time, the concentrations of ethylene and ammonia under normal conditions do not exceed hundredths . Thus, the spread of the concentration vector projection values can be 7 or more orders of magnitude [10].

**RESULTS AND DISCUSSION**

The initial information for a number of numerical experiments was the vector of reference concentrations () for four gases and the matrix (atm-1cm-1) of mass absorption coefficients of the desired gases with sizes borrowed from the literature [9], [10]. As a result of the singular decomposition of the matrix, the maximum and minimum singular numbers and were obtained. Thus, the condition number is [13].

Using a given matrix of mass absorption coefficients and the “exact” concentration vector, the exact vector of the right-hand side was calculated , which was then distorted by a random error vector (interpreted as measurement noise), distributed according to the normal law with zero mathematical expectation and a covariance matrix

(8)

in which the variances were determined by the following expression:

 (9)

where is the relative noise level specified from the interval

In what follows, the following matrix representation is used :

(10)

where , .

At the first stage of numerical research, a global regularized solution was taken as a stable solution of the SLAE (4) , defined by the relation:

(11)

where are the first columns of the matrices included in the singular decomposition   
; - matrix rank equal to 4; - “noisy” (with a given relative noise level ) vector of the volumetric absorption coefficient of the medium. The choice of the regularization parameter was carried out according to the optimality criterion [10,11].

Then a local regularizing algorithm was applied to the same initial data with iterative refinement of the noise/signal ratio; the regularized solution can be represented as [9]:

(12)

The values are estimates for the “exact” noise/signal ratios and are given by the following expression:

(13)

where , are the projections of , are the projections of the vector . The calculated vector of the global regularized solution was taken as the “starting” solution , i.e. Let us recall are the roots of the quadratic equation

(14)

it is assumed that .

The relative root-mean-square errors of the constructed regularized solutions were calculated using the formulas

(15)

The mathematical expectation operator was replaced by averaging over 30 implementations of the corresponding regularized solutions constructed using vectors .

For a global regularized solution at a noise level, the standard deviation was , for a local one - . In shows the exact and reconstructed concentrations for four gases\*, as well as the relative reconstruction errors [13].

During the described computational experiment, for some implementations, global and local regularization algorithms calculated regularized solutions, some projections of which took unphysical negative values [10]. To eliminate this drawback, a local descriptive regularizing algorithm was applied. A priori information about the non-negativity of the projections of the concentration vector was specified by a system of restrictions of the form:

(16)

where is an identity matrix of size , is a zero vector containing zero projections.

The results of this experiment for the noise level are given in table 2. The data presented in the table proves that there are no negative components in the descriptive local solution vector. In this case, the relative standard deviation of the descriptive solution is less than the error of the local and global solutions constructed without taking into account a priori information of the form (16): and . This table does not show the column containing the exact concentration values and presented in Table 1.

**TABLE 1.** Comparison of results obtained by Global, Local, and Descriptive Regularization methods

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Gas\* | Global regularization | | Local regularization | | Descriptive regularization | |
|  |  |  |  |  |  |
|  | -0.00378 | 1.83 | -0.00331 | 1.7307 | 0.00018 | 0.6027 |
|  | 0.03105 | 0.0759 | 0.03150 | 0.0625 | 0.03250 | 0.0327 |
|  | 0.01277 | 0.0055 | 0.01271 | 0.0008 | 0.01266 | 0.0031 |
|  | 0.20640 | 0.0118 | 0.20603 | 0.0099 | 0.20545 | 0.0071 |

In the described experiment, gases were used for which the scatter of concentration values was two orders of magnitude. For further research, 6 gases () with an even greater scatter of concentration values were selected. The vector of exact values was taken from [10]. For a matrix of mass absorption coefficients, the size of the condition number is determined .

To take into account the continuous attenuation coefficient, a transition was made from SLAE (4) to a system of the form

(17)

where is the size matrix obtained by adding to the right of the size matrix a unit rectangular matrix of size ; -vector of dimension , in which the first projections  contain the desired gas concentrations, and projections with numbers carry information about the value of the continuous attenuation coefficient , but with a matrix of a different dimension, was proposed by the authors of [10].

This technique for processing laser gas analysis data makes it possible to determine both gas concentrations and continuous attenuation of the medium. It should be noted that the transition to system (11) complicates the task, since it worsens the conditionality of the system: . In table 3 shows the results of a numerical experiment\* carried out by the authors [10] (concentration vector ), pseudo-solution vector , global regularized solution vector and local . To solve SLAE (17), the authors of [10] used Tikhonov’s regularization method with the choice of the regularization parameter according to the optimality criterion [9].

**ТABLE 2.** Comparison of concentration values obtained by different solution method

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Gas\* |  |  |  |  |  |
|  | 11.30 | 12.75 | 11.28 | 11.35 | 11.28 |
|  | 301 | 187 | 287 | 277 | 303 |
|  | 0.038 | 0.1507 | 0.0375 | 0.0375 | 0.0382 |
|  | 0.0509 | 1.5440 | 0.0472 | 0.0550 | 0.0489 |
|  | 0.0295 | -0.3734 | 0.0306 | 0.0317 | 0.0288 |
|  | 0.480 | -0.7831 | 0.4130 | 0.4427 | 0.445. |

For the data presented in table 2, the following relative standard deviation values were obtained:

Thus, the accuracy of the proposed local regularized solution turned out to be higher than the accuracy of the solution obtained by the authors of [10] and the accuracy of the global regularized solution.

In table 3 shows the values of the continuous attenuation coefficient  (km-1) obtained as a result of solving SLAE (17), the average value is equal to 0,67. These data are consistent with the data obtained in [10], where the average value was 0,6 (km-1) [9].

**TABLE 3.** Values of the continuous attenuation coefficient θ for different projection numbers

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Projection number | 1 | 2 | 3 | 4 | 5 | 6 |
|  | 0,7265 | 0,6910 | 0,5878 | 0,6381 | 0,7005 | 0,6798 |

The results of numerical experiments allow us to draw a conclusion about the effectiveness of using local regularizing algorithms to solve the inverse problem of gas analysis, regardless of the quantity and composition of the gases being studied [10].

**TABLE 4.** Comparison of Regularization Methods for Gas Composition Identification

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Properties | Gas\* | | | | | |
|  |  |  |  |  |  |
| Global  Regularization | 9,75 | 290 | 0,0025 | 0,0125 | 0,0395 | 0,1890 |
| Local  Regularization | 9,78 | 291 | 0,0025 | 0,0128 | 0,0370 | 0,0913 |
| Descriptive  regularization | 14,29 | 367 | 0,007 | 0,0339 | 0,252 | 0,3945 |
| Results of the work | 14,90 | 402 | 0,0068 | 0,0175 | 0,0073 | 0,3820 |

**CONCLUSION**

In conclusion, the following conclusions can be made:

The conducted numerical studies of the problem of identification of the gas composition of the atmosphere showed a higher accuracy of regularizing algorithms compared to regularizing algorithms.

In the article, regularizing algorithms allow constructing stable solutions to parametric identification problems with a wide variety of information about the parameter vector of the identified model: starting from the requirements for the "smoothness" of the desired solution and ending with information about the values or signs of the projections of the solution vector. The use of singular value decomposition both in constructing a regularized solution and in selecting the parameters of regularizing algorithms determines the computational efficiency of the presented algorithms [10].

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