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ALGORITHMS AND SOLUTION TO THE PROBLEM OF PARAMETRIC IDENTIFICATION OF THE GAS COMPOSITION OF THE ATMOSPHERE

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the capacitive mode of a parallel circuit or vice versa. This does not take into account the fact that of the equivalent modes, only 3 is unstable for a series circuit, and point 7 is unstable for a parallel circuit.

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ALGORITHMS AND SOLUTION TO THE PROBLEM OF PARAMETRIC IDENTIFICATION OF THE GAS COMPOSITION OF THE ATMOSPHERE

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Abstract. *This article discusses the problem of identifying the gas composition of the atmosphere, which has important practical significance and allows us to illustrate the advantages of the proposed regularizing solution algorithms. Every ear, human industrial activity increasingly aggravates the problem of environmental protection. Among the diverse human impacts on nature, air pollution occupies a special place. Every ear, up to 500 thousand various pollutants are emitted into the atmosphere. In this regard, the task of monitoring the composition of the atmosphere is very relevant. Numerical studies of the problem of identifying the gas composition of the atmosphere have*

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shown higher accuracy of local regularizing algorithms compared to global regularizing algorithms. The local regularization algorithm is shown to perform well when reconstructing solutions to projections of the concentration vector, as well as with a scatter of order projection values.

Keywords: *coefficient, proportionality, spectral lines, regularizing, molecular absorption, algebraic equations, dispersion estimation, air aerosols, ill-conditioned, algorithm, conditionality, mathematical expectation, covariance matrix.*

Annotatsiya: *Ushbu maqolada atmosferaning gaz tarkibini aniqlash muammosi ko'rib chiqiladi, bu muhim amaliy ahamiyatga ega va taklif qilingan tartibga solish algoritmlarining afzalliklarini ko'rsatishga imkon beradi. Har bir insonning sanoat faoliyati atrof-muhitni muhofaza qilish muammosini tobora kuchaytirmoqda. Insonning tabiatga ta'sirining xilma-xilligi orasida havoning ifloslanishi alohida o'rin tutadi. Har bir quloqdan atmosferaga 500 minggacha turli ifloslantiruvchi moddalar chiqariladi. Shu munosabat bilan atmosfera tarkibini kuzatish vazifasi juda dolzarbdir. Atmosferaning gaz tarkibini aniqlash muammosining raqamli tadqiqotlari global tartibga solish algoritmlariga nisbatan mahalliy tartibga solish algoritmlarining yuqori aniqligini ko'rsatdi. Mahalliy tartibga solish algoritmi konsentratsiya vektorining proyeksiyalariga yechimlarni qayta qurishda, shuningdek tartibli proyeksiya qiymatlarining tarqalishi bilan yaxshi ishlashi ko'rsatilgan.*

Tayanch so‘zlar: *koeffitsient, mutanosiblik, spektral chiziqlar, tartibga solish, molekulyar yutilish, algebraik tenglamalar, dispersiyani baholash, havo aerozollari, yomon shartli, algoritm, shartlilik, matematik kutish, kovariatsiya matritsasi.*

Аннотация: *В данной статье рассматривается проблема идентификации газового состава атмосферы, имеющая важное практическое значение и позволяющая проиллюстрировать преимущества предлагаемых регуляризирующих алгоритмов решения. С каждым годом производственная деятельность человека все больше обостряет проблему охраны окружающей среды. Среди многообразных воздействий человека на природу загрязнение воздуха занимает особое место. Ежегодно в атмосферу выбрасывается до 500 тысяч различных загрязняющих веществ. В связи с этим задача мониторинга состава атмосферы весьма актуальна. Численные исследования задачи идентификации газового состава атмосферы показали более высокую точность алгоритмов локальной регуляризации по сравнению с алгоритмами глобальной регуляризации. Показано, что алгоритм локальной регуляризации хорошо работает при восстановлении решений по проекциям вектора концентрации, а также при разбросе значений проекций порядка.*

Ключевые слова: *коэффициент, пропорциональности, спектральных линий, регуляризирующих, поглощения молекул, алгебраических уравнений, оценки дисперсии, воздухе аэрозолей, плохо обусловленными, алгоритм, обусловленности, математическим ожиданием, ковариационной матрица.*

Introduction

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 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. 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 [54;103]. 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.

Research Methods and the Received Results

The volumetric attenuation coefficient of a medium $\mu(\lambda)$ for radiation with a wavelength λ 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.

$$I(\lambda) = I_0(\lambda) \cdot e^{-\mu(\lambda)L} \quad (1)$$

where $I(\lambda)$ and $I_0(\lambda)$ (W/cm2) are the radiation intensity, respectively, at the beginning and at the end of an atmospheric channel of length L; the exponent is called the optical thickness of the layer.

On the other hand, the measured volumetric attenuation coefficient of the medium $\mu(\lambda)$ for an isolated absorption line is related to the concentration of the target gas by the relation [51;103]:

$$\mu(\lambda) = K(\lambda) \cdot \rho, \quad (2)$$

where ρ is the concentration of the desired gas, averaged along the propagation path of the laser beam, $K(\lambda)$ is the mass absorption coefficient of the desired gas at wavelength λ.

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

$$\mu(\lambda_i) = \sum_{j-1}^{M} K_j(\lambda_i) \cdot \rho_j \quad (3)$$

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

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 CO_2 is the laser with a fixed wavelength and the possibility of its discrete tuning. Then, if the measurements were carried out at N lengths, equation (3) can be rewritten as a system of linear algebraic equations

$$K \cdot \rho = f \quad (4)$$

in which K is a matrix of the size $(N \times M)$ of the mass absorption coefficients of the M desired gases at N measurement wavelengths, $\rho - M$ - a dimensional vector of concentrations; $f - N$ - dimensional vector of the volumetric absorption coefficient of the medium with projections $f_i = \mu(\lambda_i)$. Based on the measurement results, taking into account (1), these projections can be calculated as follows:

$$f_i = \frac{1}{L} \cdot \ln\left(\frac{I_0(\lambda_i)}{I(\lambda_i)}\right), \; i = 1, 2, ..., N. \quad (5)$$

It is assumed that the vector of the right side of system (4) contains a vector of measurement noise η with zero mean $(M[\eta] = 0_N)$ and a covariance matrix $V_\eta = M\left[\eta\eta^T\right]$, which has a diagonal structure $V_\eta = diag\left\{\sigma_1^2, \sigma_2^2, ..., \sigma_N^2\right\}$. To estimate the dispersion of the i-measurement, the following formula was proposed in [58], [10]:

$$\sigma_i^2 = \frac{1}{n \cdot L^2}\left\{\left[\frac{\sigma_{I_0}}{I_0}\right]^2 \left(1 + \exp\left[2\ddot{\ddot{f}}_i \cdot L\right]\right) + \left(\frac{\sigma_K}{K}\right)^2\right\} \quad (6)$$

where n is the number of measurements at a wavelength λ_i; $\ddot{\ddot{f}}_i$ - average value calculated from sales f_i; $\frac{\sigma_K}{K}$-relative error of the optics-electronic path; $\frac{\sigma_{I_0}}{I_0}$ - relative error in measuring the radiation intensity at the entrance to the atmosphere; L - length of the route. The values of $\frac{\sigma_K}{K}$ and $\frac{\sigma_{I_0}}{I_0}$ do not exceed 1% for the equipment used by the authors of [58].

In the general case, in the presence of aerosols and vapors H_2O, equation (4) takes the form:

$$K \cdot \rho + \theta = f \quad (7)$$

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

Systems (4) and (7) are ill-conditioned, which causes instability of their solutions with respect to errors η 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 H_2O in mid-latitudes in winter is $5.88 \cdot 10^3 - (ppm)$ and $1.56 \cdot 10^4 - (ppm)$ - in summer. At the same time, the concentrations of ethylene and ammonia under normal conditions do not exceed hundredths $(1\ ppm = 10^{-6}\ amм)$. Thus, the spread of the concentration vector projection values can be 7 or more orders of magnitude.

Results and discussion

The initial information for a number of numerical experiments was the vector of reference concentrations $\bar{\rho}$ (ppm) for four gases and the matrix (atm-1cm-1) of mass absorption coefficients of the desired gases with sizes 100×4 borrowed from the literature [60,102], [10]. As a result of the singular decomposition of the matrix, the maximum and minimum singular numbers $\lambda_{\max} \approx 33.80$ and $\lambda_{\min} \approx 0.0022$ were obtained. Thus, the condition number is $cond(K) \approx \frac{\lambda_{\max}}{\lambda_{\min}} \approx 15462$.

Using a given matrix of mass absorption coefficients K and the "exact" concentration $\bar{\rho}$ vector, the exact vector of the right-hand side was calculated $\bar{f}$, which was then distorted by a random error vector η (interpreted as measurement noise), distributed according to the normal law with zero mathematical expectation and a covariance matrix

$$V_\eta = diag\left\{\sigma_1^2, \sigma_2^2, ..., \sigma_\eta^2\right\}, \quad (8)$$

in which the variances were determined by the following expression:

$$\sigma_i^2 = \left(\delta_f \cdot \frac{\left|\bar{f}_i\right|}{2}\right)^2, \; i = 1, ..., N, \quad (9)$$

where $\delta_f = \|\eta\| / \left\|\bar{f}\right\|$ is the relative noise level specified from the interval $[0.0001, 0.15]$.

In what follows, the following matrix representation is used V_η:

$$V_\eta = \sigma_\eta^2 \cdot C_\eta, \quad (10)$$

where $\sigma_\eta^2 = \max \sigma_i^2$,

$$C_\eta = diag\left\{\frac{\sigma_1^2}{\sigma_\eta^2}, \frac{\sigma_2^2}{\sigma_\eta^2}, ..., \frac{\sigma_N^2}{\sigma_\eta^2}\right\}.$$

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

$$\rho_\alpha = \sum_{j=1}^{\rho}\left[\frac{\lambda_j}{\lambda_j^2 + \alpha m(\lambda_j)} \cdot \left\langle u_j, C_\eta^{-1/2}\tilde{f}\right\rangle\right]\nu_j, \quad (11)$$

where u_j, ν_j are the first ρ columns of the matrices U, V included in the singular decomposition $C_\eta^{-1/2}K = U \wedge V^T$; ρ - matrix rank K equal to 4; $\tilde{f} = \bar{f} + \eta$ - "noisy" (with a given relative noise level δ_f) vector of the volumetric absorption coefficient of the medium. The choice of the regularization parameter α was carried out according to the optimality criterion.

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

$$\rho_S = \sum_{j=1}^{\rho}\left[\frac{1}{\lambda_j(1+\bar{S}_j)} \cdot \left\langle u_j, C_\eta^{-1/2}\tilde{f}\right\rangle\right]\nu_j \quad (12)$$

The values $\bar{S}_j$ are estimates for the "exact" noise/signal ratios S_j and are given by the following expression:

$$\hat{S}_j = \begin{cases} S_{j,1}^*, \ if \ \tilde{S}_j^+ \le 1/4 \ u \ 0 \le S_j^{(0)} < S_{j,2}^*; \\ S_{j,1}^*, \ if \ \tilde{S}_j^+ \le 1/4 \ u \ S_j^{(0)} = S_{j,2}^*; \\ 0, \quad if \ \tilde{S}_j^+ \le 1/4 \ u \ S_j^{(0)} > S_{j,2}^*; \\ 0, \quad if \ \tilde{S}_j^+ > 1/4; \end{cases} \quad (13)$$

Where $\tilde{S}_j^+ = \sigma_\eta^2 / \tilde{y}_j^2$, $S_j^{(0)} = \sigma_\eta^2 / (\lambda_j x_j^{(0)})^2$, $j = 1,..., \rho = 4$, $\tilde{y}_j$ are the projections of $\left\langle u_j, C_\eta^{-1/2}\tilde{f}\right\rangle$, $x_j^{(0)}$ are the projections of the vector $x^{(0)} = V_\rho^T \rho^{(0)}$. The calculated vector of the global regularized solution $\rho^{(0)}$ was taken as the "starting" solution ρ_{α_w}, i.e. $x^{(0)} = V^T \rho_{\alpha_w}$ Let us recall $S_{j,1}^*, S_{j,2}^*$ are the roots of the quadratic equation

$$(S_j^*)^2 + \left(2 - \frac{1}{\bar{S}_j^+}\right)S_j^* + 1 = 0 \quad (14)$$

it is assumed that $S_{j,1}^* \le S_{j,2}^*$.

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

$$\Delta_\alpha(\rho) = \frac{M\left[\left\|\tilde{\rho}_\alpha - \bar{\rho}\right\|^2\right]}{\left\|\bar{\rho}\right\|^2}, \ \Delta_S(\rho) = \frac{M\left[\left\|\tilde{\rho}_S - \bar{\rho}\right\|^2\right]}{\left\|\bar{\rho}\right\|^2} \quad (15)$$

The mathematical expectation operator was replaced by averaging over 30 implementations of the corresponding regularized solutions constructed using vectors $\tilde{f}^{(n)} = \bar{f} + \eta^{(n)}$, $n = 1,..., 30$.

For a global regularized solution at a noise level, $\delta_j = 0.05$ the standard deviation was $\Delta(\rho_\alpha) = 1,03 \cdot 10^{-3}$, for a local one - $\Delta(\rho_S) = 5,72 \cdot 10^{-4}$. In table Table 4.1 shows the exact and reconstructed concentrations for four gases*, as well as the relative reconstruction errors.

Table 1

Gas*	$\bar{\rho}_j$	Global regularization		Local regularization	
		ρ_{α_j}	$\frac{\left\|\bar{\rho}_j - \rho_{\alpha_j}\right\|}{\bar{\rho}}$	ρ_{S_j}	$\frac{\left\|\bar{\rho}_j - \rho_{S_j}\right\|}{\bar{\rho}_j}$
NH_3	0,00453	0,00441	0,0265	0,00451	0,0044
O_3	0,03360	0,03350	0,0030	0,03352	0,0024
C_2H_4	0,01270	0,01275	0,0040	0,01271	0,0008
C_6H_6	0,20400	0,20475	0,0172	0,20425	0,00122

During the described computational experiment, for some implementations, global and local regularization $\tilde{f}^{(n)}$ algorithms calculated regularized solutions, some projections of which took unphysical negative values. 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:

$$-I_{M\times M}\cdot\rho<0_M \qquad (16)$$

where $I_{M\times M}$ is an identity matrix of size $M\times M$, 0_M is a zero vector M containing zero projections.

Conclusion

The results of this experiment for the noise level $\delta_j=0.05$ 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): $\Delta(\rho_\alpha)=1.90\cdot10^{-3}$, $\Delta(\rho_S)=1.65\cdot10^{-3}$ and $\Delta(p_S^*)=5.18\cdot10^{-4}$. This table does not show the column containing the exact concentration values $\bar{\rho}_j$ and presented in Table 1.

Table 2

Gas*	Global regularization		Local regularization		Descriptive regularization	
	ρ_{α_j}	$\frac{\lvert\bar{\rho}_j-\rho_{\alpha_j}\rvert}{\bar{\rho}}$	ρ_{S_j}	$\frac{\lvert\bar{\rho}_j-\rho_{S_j}\rvert}{\bar{\rho}_j}$	$\rho^*{}_{S_j}$	$\frac{\lvert\bar{\rho}_j-\rho^*{}_{S_j}\rvert}{\bar{\rho}_j}$
NH_3	-0.00378	1.83	-0.00331	1.7307	0.00018	0.6027
O_3	0.03105	0.0759	0.03150	0.0625	0.03250	0.0327
C_2H_4	0.01277	0.0055	0.01271	0.0008	0.01266	0.0031
C_6H_6	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 ($M=6$) with an even greater scatter of concentration values were selected. $H_2O, CO_2, NH_3, O_2, C_2H_2, C_6H_6$. The vector of exact values was taken from [36]. For a matrix of mass absorption coefficients, the size of the 16×6 condition number is determined $cond(K)\approx18319$.

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

$$W\cdot\psi-f \qquad (17)$$

where W is the size $N\times(2\cdot M)$ matrix obtained by adding to the right of the K size matrix $N\times M$ a unit rectangular matrix of size $N\times M$; ψ -vector of dimension $2M$, in which the first projections M contain the desired gas concentrations, and projections with numbers $j=M+1,...,2\cdot M$ carry information about the value of the continuous attenuation coefficient θ, but with a matrix of W a different dimension, was proposed by the authors of [58].

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: $cond(W)\approx41806$. In table Figure 3 shows the results of a numerical experiment* carried out by the authors [58] (concentration vector ρ_T), pseudo-solution vector ρ_{MHK}, global regularized solution vector ρ_α and local ρ_S. To solve SLAE (17), the authors of [36] used Tikhonov's regularization method with the choice of the regularization parameter according to the optimality criterion.

Table 3

Gas*	$\bar{\rho}$	ρ_{MHK}	ρ_T	ρ_α	ρ_S
H_2O	11.30	12.75	11.28	11.35	11.28
CO_2	301	187	287	277	303
NH_3	0.038	0.1507	0.0375	0.0375	0.0382
O_2	0.0509	1.5440	0.0472	0.0550	0.0489
C_2H_2	0.0295	-0.3734	0.0306	0.0317	0.0288
C_6H_6	0.480	-0.7831	0.4130	0.4427	0.445.

For the data presented in table. 3, the following relative standard deviation values were obtained:

$$\Delta(\rho_{MHK}) = 1.43,\ \Delta(\rho_{\gamma}) = 2.16 \cdot 10^{-3},\ \Delta(\rho_{\alpha}) = 3.30 \cdot 10^{-3}\ u\ \Delta(\rho_{S}) = 4.40 \cdot 10^{-4}.$$

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 [58] and the accuracy of the global regularized solution.

In table Figure 4 shows the values of the continuous attenuation coefficient θ (km^{-1}) obtained as a result of solving SLAE (17), the average value $\overline{\theta}$ is equal to 0.67. These data are consistent with the data obtained in [58], where the average value $\overline{\theta}_T$ was 0.6 (km-1).

Table 4

Projection number	1	2	3	4	5	6
θ	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.

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