AVAILABLE INFORMATION FOR DETERMINATION OF OPTICAL PARAMETERS OF ATMOSPHERIC LAYERS FROM MEASUREMENTS OF SPECTRAL RADIATION FLUX AT DIFFERENT LEVELS IN THE ATMOSPHERE. III. DETERMINATION OF OPTICAL PARAMETERS OF LAYERS IN THE INHOMOGENEOUS MULTILAYERED ATMOSPHERE (NUMERICAL EXPERIMENT)

O.B. Vasil'ev and A.V. Vasil'ev

St. Petersburg State University,
Scientific –Research Institute of Physics at the St. Petersburg State University
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In this paper, we present some results of mathematical modeling of the conditions for solving the inverse problem on determination of optical parameters of atmospheric layers from the data of measurements of hemispherical spectral flux of radiation at different levels in the atmosphere. The iteration process used in the paper for solving the inverse problem is shown to be convergent even for rather rough zero-order approximation. It is also shown that the proposed algorithm can be successfully used for processing of the data of real experiments.

Statement of the inverse problem and technique for its solution have been considered in Refs. 1 and 2, as well as information content of solar radiation flux with respect to the optical parameters of atmospheric layers has been demonstrated. This paper is the continuation of the aforementioned papers, so we describe a specific calculation algorithm for solving the inverse problem without repetition of basic formulas and conclusions keeping designations that have been already used. As a development of the approach considered in the late 60s and early 70s,[3,4] the inverse problem is suggested to be solved by combination of direct modeling and method of statistical regularization. The algorithm is checked in a closed numerical experiment. [Such an approach was studied earlier by Krekov (see, for example, Refs. 5 and 6) and Naats].

In order to be certain that the selected algorithm is correct and the obtained solutions are adequate to the real parameters of the atmosphere, the numerical experiment has been carried out and its results are described in this paper.

The essence of the numerical experiment is the following: some model of the atmosphere that further is referred to as "real" is assigned, then the direct problem is solved for it (i.e., upward and downward radiation flux is calculated), and the values of the flux are considered to be the results of experimental measurements; the inverse problem is solved for these "measurements." Comparison of the "real" model of the atmosphere and the results of solving the inverse problem makes it possible to conclude about the correctness of its solution.

Let us briefly describe an algorithm for the numerical experiment including the technique for solving the inverse problem.

1. The parameters of the problem are specified that are taken to be known exactly: the number of atmospheric layers (see Ref. 2), zenith angle of the Sun, surface albedo, and solar constant.

2. The "real" model of the atmosphere is assigned by the vector $\mathbf{X}_R$ whose components are the optical thicknesses of the layers, single scattering albedos of the layers, and elongation of the scattering phase functions of the layers (for employed parametrization of the atmosphere, see Ref. 2).

3. The direct problem is solved for the model $\mathbf{X}_R$, i.e., experimental measurements $\mathbf{F} = K(\mathbf{X}_R)$ are modeled, where K is the operator of solving the direct problem, and $\mathbf{F}$ are the "measured" radiation fluxes. The direct problem is solved by the Monte Carlo method (see below), so in addition to the measurement vector $\mathbf{F}$, the vector of the variance of measurements Σ is obtained. Further we interpret it as a diagonal matrix of corresponding variances. The direct problem has been solved with an accuracy no less than 1.5% for each value of the flux. It corresponds to the experimental error, so we need not to add any "random" errors.

4. Then we "forget" the "real" model of the atmosphere and consider the quantities $\mathbf{F}$ and Σ to be the results of some experimental measurements of unknown atmospheric parameters. In order for these parameters to be reconstructed, we solve the inverse problem by the method of statistical regularization.[7]

5. The zero–order approximation is selected, that is, the vector $\mathbf{X}_0$ and the vector of *a priori* variances $\mathbf{D}$ that we further interpret as a diagonal matrix of corresponding variances. The *a priori* variances are selected from general physical considerations for the range of possible variation of the atmospheric layer parameters.

6. The nonlinear inverse problem is solved by iteration technique.[8] The iteration cycle is over $i = 0, 1, \ldots$.

7. Then the flux and its derivative are calculated in the ith approximation: $\mathbf{F}_i = K(\mathbf{X}_i)$, $A_i = R(\mathbf{X}_i)$, where R is the operator of calculating the derivatives, and A_i is the matrix of partial derivatives of the flux in each layer with respect to its parameters (technique for calculating the matrix A is described below).

8. Fisher's matrix is calculated by the formula $M_i = (A_i^+ \Sigma^{-1} A_i + D^{-1})^{-1}$. The diagonal elements of the matrix M_i are the *a posteriori* variances for the model $\mathbf{X}_i$.

9. The "measured" flux **F** is compared with the calculated one $\tilde{\mathbf{F}}_0$ in the zero–order approximation. If they agree (within the limits of the double root–mean–square error), the zero–order approximation is assumed to be correct. This approximation with the corresponding *a posteriori* variance is considered to be the solution of inverse problem. The criterion for termination of iterations is the difference between the *i*th and the preceding approximations $\mathbf{X}_i - \mathbf{X}_{i-1}$. In the numerical experiment, we terminated the iteration process in the interactive mode. Further in processing the real experiments the criteria for automatic termination of iterations will be selected.

10. If iterations are continued, the next approximation is calculated by the formula

$$\mathbf{X}_{i+1} = \mathbf{X}_0 + M_i A_i^+ \Sigma^{-1} (\mathbf{F} - \tilde{\mathbf{F}}_i + A_i (\mathbf{X}_i - \mathbf{X}_0)),$$

and calculations are repeated starting from item 7.

11. After termination of iterations, the solution of the inverse problem is considered to be the vector $\mathbf{X}_i$ and variances of its components, i.e., the diagonal elements of the matrix M_i.

12. In order to check the correctness of the solution of the inverse problem, the "measured" and calculated flux **F** and $\tilde{\mathbf{F}}_i$ are compared for real and retrieved models $\mathbf{X}_R$ and $\mathbf{X}_i$. Their good retrieval accuracy is indicated by their agreement within the limits of the double *a posteriori* root–mean–square deviations (RMSD).

Now let us dwell on the technique for solving the direct problem and calculating the partial derivatives of the flux. The Monte Carlo method was used in Ref. 2 for solving the transfer equation, and the technique of correlated trajectories of the Monte Carlo method was employed in calculating the derivatives. Its use in the first calculations was reasoned by the fact that the preliminary calculations were carried out. Their purpose was only to demonstrate that the amount of information was sufficient for the solution of the problem. However, the more optimal technique[9] developed at the Computer Center of the Siberian Branch of the Russian Academy of Sciences was used for solving the inverse problem, capable of calculating the derivatives simultaneously with the flux.

Unfortunately, although the calculation algorithm is simple, it is rather cumbersome (this is peculiar to all algorithms of the Monte Carlo method), so we do not present it here. Let us only briefly describe the basic principles of calculating the derivatives and the peculiarities of their calculation as applied to our problem.

Derivatives are calculated simultaneously with modeling of flux, i.e., using the same photon trajectories. To calculate the derivatives, the special photon weights are introduced that are equal to the sum of the logarithmic derivatives of the probability of transition between the points of phase space and the photon local weight. It is clear that the corresponding formulas depend on a specific calculation technique (on the parameters to be modeled and algorithms for modeling).

Let us use the algorithm for modeling the weighted functions with analytical averaging over the probabilities of photon absorption and leaving the medium as well as with local estimates of the flux,[10] with the optical thickness being used as a vertical coordinate in the atmosphere, what significantly simplifies all calculations. The arrangement of specific expressions for the probability of photon transition between the points of the phase space and of the local estimates of the flux as well as of their differentiation with respect to the optical parameters of the atmospheric layers is not difficult. We omit the corresponding derivations because of limitations on the length of the article.

We also note that the comparison between the "measured" and calculated values of the flux is used in the algorithm. Since "measurements" in our numerical experiment are at the same time calculations, the method of correlated trajectories[10] is used for comparison between the values of the flux in order to exclude the effect of statistical error of the Monte Carlo method. Its essence is the following. The same photon trajectories are used for modeling of the "measured" and "calculated" values of the flux. Therefore, their difference is determined only by various atmospheric models.

Nine numerical experiments on solving the inverse problem for different "real" models of the atmosphere were carried out by the given algorithm. Calculated results are given in Table I incorporating the "real" model of the atmosphere (optical thickness of the layers τ, single scattering albedo in the layer Λ, and elongation of the scattering phase function G), the zero–order approximation (identical for all experiments), and the results of solving the inverse problem (values of the retrieved optical parameters of the atmospheric layers and *a posteriori* variances of these parameters) for each experiment. Here n denotes the number of iterations.

The following models were selected for the experiments: "thin" one–layer (the first experiment), "thin" five–layer homogeneous (the second experiment), "thin" five–layer inhomogeneous (the third experiment), "average" one–layer (the fourth experiment), "average" five–layer homogeneous (the fifth experiment), "average" five–layer inhomogeneous (the sixth experiment), "thick" one–layer (the seventh experiment), "thick" five–layer homogeneous (the eighth experiment), and "thick" five–layer inhomogeneous (the ninth experiment). The zenith angle of the Sun was taken to be 45° for all calculations, and the surface albedo was 30%.

Calculations were carried out on an IBM –PC/286. Execution time varied from a few minutes to several hours depending on the complexity of the model (in particular, on the number of layers and their optical thickness τ).

The principal results of the numerical experiment are the following.

For "thin" models, the optical thickness is retrieved well, the single scattering albedo – worse, and the elongation of the scattering phase function practically cannot be retrieved. Especial attention should be paid to the results of the third experiment, where the inhomogeneity of the atmosphere was retrieved well in spite of the fact that the zero-–order approximation was homogeneous. Obviously, the good retrieval of the optical thickness for the "thin" atmosphere is explained by the fact that due to the small contribution of scattering, the amount of information on the optical thickness contained in the flux is greater than that on the single scattering albedo and scattering phase function.

For "average" atmospheric models, the optical thickness and the single scattering albedo are retrieved well. Let us also pay attention to the results of the sixth experiment. The vertical profile of the optical thickness was not retrieved here from the homogeneous zero–order approximation (as for the "thin" model), but the vertical profile of the single scattering albedo was retrieved well. Therefore, due to scattering, the amount of information on the optical thickness contained in flux becomes less than that of information on the single scattering albedo.

For the "thick" models, the dependence of the results of solving the inverse problem on the zero-–order approximation becomes pronounced. Actually, the algorithms for statistical regularization give the solutions that are most similar to the zero–order approximation, so the unique solution, if it exists, depends on the zero-–order approximation.

TABLE I. Results of the numerical experiments on solving the inverse problem.

"Real" model			Zero-–order appoximation			Result of solving the inverse problem (the RMSD is given in parenthesis)			
1			2			3			
The first experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
0.2	0.9	13	0.6	0.85	10	12	0.19(0.02)	0.88(0.03)	8(6)
The second experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
0.04	0.09	13	0.12	0.85	10	11	0.036(0.005)	0.87(0.06)	11(7)
0.04	0.09	13	0.12	0.85	10		0.040(0.007)	0.88(0.06)	9(6)
0.04	0.09	13	0.12	0.85	10		0.040(0.008)	0.88(0.06)	8(7)
0.04	0.09	13	0.12	0.85	10		0.040(0.009)	0.87(0.06)	10(7)
0.04	0.09	13	0.12	0.85	10		0.040(0.009)	0.88(0.05)	10(7)
The third experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
0.02	0.75	6	0.12	0.85	10	8	0.027(0.003)	0.83(0.07)	10(7)
0.03	0.8	9	0.12	0.85	10		0.033(0.005)	0.83(0.06)	11(7)
0.04	0.85	13	0.12	0.85	10		0.049(0.007)	0.80(0.05)	11(7)
0.05	0.9	17	0.12	0.85	10		0.041(0.009)	0.88(0.05)	9(7)
0.06	0.95	20	0.12	0.85	10		0.061(0.009)	0.91(0.05)	13(7)
The fourth experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
0.5	0.9	14	0.6	0.85	10	8	0.43(0.04)	0.89(0.02)	8(7)
The fifth experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
0.1	0.9	14	0.12	0.85	10	6	0.086(0.007)	0.88(0.05)	11(7)
0.1	0.9	14	0.12	0.85	10		0.089(0.011)	0.87(0.06)	8(5)
0.1	0.9	14	0.12	0.85	10		0.097(0.012)	0.86(0.05)	9(6)
0.1	0.9	14	0.12	0.85	10		0.088(0.011)	0.90(0.05)	9(7)
0.1	0.9	14	0.12	0.85	10		0.087(0.010)	0.87(0.04)	9(7)
The sixth experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*		Λ	*G*
0.07	0.75	5	0.12	0.85	10	7	0.105(0.007)	0.81(0.05)	12(7)
0.09	0.8	8	0.12	0.85	10		0.099(0.009)	0.83(0.05)	12(6)
0.11	0.85	13	0.12	0.85	10		0.095(0.01)	0.84(0.05)	11(6)
0.11	0.9	16	0.12	0.85	10		0.109(0.01)	0.88(0.04)	10(7)
0.12	0.95	20	0.12	0.85	10		0.090(0.01)	0.93(0.04)	9(7)
The seventh experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
1.8	0.9	14	0.6	0.85	10	11	1.28(0.12)	0.86(0.02)	7(7)

TABLE I (continued).

1			2			3			
The eighth experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
0.36	0.9	14	0.12	0.85	10	8	0.18(0.03)	0.86(0.06)	3(2)
0.36	0.9	14	0.12	0.85	10		0.23(0.03)	0.87(0.05)	5(5)
0.36	0.9	14	0.12	0.85	10		0.26(0.02)	0.80(0.04)	9(6)
0.36	0.9	14	0.12	0.85	10		0.25(0.02)	0.84(0.04)	9(6)
0.36	0.9	14	0.12	0.85	10		0.24(0.02)	0.86(0.02)	9(7)
The ninth experiment									
τ	Λ	*G*	τ	Λ	*G*	*n*	τ	Λ	*G*
0.21	0.75	5	0.12	0.85	10	9	0.28(0.02)	0.81(0.04)	10(6)
0.27	0.8	8	0.12	0.85	10		0.27(0.02)	0.80(0.03)	10(6)
0.33	0.85	13	0.12	0.85	10		0.27(0.02)	0.84(0.03)	10(7)
0.33	0.9	16	0.12	0.85	10		0.23(0.02)	0.85(0.03)	8(7)
0.36	0.95	20	0.12	0.85	10		0.21(0.03)	0.94(0.02)	6(6)

The results of the seventh to ninth experiments are really the solutions of the inverse problem, since the difference between the values of the flux calculated by the "initial" and "retrieved" models, is less than the double RMSD of each layer.

We have specially selected the zero–order approximation to be essentially different from the initial model in order to investigate convergence of the iterations. The results of all nine experiments show that the iterations really converge, though the solution for "thick" models differ from the "real" model. In this connection, for processing of the results of real but not "numerical" experiments, we recommend to select another zero-–order approximation, if the solution differs essentially from the employed zero-–order approximation.

We note that the elongation of the scattering phase function G cannot be retrieved in our nine experiments (*a posteriori* variance was close to *a priori* one). Really, the calculations of the information content performed in Ref. 2 show that the information on the scattering phase function may be obtained from measurements of the hemispheric flux only at rather large optical thicknesses and "favorable" combination of the other parameters. By the way, the eighth experiment indicates the feasibility of rough retrieval of the elongation of the scattering phase function for two first layers.

Thus the results of numerical experiments allow us to make a promising conclusion about feasibility of retrieval of the vertical profiles of the atmospheric parameters from experimental hemispheric flux measured at different levels in the cloudless atmosphere. Such measurements were carried out over several years in the Laboratory of ShortWave Radiation of the Scientific–Research Institute of Physics at the Leningrad State University.[11,12]

We note that in numerical experiments, in order to check the convergence of iterations, we specially selected some "average" zero–order approximation, which differed essentially from the "real" model, and large *a priori* variance. In processing of the results of real experiments, one can select the mean climatic model of the atmosphere for the region under investigation and corresponding *a priori* variance as a zero–order approximation. One also can use the estimates of separate parameters of the atmosphere obtained in a two–flux approximation[11] as a zero-–order approximation. It should increase the accuracy of solving the inverse problem and decrease the number of iterations.

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