EFFICIENT TECHNIQUE FOR LINE-BY-LINE CALCULATING THE TRANSMITTANCE OF THE ABSORBING ATMOSPHERE

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A new algorithm for calculating the transmittance has been developed that includes recent advances in the line-by-line calculation method. The high speed of operation is provided due to preliminary selection of absorption lines, frequency grid optimization, and reduction of inhomogeneous path to equivalent homogeneous one.

INTRODUCTION

It is well known that the line-by-line method of calculation of the absorption characteristics of a gas medium is standard and is applied for verification of approximate models of transmittance and for direct modeling of the radiative transfer in molecular absorbing media. In this connection, development and creation of new highly efficient algorithms are urgent problems of indubitable interest for specialists. In this paper, we briefly describe a new algorithm including recent advances in the line-by-line method of calculation of the transmittance.[1]

The main directions of investigations that are being carried out by different scientific groups in order to reduce the time of transmittance calculation by the line-by-line method are the following[2]: 1) selection of absorption lines, 2) optimization of frequency grid, 3) reduction of inhomogeneous path to homogeneous one, 4) cutting absorption line profile, 5) separation of procedures for calculation of the selective and continuum absorption, 6) separation of frequency and altitude dependence of the optical thickness in line wings for inhomogeneous path, and 7) optimization of the algorithm for calculating the Voigt profile. In this paper, we consider the first three directions.

1. SELECTION OF ABSORPTION LINES

Gas absorption lines of different intensity in different bands may fall within a given spectral range $\Delta\nu$. The range of line intensity variations is quite wide, and the number of lines can be large. This leads to a significant increase in the calculation time. On the other hand, there are some lines in the spectral range $\Delta\nu$ whose contribution into the absorption is negligible. In the case of overlap of different gas bands, the number of lines can reach several hundreds of thousands (for example, the number of lines of the first six gases in the HITRAN–91 atlas[3] is about 120 000 in the 500–1300 cm^{-1} range). However, taking into account different amount of these gases in the atmosphere, only few thousands of lines give a real contribution to the absorption. So it is reasonable to take into account only these lines and exclude the remainder from calculation procedure. For this purpose, efficient criteria for the selection of lines are necessary.

The well-known criteria[4] are based on excluding the lines whose intensity (or absorption coefficient) is less than a given threshold value. Other criteria are based on estimating the optical thickness.[2,5] In our algorithm for calculating the transmittance we also use the criterion of line exclusion on the basis of estimating the optical thickness.[6] The criterion includes two selections, the general and altitude ones. For general selection, the optical thickness is estimated using approximate formulas for the line center and wing depending on the line position in the selected wavelength range (Fig. 1).

The rule of removing lines from calculations has the following form for the general selection[7]:

$$S_{0ij} < \varepsilon / W_{cj} \quad , \quad \nu_{ij} \in [\nu_1 - \Delta\nu_c, \nu_2 + \Delta\nu_c] \ , \tag{1}$$

$$\frac{S_{0ij}\,\gamma_{0ij}}{(\nu_{1,2} - \Delta\nu_{i,j})^2} < \varepsilon\,\delta / W_{wj} \ ,$$

$$\nu_{i,j} \in [\nu_1^*, \nu_1^* + \Delta\nu_w] \cup [\nu_2^* - \Delta\nu_w, \nu_2^*] \ , \tag{2}$$

where ε and δ are the given threshold values; $\Delta\nu$ (Fig. 1) is the spectral interval of averaging of the transmittance function calculated at a point ν_0; $\Delta\nu_c$ is the spectral interval beyond $\Delta\nu$ in which the selection is made by line centers; $\Delta\nu_w$ is the spectral interval in which the selection is made by line wings;

$$W_{cj} = 0.47 \int_{z_1}^{z_2} \varphi_1(z)\,\frac{\rho_j(z)}{\gamma_V(z)}\,dz \ ,$$

$$W_{wj} = \int_{z_1}^{z_2} \varphi_2(z)\,\rho_j(z)\,dz$$

are the absorbing masses of the jth gas in the line center (W_{cj}) and wing (W_{wj}); S_{0ij}, γ_{0ij}, and ν_{ij} are the intensity, Lorentz half-width, and center frequency of the ith line of the jth gas, respectively; $\gamma_V(z)$ is the Voigt line half-width calculated in the Matveev approximation[8]; $\varphi_1(z)$ and $\varphi_2(z)$ are the known functions of pressure and temperature; and ρ_j is the jth gas concentration.

The lines after the first selection are subject to the second selection whose essence is the following. The altitude z_{0i} is estimated for each line, above which (for upward path) or below which (for downward path) the contribution to the optical thickness is negligible. The rule for line removing has the following form for this selection:

$$\tau(z_{0i}, z_2) \le \varepsilon. \quad (3)$$

The altitude selection leads to the decrease of the number of lines to be considered as the layer thickness increases.

Examples of selection of the absorption lines are given in Tables I and II. It is seen that the number of lines can decrease by more than an order of magnitude after the first selection. The altitude selection (Table II) for the 40 km layer is most efficient for water vapor, because 90% of the atmospheric moisture is concentrated in the lower 5 km layer.

Figure 2 shows the CO_2 transmittance spectrum for the 50 km layer (*a*) and the relative error (*b*) due to excluding a line by criteria (1)–(3). The error does not exceed 0.4%.

Under certain modeling conditions, the spectral transmittance error due to absorption line selection may reach a few percents (for example, it reaches 3% for the ozone transmittance in the 1039.5–1040 cm^{-1} spectral range in the 50 km layer). However, this error does not affect essentially the accuracy of calculating the total transmittance (the total transmittance error did not exceed 0.5% in all the examples being considered). In addition, it can be reduced due to the selection of the threshold values ε and δ in Eqs. (1)–(3), if necessary. A decrease in the calculation time due to the selection can be one order of magnitude or more under certain conditions.

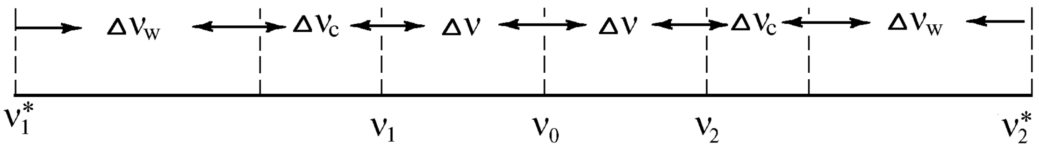

FIG. 1. General line selection diagram: $\Delta\nu$ is the spectral interval of averaging of the transmittance function calculated at the point ν_0; $\Delta\nu_c$ is spectral interval beyond $\Delta\nu$ in which the selection is made by line centers; $\Delta\nu_w$ is the spectral interval in which the selection is made by line wings.

TABLE I. General selection of absorption lines.

Spectral range, cm^{-1}	The number of lines, HITRAN-91	Gases	The number of lines after selection
4723–4764	1324	all	703
4000–4050	1956	all	124
500–1300	118913	the first six gases	11819

TABLE II. Altitude selection of absorption lines in the 40 km *layer.*

Altitude, km	The number of lines		
	H_2O 10095–10105 cm^{-1}	CO_2 721.5–722.5 cm^{-1}	O_3 1039.5–1040 cm^{-1}
0	19	157	205
5	4	95	194
10	1	66	181
20	0	35	113
30	0	17	86
40	0	12	35

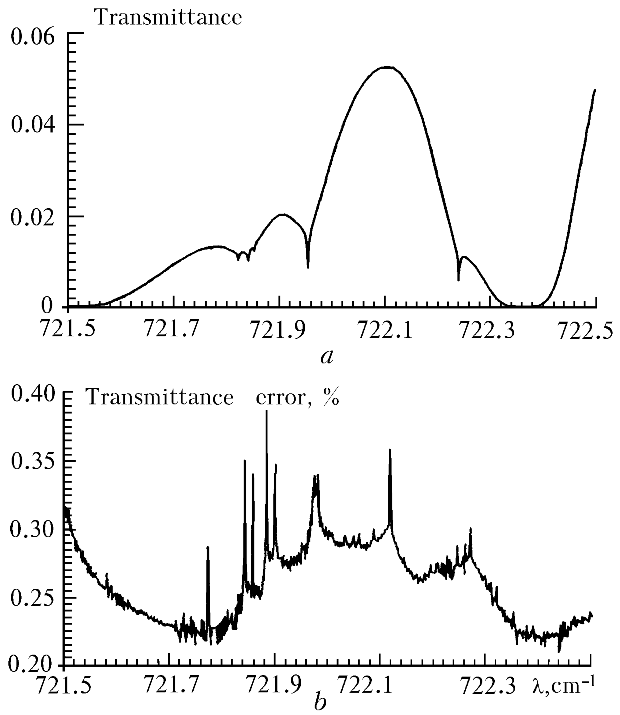

FIG. 2. CO_2 *transmittance spectrum in the* 50 km *layer (a) and the relative transmittance error due to exception of absorption line by the criteria (1)–(3) (b).*

2. FREQUENCY GRID OPTIMIZATION

When calculating the total transmittance, it is necessary to calculate the spectral transmittance (integrand function) on a frequency grid. As a rule, a uniform grid is used that provides the high accuracy of total transmittance calculations, with the calculation time being inversely proportional to the grid step.

The algorithms have been used in recent years with non-uniform adaptive step that take into account the oscillating behavior of the integrand function.[4,5,9-12] We use here the more effective multigrid technique proposed in Refs. 9 and 10. The essence of this technique is the following. A series of homogeneous grids whose step decreases according to the rule $h_l = h_0 2^l$, where h_0 is the finest grid step, and l is the serial grid number, is used instead of inhomogeneous frequency grid. We usually use $\gamma_V/4$ as h_0, where γ_V is the Voigt half-width of a line.

The absorption coefficients are calculated only at the nodes of a grid whose serial number increases as the frequency separation from the line center increases. Linear or quadratic interpolation is applied to calculate the absorption coefficients at intermediate frequencies. The multigrid technique allows us to minimize the transmittance calculation time in the given spectral range $\Delta\nu$ and to ensure the required accuracy.

We note that this frequency grid optimization technique is similar to the technique used by Smith et al.[13] The functions $Q_i(\nu)$ used to represent the initial absorption line profile $f(\nu)$ are the analogue of grids with different step h_l. The step size is multiple of four.

The time decrease provided by such a multigrid algorithm may be more than an order of magnitude.[9,10]

3. REDUCTION TO A HOMOGENEOUS PATH

The longest calculation time is necessary for calculating the total transmittance of an inhomogeneous path. In this case, it is necessary to calculate the integral over the altitude at each grid node. When using 11 grids, the number of grid nodes is approximately 90 for the spectral range $\Delta\nu = 1$ cm^{-1} and the minimum step $h_0 = \gamma_d/4$ in the 10 μm wavelength range. In this case, the largest grid step is about 0.25 cm^{-1}. For the spectral interval $\Delta\nu = 10$ cm^{-1}, 40 more nodes are required. In this case, the number of integrals over the altitude will be approximately 130 N, where N is the number of absorption lines.

To decrease the calculation time, one can apply the Courtis-Godson idea[14] to replace an inhomogeneous path by equivalent homogeneous one. It is well known that two parameters are introduced in this case: the first means the absorbing mass U_{ij}, and the second means the mean weighted pressure or the mean weighted half-width $\overline{\gamma}_{ij}$ being equal to

$$U_{ij} = \int\limits_{z_1}^{z_2} S_{ij}\, \rho_j\, dz , \qquad \overline{\gamma}_{ij} = \frac{\int\limits_{z_1}^{z_2} S_{ij}\, \gamma_{ij}\, \rho_j\, dz}{\int\limits_{z_1}^{z_2} S_{ij}\, \rho_j\, dz} , \qquad (4)$$

where S_{ij} and γ_{ij} are the intensity and the half-width of the ith line of the jth gas, respectively. Results of modeling show that for such definition of the parameter γ_{ij} it is possible to describe adequately only the wing of the reduced optical thickness, underestimating it in the line center. We use other definition of the parameter γ_{ij} calculated on the basis of two asymptotic approximations for the wing and the center of the line. In the case of the Lorentz profile, the parameters U_{ij} and γ_{ij} have the form

$$U_{ij} = \int\limits_{z_1}^{z_2} S_{ij}\, \gamma_{ij}\, \rho_j\, dz , \qquad \overline{\gamma}^{\,2}_{ij} = \frac{U_{ij}}{\int\limits_{z_1}^{z_2} \frac{S_{ij}\, \rho_j}{\gamma_{ij}}\, dz} . \qquad (5)$$

It is also easy to determine the parameters U_{ij} and $\overline{\gamma}_{ij}$ for the Voigt profile.

For the Lorentz profile, the reduced optical thickness has the form

$$\tau_{ij} = \frac{U_{ij}}{\pi[(\nu - \nu_{ij})^2 + \overline{\gamma}_{ij}^2]} . \tag{6}$$

One can see from Eqs. (5) and (6) that for the reduced optical thickness it is necessary to calculate only two integrals over altitude for each absorption line (three integrals for each line for the Voigt profile), which makes it possible to decrease essentially the calculation time.

Calculations of transmittance in different spectral ranges show that the error of reducing does not exceed 0.5%, whereas the time decreases 4–5 times.

CONCLUSION

By combination of powerful techniques for acceleration of the line-by-line calculations such as the absorption line selection, multigrid algorithm, and reduction of inhomogeneous path to homogeneous one, into a calculation procedure, a new algorithm has been created for calculating the transmittance. This algorithm is now one of the fastest known algorithms.

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REFERENCES

1. A.A. Mitsel', I.V. Ptashnik, K.M. Firsov, and B.A. Fomin, in: *Abstracts of Reports at the Second Interrepublic Symposium on Atmospheric and Oceanic Optics,* Tomsk (1995), pp. 31–32.
2. A. Chedin, H. Fisher, K. Kunzi, et al., eds., *Report on the ITRA, International Radiation Commission Working Group on Remote Sensing*, University of Maryland (1988), 220 pp.
3. L.S. Rothman, R.R. Gamache, R.H. Tipping, et al., J. Quant. Spectrosc. Radiat. Transfer **48**, 469–507 (1992).
4. A.A. Mitsel' and V.P. Rudenko, "*Software package for calculation of energy losses of optical Radiation in the atmosphere,B* Preprint No. 57, Institute of Atmospheric Optics, Tomsk (1988), 56 pp.
5. S.V. Afonin and A.G. Gendrin, in: *Software Support for Atmospheric Optics Problems* (Nauka, Novosibirsk, 1988), pp. 38–65.
6. A.A. Mitsel' and K.M. Firsov, Atmos. Oceanic Opt. **7**, No. 10, 779–780 (1994).
7. A.A. Mitsel and K.M. Firsov, J. Quant. Spectrosc. Radiat. Transfer (in print) (1995).
8. V.S. Matveev, Zh. Prikl. Spektrosk. **16**, No. 2, 228 (1972).
9. B.A. Fomin, "*Effective line-by-line technique for calculating radiation absorption in gases,B* Preprint IAE–5658/1, Russian Research Center "Kurchatov Institute," Moscow (1993), 13 pp.
10. B.A. Fomin, A.N. Trotsenko, and S.V. Romanov, Atmos. Oceanic Opt. **7**, Nos. 11–12, 786–789 (1994).
11. O. Valdar, J. Quant. Spectrosc. Radiat. Transfer **26**, No. 4, 381–384 (1981).
12. O. Valdar, J. Quant. Spectrosc. Radiat. Transfer **29**, No. 5, 407–411 (1983).
13. H.J.P. Smith, D.J. Dube, M.E. Gardner, et al., *FASCOD–Fast Atmospheric Signature Code (Spectrum Transmittance and Radiance)*, Report AFGL–TR–78–0081 (1978), 140 pp.
14. R.M. Goodie, *Atmospheric Radiation* [Russian translation] (Mir, Moscow, 1966), 522 pp.