Aggregate method for calculating atmospheric absorption with 20 cm^{-1} spectral resolution

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A new method for calculating the atmospheric absorption using parametric models of absorption bands is described. Model parameters are chosen based on the data obtained by the line-by-line (LBL) method. A possibility to choose an optimal model for a given spectral region is provided for. Modeling results are presented and compared with realistic data.

Introduction

The main characteristic of the radiative transfer equation is the transmission function of an atmospheric layer in a given zenith direction. It is used for calculation of fluxes of both the thermal and shortwave radiation in spectral regions occupied by absorption bands of atmospheric gases.

Depending on the problems of atmospheric optics to be solved, the transmission functions should be known with either high (for example, for interpretation of satellite data) or low spectral resolution (for example, for solution of radiation-climate problems). The transmission function with medium and low resolution is now often calculated using empiric methods, methods based on models of absorption bands, and the line-by-line method.

The line-by-line method of calculation of the transmission function has no restrictions connected with spectral resolution and allows calculation of the transmission for any spectral interval. However, its main disadvantage is long time needed for computation in a wide wavelength region.

Empiric methods and methods based on models of absorption bands are parametric: their parameters are determined from fitting to laboratory data or data obtained by the line-by-line method. They are commonly used to calculate the extinction of broadband atmospheric radiation. The empirical method form the foundation of the corresponding calculation techniques, such as SOI (State Optical institute),[1] SIAO (State Institute of Applied Optics),[2] LOWTRAN,[3] and MGO (Main Geophysical Observatory).[4] In this case, the transmission function depends on the absorbing mass of a gas and some parameter (or parameters). Both the form of the function itself and its parameters are determined from experimental data.

The LOWTRAN technique in the form of a software package has received the widest practical usage. The advantage of this technique is high speed, and its disadvantage is low accuracy. Besides, it is inapplicable to analytical calculations when solving some radiative problems.

The aggregate method for calculating the transmission function is based on model representation of absorption bands (also depended on parameters).[5] According to intention of the authors of the method, every model is applied to that spectral interval, in which its accuracy is the best. The advantages of the aggregate method are (a) high speed in computation of the transmittance (parameters for every wavelength are considered to be constant) and (b) the possibility of analytical calculations when solving radiative problems.

The disadvantages of the aggregate method[5] are the absence of the applicability boundaries and low accuracy. It should be also noted that the parameters of this technique in different wavelength regions are determined at different spectral resolutions.

In this paper, we propose a new aggregate method that differs from the technique of Ref. 5 in that:

(1) all parameters are fitted at a fixed spectral resolution of 20 cm^{-1};

(2) to fit the parameters, the absorption values, calculated by the LBL method, are used;

(3) parameters for all gases (water vapor, carbon dioxide, ozone, N_2O, and methane were considered) are calculated in the wavelength region from 330 to 10000 cm^{-1} (1–30 μm) with a step of 5 cm^{-1}.

Models of absorption

Theoretical models are based on an idealized representation of absorption bands as various models permitting their analytical description. These models are parametric, and the parameters themselves are determined from experimental data or calculated directly for different values of thermodynamic parameters of a medium. The models of spectra and their approximation were described in detail in Refs. 5–8 and 12.

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The aggregate method uses the following models[5]:

1. Approximation of a strong line of the Goody model:

$$A(\lambda) = 1 - \exp[-\sqrt{W^* k_1(\lambda)}], \quad (1)$$

where $A(\lambda)$ is the gas absorption at a given wavelength; $k_1(\lambda)$ is a spectral parameter; W^* is the equivalent absorbing mass, in cm DL, calculated by the equation for a vertical path with the zenith angle θ:

$$W^* = \int_{z_1}^{z_2} \rho \frac{P(z)}{P_0} \left(\frac{T_0}{T(z)}\right)^{0.5} B(z,\theta)\mathrm{d}z, \quad (2)$$

or by the equation for a horizontal path of the length L:

$$W^* = \rho \frac{P(z)}{P_0} \left(\frac{T_0}{T(z)}\right)^{0.5} L. \quad (3)$$

Here $B(z,\theta) = \dfrac{(R+z)}{\sqrt{(R+z)^2 - (R+z_1)^2 \sin^2\theta}}$ (4)

is a function of the beam path; R is the Earth's radius; ρ is the concentration of a gas, in g/cm^3; z_1 and z_2 are the boundaries of the absorbing layer; L is the path length, in cm; $P(z)$ is the air pressure, in Torr; $T(z)$ is the air temperature, in K; P_0 = 760 Torr; T_0 = 273 K. This model includes only one fitting parameter $k_1(\lambda)$.

2. Goody model of a band:

$$A(\lambda) = 1 - \exp\left(-\frac{S}{d}\frac{W}{\sqrt{1 + \frac{2}{\bar{p}}\frac{SW}{2\pi\gamma_0'}}}\right), \quad (5)$$

where $W = \rho(z)L$ is the content of an absorbing gas for the horizontal path and $W = \int_{z_1}^{z_2} \rho(z) B(z,\theta)\mathrm{d}z$ - for the vertical path;

$$\bar{p} = \frac{P_0}{W} W^*; \quad \gamma_0' = \frac{\gamma_0}{P_0}, \quad (6)$$

γ_0 is the Lorentz halfwidth determined at $p = P_0 =$ = 760 Torr.

This model includes two fitting parameters: S/d and $S/2\pi\gamma_0'$.

3. Modified Goody model:

$$A(\lambda) = 1 - \exp\left(-\frac{W k_3(\lambda)}{\sqrt{1 + \frac{k_3(\lambda) W}{4\bar{p} k_4(\lambda)}}}\right), \quad (7)$$

where $k_3(\lambda)$ and $k_4(\lambda)$ are fitting parameters; W is the gas content calculated by

$$W = \int_{z_1}^{z_2} \frac{P_g(z)}{P(z)} \frac{P(z)}{P_0} \frac{T_0}{T(z)} B(z,\theta)\mathrm{d}z, \quad (8)$$

where $P_g(z)$ is the gas pressure.

4. Elsasser model:

$$A(\lambda) = \mathrm{sh}\beta \int_0^b J_0(t) \exp(-t\ \mathrm{ch}\beta)\ \mathrm{d}t; \quad (9)$$

$$\beta = \frac{2\pi\gamma_0'}{d}\ \bar{p};\ \bar{p} = \frac{P_0}{W} W^*; \quad (10)$$

$$b = \frac{S/d}{\mathrm{sh}\beta} W;\ x = \frac{S/d}{(2\pi\gamma_0'/d)\bar{p}} W = \frac{b\ \mathrm{sh}\beta}{\beta}, \quad (11)$$

where $J_0(t)$ is the zero-order Bessel function; W is the gas content (8), and the rest are explained in the above models.

The parameters of this model are S/d and $2\pi\gamma_0'/d$.

5. Approximation of a strong line of the Elsasser band:

$$A = \Phi(\sqrt{\beta^2 x/2}), \quad (12)$$

where $\Phi(t) = \dfrac{2}{\sqrt{\pi}} \int_0^t \mathrm{e}^{-z^2}\mathrm{d}z$.

Equation (12) for calculating the absorption uses the data that were prior used for calculation of the parameter β by Eq. (10) and the parameter x by Eq. (11).

The value of W^* is calculated by the equation

$$W^* = \int_{z_1}^{z_2} \frac{P_g(z)}{P(z)} \left(\frac{P(z)}{P_0}\right)^2 \left(\frac{T_0}{T(z)}\right)^{1.5} B(z,\theta)\mathrm{d}z. \quad (13)$$

The parameters of this model coincide with the parameters of the simple Elsasser model (S/d and $2\pi\gamma_0'/d$).

For some sections of the spectrum, the equation

$$A(\lambda) = \Phi\left[\sqrt{W^* k_5(\lambda)}\right] \quad (14)$$

is used instead of Eq. (12). In Eq. (14), W^* is calculated by Eq. (13), and $\Phi(t)$ is calculated by Eq. (12); $k_5(\lambda)$ is the parameter of the model.

6. Elsasser model with temperature dependence:

In this model, the main equations are Eqs. (9)–(11), in which the parameters S/d and $2\pi\gamma_0'/d$ are set by the equations

$$\frac{S}{d} = \frac{a_1 \exp(-a_2/T_h)}{T_h^2};$$
$$\frac{2\pi\gamma_0'}{d}\frac{S}{d} = \frac{a_3 \exp(-a_4/T_h)}{T_h^2}, \quad (15)$$

including four fitting parameters: a_1, a_2, a_3, and a_4. In Eq. (15), T_h is the temperature of an equivalent homogeneous layer.

7. Modified Elsasser model:

The absorption function is determined by Eq. (9), and the parameter β is constructed as

$$\beta = \left(\frac{2\pi\gamma_0'}{d}\right)\left(\frac{\bar{p}}{P_0}\right)^{c(\lambda)} = \beta_0\left(\frac{\bar{p}}{P_0}\right)^{c(\lambda)}. \qquad (16)$$

The parameters here are β_0, $c(\lambda)$, and S/d. The pressure $\bar{p}$ is calculated by Eq. (10), and W and W^* are calculated by Eqs. (8) and (13).

Calculation of model parameters

The parameters $k_1(\lambda), \ldots, k_m(\lambda)$ of some model are determined with the use of the least-square method. Initial data are obtained with the use of the LBL method and the HITRAN–96 spectral database. The minimizing functional $Q[k_1(\lambda), \ldots, k_m(\lambda)]$ is determined by the equation

$$Q[k_1(\lambda), \ldots, k_m(\lambda)] =$$

$$= \sum_{i=1}^{n} \{A_i(\lambda) - f[W_i, k_1(\lambda), \ldots, k_m(\lambda)]\}^2 \to \min, \qquad (17)$$

where $A_i(\lambda) = A(W_i, \lambda)$ is the absorption calculated by the LBL method with the resolution of 20 cm^{-1}, $f[W_i, k_1(\lambda), \ldots, k_m(\lambda)]$ is the absorption model, W_i is the absorbing mass of a gas, $k_1(\lambda), \ldots, k_m(\lambda)$ are the parameters of the given model.

The determined parameters $k_1(\lambda), \ldots, k_m(\lambda)$ are stored as a file. Table 1 presents a fragment of such a file.

Table 1. Example of the table of parameters for ozone at the absorbing mass from 0.0006876638 to 0.0017392 cm DL

Model identifier	Wavenumber, cm^{-1}	The first parameter	The second parameter
3	770	0.04949438	0.2247906
2	775	0.04140093	0.02793893
3	780	0.03363267	0.1807833
3	785	0.02724842	0.1463426
3	790	0.02093796	0.1234225
3	795	0.01681563	0.09007432
3	800	0.01319392	0.07917236

The first column of the Table gives the identification number of a model (in this table, the Goody model of a band has number 2, the modified Goody model has number 3, and so on). The second column gives the wavenumber in reciprocal centimeters. The following columns present the model parameters.

For comparison, Table 2 presents the parameters of the methods from Ref. 5.

The computer program provides for the capability of choosing the optimal model for a given wavelength by minimizing the functional (17): the absorption model $f_j[k_1(\lambda), \ldots, k_m(\lambda)]$, for which the functional (17) is minimal, is taken as the optimum.

Table 2. Example of the table of parameters for the aggregate method from Ref. 5 for ozone

Model identifier	Wavenumber, cm^{-1}	The first parameter	The second parameter
3	769.8229	0.0365	1.14
3	772.2008	0.0338	1.14
3	773.9938	0.0315	1.14
3	775.7952	0.0292	1.14
3	778.2101	0.0271	1.14
3	780.0312	0.0251	1.14
3	781.8608	0.0230	1.14
3	783.6991	0.0210	1.14
3	786.1635	0.0192	1.14
3	788.0221	0.0176	1.14
3	789.8894	0.0161	1.14
3	791.7656	0.0144	1.14
3	794.2812	0.0133	1.14
3	796.1783	0.0120	1.14
3	798.0846	0.0109	1.14
3	800.0000	0.0100	1.14

Calculation of the gas mixture transmittance

Let us now consider the problem of radiation absorption by a gas mixture. For monochromatic radiation, the transmittance of a gas mixture is equal to the product of their transmittances $T_1(\nu)$ and $T_2(\nu)$ at the frequency ν:

$$T_\Sigma(\nu) = T_1(\nu)\, T_2(\nu), \qquad (18)$$

where T_1 is the transmittance of the first gas (in the absence of the second gas), and T_2 is the transmittance of the second gas (in the absence of the first gas).

When the transmittance is calculated with a medium (20 cm^{-1}) spectral resolution, no exact solution of the problem of band overlapping for a gas mixture in the model representation of absorption spectra exists.

Nevertheless, the rule (18) is used in calculations. In the papers by Burch,[9] Hoover,[10] and Tubbs,[11] it is shown that the product rule is fulfilled accurate to several percent under the following conditions:

(1) the interval $\Delta\nu$ is wide enough to include, at least, several lines of each gas;

(2) the positions of lines of two gases are not related to each other by some functional dependence;

(3) the partial pressure of a buffer gas is much higher than the partial pressure of absorbing gases.

The rule (18) allows the calculation of transmittance of a gas mixture to be reduced to calculation of transmittances of individual gases. This significantly alleviates the problem.

Results of modeling

For analysis, the calculated results given by different methods should be compared with realistic values obtained based on current spectroscopic data.

Figure 1 shows the relative error in calculation of the radiation absorption due to water vapor by the methods from Ref. 5. From this plot we can conclude that the calculation by the methods from Ref. 5 often disagrees with the realistic data. This can be explained, first of all, by the fact that the aggregate method was developed more than 20 years ago, and there were no such accurate data at that time (as compared to the current data).

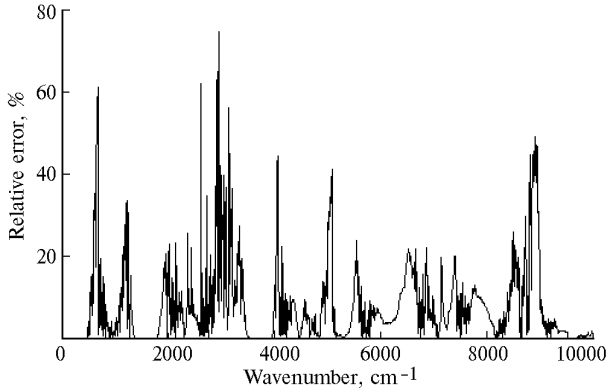

Fig. 1. Relative error in calculation of absorption due to water vapor by the methods from Ref. 5; vertical path (0–100 km), zenith angle is equal to zero, meteorological model of midlatitude summer.

Figure 2 shows the relative error in calculation of water vapor absorption by the LOWTRAN–7 methods (with the spectral resolution of 20 cm^{-1}). One can see that the average error is 15%, and at some wavelengths it exceeds 30%. This can be explained by the above-mentioned disadvantages of empirical methods.

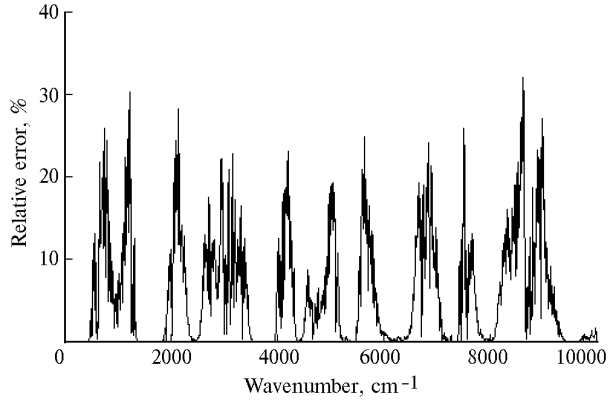

Fig. 2. Relative error in calculation of water vapor absorption by the LOWTRAN–7 methods. The conditions are the same as in Fig. 1.

Figure 3 shows the relative error in calculation of water vapor absorption with the new technique. The calculation was made for the model of midlatitude summer after fitting of model parameters using 100 meteofiles (the range of absorbing mass was taken as wide as possible: from $2.8 \cdot 10^{-15}$ to 25.6 cm DL).

It is seen that calculation by the new technique not always agrees with the realistic data and remains at the level of the error given by the LOWTRAN–7 technique.

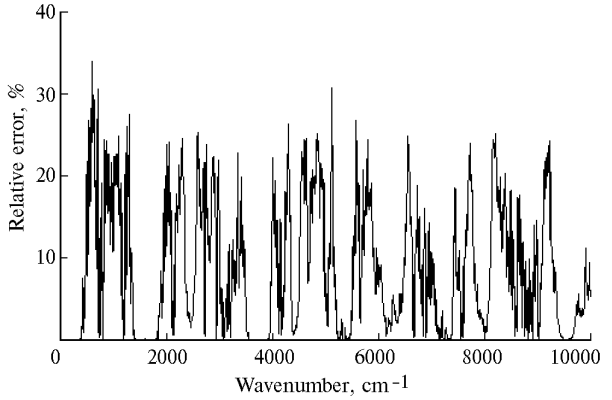

Fig. 3. Relative error in calculation of water vapor absorption by the new technique after fitting of the parameters of Eq. (17) in one of the maximum possible range of absorbing mass. The conditions are the same as in Fig. 1.

To improve the accuracy, the range of absorbing mass was divided into 100 subranges. Then Eq. (17) was minimized (and the corresponding parameters were sought for) in every subrange. As a result, the relative error decreased down to several percent (Fig. 4).

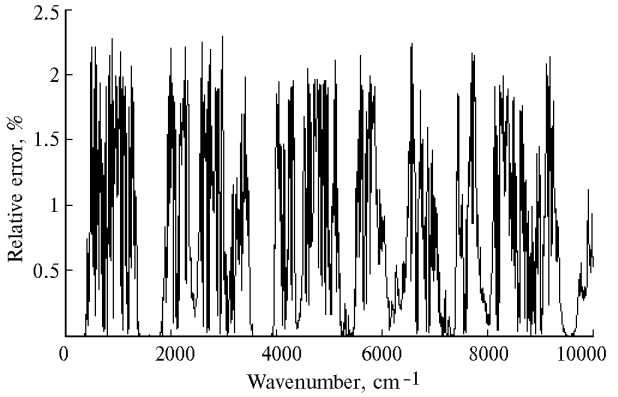

Fig. 4. Relative error in calculation of water vapor absorption by the new technique after fitting of the parameters of Eq. (17) in 100 subranges of the maximum possible range of absorbing mass. The conditions are the same as in Fig. 1.

These figures demonstrate the significant improvement of the accuracy of the aggregate methods (the error is less than 3%) for water vapor. For other gases the situation is similar. The accuracy is increased due to division of the range of absorbing mass into subranges. As a result, the computer memory needed for storage of the information on the parameters increases. This is an inevitable charge for the increase in accuracy.

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References

1. M.S. Kiseleva, V.S. Neporent, and E.O. Fedorova, Izv. Akad. Nauk SSSR, Ser. Fiz. Atmos. Okeana **3**, No. 5, 640–649 (1967).

2. V.L. Filippov, S.D. Kozlov, N.A. Rumyantseva, A.S. Makarov, and N.M. Ziatdinova, "Atmospheric transmittance in 1–14 μm region with high visibility range," Izv. Vyssh. Uchebn. Zaved., Ser. Fizika, Dep. VINITI No. 2483–4 (1984), 52 pp.
3. F.X. Kneizys, E.P. Shettle, W.O. Gallery, J.H. Chetwynd, L.W. Abreu, J.E.A. Selby, S.A. Clough, and R.W. Fenn, *Atmospheric Transmittance. Radiance. Computer Code LOWTRAN 6*, AFGL–TR–83–0187 (Hanscom, AFB, Mass., 1983), 200 pp.
4. A.M. Brounshtein and A.D. Frolov, Trudy Gl. Geofiz. Obs., Issue 496, 70–79 (1985).
5. W.L. Wolf, G.J. Zissis, S. Chapter, and A.J. La Rocca, eds., *The Infrared Handbook. Atmospheric Absorption* (Washington, 1978), pp. 5-1–5-132.
6. R.M. Goody, *Atmospheric Radiation* (Clarendon Press, Oxford, 1964).
7. S.S. Penner, *Quantitative Molecular Spectroscopy and Gas Emissivities* (Addison-Wesley, Reading, Mass., 1969).
8. V.E. Zuev, *Propagation of Visible and Infrared Radiation in the Atmosphere* (Halsted Press, New York, 1974).
9. D.E. Burch, J.N. Howard, and D. Williams, J. Opt. Soc. Am., No. 46, 452–455 (1956).
10. G.M. Hoover, C.E. Hathaway, and D. Williams, Appl. Opt., No. 6, 481–487 (1967).
11. L.D. Tubbs, C.E. Hathaway, and D. Williams, Appl. Opt., No. 6, 1422–1423 (1967).
12. A.A. Mitsel and K.M. Firsov, Atmos. Oceanic Opt. **13**, No. 2, 162–179 (2000).