

A NEW METHOD OF TREATING OVERLAPPING ABSORPTION BANDS OF ATMOSPHERIC GASES IN RADIATIVE TRANSFER PARAMETERIZATION

K.M. Firsov and T.Yu. Chesnokova

*Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk
Received September 1, 1997*

A method of longwave radiative transfer parameterization for the Earth's atmosphere is described. Spectral line parameters are used to calculate characteristics of molecular absorption. The k -distribution technique is shown to provide uncertain calculation of the frequency dependence of the transformed coefficient of molecular absorption. So, a phenomenological scheme has been constructed to treat overlapping gas absorption bands, which ensures higher level of parameterization of transmission functions than traditional techniques can provide. In comparison with line-by-line (LBL) techniques, this method calculates the transmission functions along any atmospheric path with an accuracy better than 1–2%.

INTRODUCTION

The atmospheric radiative transfer calculations in current climatological problems must be computationally fast yet exact, what in essence is incompatible.^{1,2} So, currently a considerable researcher effort is directed toward creating efficient radiative transfer parameterizations, i.e., towards reaching a compromise between computational cost and accuracy. This paper presents a method of parameterizing the transmission functions in the case of overlapping absorption bands of atmospheric gases.

In order to give an idea of how molecular absorption is incorporated in radiation calculations, we consider the solution of longwave radiative transfer equation in the clear atmosphere in the form¹

$$F^{\uparrow}(z) = \int_0^{\infty} \pi B_{\nu}(z_0) T_{\nu}^f(z, z_0) d\nu + \int_0^z \int_0^{\infty} \pi B_{\nu}(z') \frac{dT_{\nu}^f(z, z')}{dz'} dz' d\nu, \quad (1)$$

$$F^{\downarrow}(z) = \int_0^z \int_0^{\infty} \pi B_{\nu}(z') \frac{dT_{\nu}^f(z, z')}{dz'} dz' d\nu, \quad (2)$$

where $F^{\uparrow}(z)$ and $F^{\downarrow}(z)$ are the upward and downward fluxes through the level z ; $B_{\nu}(z)$ is the Planck function; $T_{\nu}^f(z, z')$ is the diffuse transmission function given by the following expression:

$$T_{\nu}^f(z, z') = 2 \int_0^1 \exp \left\{ -\frac{1}{\mu} \tau(\nu, z, z') \right\} d\mu, \quad (3)$$

where μ is the cosine of zenith angle,

$$\tau(z, z') = \int_z^{z'} K(\nu, p(h), T(h)) \rho(h) dh, \quad (4)$$

$\tau(z, z')$ is the optical depth of the layer $z-z'$; $K(\nu, p(h), T(h))$ is the molecular absorption coefficient, which is a function of the pressure p and temperature T ; and $\rho(h)$ is the gas concentration.

Spectral analyses usually assume Voigt line shape for individual spectral lines, which is a convolution of the Doppler and Lorentzian line shapes and includes an improper integral. Furthermore, absorption coefficient calculations generally involve summation over a large number of spectral lines (numbering 10^5 in ozone absorption bands, for example), which in essence represents an extra integration. It should be noted that frequency integration is integration of rapidly varying functions. Despite great recent effort to improve algorithms of molecular absorption calculation,^{3,4} direct methods, even used in simple case like our, are very much computationally expensive.

Radiative transfer parameterizations are generally started by assuming the approximation

$$T_{\nu}^f(z, z') = \exp \left\{ -\frac{1}{\mu_0} \tau(z, z') \right\}, \quad (5)$$

where $\mu_0 = 1.66$. As pointed out in Ref. 5, this affects only the downward fluxes in the lower troposphere, with overall error not exceeding 1 W/m^2 .

Further standard step is to divide the frequency integration interval into the subintervals $\Delta\nu$, within which the Planck function can be considered constant, what finally yields equations of the type of (1) and (2), but with $T_{\nu}^f(z, z')$ now meaning the average

transmission function over the spectral interval $\Delta\nu$ (Refs. 1 and 2)

$$T_{\nu}^f(z, z') = \frac{1}{\Delta\nu} \int_{\Delta\nu} \exp \left\{ -\frac{1}{\mu_0} \int_z^{z'} K(\nu, p(h), T(h)) \rho(h) dh \right\} d\nu. \tag{6}$$

Thus, the task of parameterizing the transfer equation is essentially that of parameterizing the transmission function as given by expression (6). Of notice is that the diffusion factor as given by Eq. (5) is not to be necessarily used to parameterize the transfer equation (e.g., see Refs. 6 and 7).

PARAMETERIZATION OF TRANSMISSION FUNCTIONS IN CASE WHEN A SINGLE GAS ABSORBS

A well recognized fact now is that due to poor model representations of the absorption spectra, particularly those of carbon dioxide and ozone absorption, large errors can be obtained.^{1,5,8} For the sake of less errors, the standard Curtis-Godson method⁹ is frequently abandoned with the result being a complicated functional dependence of the transmission function on meteorological parameters, and not always a success. The 1990 intercomparison of radiation codes has demonstrated that calculated data seriously disagree and errors are an order of magnitude higher than the required values, even with a purely molecular atmosphere (with no scattering and clouds present).¹⁰ These discrepancies mostly stem from the difference in used parameterizations of molecular absorption parameters, that enter into the transfer equation.

Using the Laplace transform, the transmission function can be represented as a series of exponentials (in the foreign literature, this method is commonly referred to as the "k-distribution" technique), which transformation increases the approximation accuracy and favors parameter estimation. In addition, the exponential representation of transmission functions is a convenient approximation for solving the transfer equation in a scattering medium.^{11,12}

Upon the Laplace transform, the transmission function takes the following form¹²:

$$T = \int_0^1 \exp \{-\tau(g)\} dg, \tag{7}$$

where $\tau(g)$ is the optical depth, the exponent under the integral in Eq. (6) is

$$g(\tau) = \frac{1}{\nu_2 - \nu_1} \int_{\nu_1}^{\nu_2} W(\nu) d\nu, \tag{8}$$

$$W(\nu) = \begin{cases} 1, & \tau(\nu) < \tau, \\ 0, & \tau(\nu) > \tau. \end{cases} \tag{9}$$

The $g(\tau)$ calculation reduces to summing the intervals for which the condition $\tau(\nu) < \tau$ holds. Consequently, $g(\tau)$ is a monotonically increasing function whose inversion readily yields $\tau(g)$. The numerical implementation is quite trivial. To evaluate $\tau(g)$, it is necessary to calculate the absorption coefficients by uniformly incrementing frequency and then to sort the resulting array in ascending order.

In Refs. 11 and 13, the transmission functions were derived using the relations

$$T = \int_0^{\infty} f(\tau) \exp\{-\tau\} d\tau, \tag{10}$$

where

$$f(\tau_i) = \frac{1}{\nu_2 - \nu_1} \sum_j \left| \frac{\Delta\nu_j}{\Delta\tau_i} \right| W(\tau_i, \tau_{i+1}). \tag{11}$$

The function $W(\tau_i, \tau_{i+1})$ is nonzero (equal to unity) for those spectral intervals where the condition $\tau_i < \tau(\nu) < \tau_{i+1}$ is satisfied. To find out how Eqs. (7)–(9) and Eqs. (10)–(11) are interrelated, we adopt the relation¹²

$$g(\tau) = \int_0^{\tau} f(\vartheta) d\vartheta, \tag{12}$$

from which it follows that

$$f(\tau) = \frac{dg}{d\tau} \Rightarrow f(\tau) \Delta\tau \approx g(\tau + \Delta\tau) - g(\tau). \tag{13}$$

The validity of Eq. (13) rests upon the fact that $g(\tau)$ is a smooth, monotonically increasing, and everywhere differentiable function. From Eqs. (13) and (8) it follows that, to calculate $f(\tau) \Delta\tau$, it is necessary to sum spectral intervals for which the condition $\tau < \tau(\nu) < \tau + \Delta\tau$ is satisfied; thus the relationship between Eqs. (11) and (8) can readily be established. It should be noted that the intermediate $f(\tau)$ calculations lead to extra complication of the numerical realization and, moreover, the numerical differentiation always increases the error. By means of equations (7)–(9), we change from the rapidly varying function $\tau(\nu)$ to the monotonic function $\tau(g)$, and that is all. Any time the atmospheric thermodynamic parameters change, we have to recalculate $\tau(\nu)$ by the LBL method and then convert it to $\tau(g)$; thus, the parameterization problem has not been solved. In this sense, no improvement is gained over traditional LBL method because most computer time goes into the $\tau(\nu)$ computation rather than the frequency integration.^{3,4}

Therefore, $\tau(g)$ parameterization is required in order to cope with the atmospheric variability. That can be done using either the method of reduced absorbing mass^{11,14} "scale approximation" or the c - k -correlation technique^{6,13} which approximates the optical depth as

$$\tau(g, z, z') = \int_z^{z'} K(g, p(h), T(h)) \rho(h) dh, \quad (14)$$

where $K(g, p(h), T(h))$ are the absorption coefficients at frequency g and height h . The c - k -correlation can be qualitatively interpreted as follows: it is valid when the molecular absorption coefficients, corresponding to the same frequency g , have altitude independent positions in the transformed spectrum $k(g)$. To evaluate $K(g)$, it is necessary to calculate $K(n)$ by uniformly incrementing frequency within the interval ν_1 - ν_2 , and then to sort the resulting array in ascending order and to scale the spectral interval by $\Delta\nu$. That is, physically this approximation is based upon the fact that the spectral dependence of molecular absorption coefficient changes quite similarly with altitude for all spectral lines. Slight deviations are to be expected near the centers of weak lines, however their contributions are deemed insignificant under the conditions of the real atmosphere. The validity of c - k -correlation was evaluated numerically in Refs. 6 and 13. The error of transmission function calculation did not exceed 1%.

Because of the smoothness of the integrand in Eq. (7), depending on the quadrature formulas used, 5 to 10 expansion terms are sufficient to evaluate the integral, that is

$$T_v^f(z, z') = \sum_{i=1}^n C_i \times \exp \left\{ -\frac{1}{\mu_0} \int_z^{z'} K(g_i, p(h), T(h)) \rho(h) dh \right\}. \quad (15)$$

Based on our previous experience, a few fixed pressures and temperatures are sufficient to calculate an array of absorption coefficients $K(g_i, p_j, T_k)$, and in turn the number 10^3 of the latter is sufficient to calculate transmission functions for a wide range of atmospheric conditions.

Figures 1 and 2 show typical altitude and temperature behaviors of the absorption coefficients.

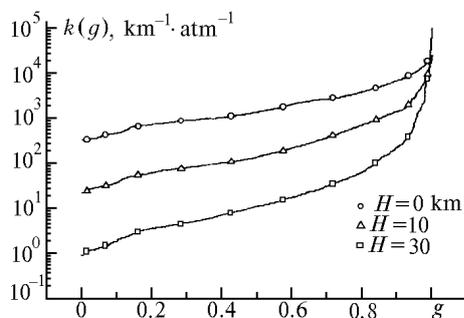


FIG. 1. Altitude behavior of the coefficient $k(g)$.

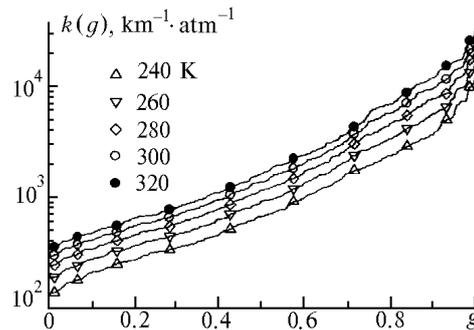


FIG. 2. Temperature dependence of absorption coefficient. Circles show $k(g)$ values corresponding to the Gaussian quadrature nodes.

OVERLAPPING ABSORPTION BANDS

It can be stated that many approaches and methods have recently been developed that allow fairly efficient parameterization of the transmission function for the case of inhomogeneous atmosphere, however provided a single absorbing gas is considered.

When absorption bands of two or more gases overlap, total transmission is approximated as a product of transmission functions of individual gases. This is the approximation deficiency, because the multiplication of transmission functions as exponential series results in exorbitant number of expansion terms, which is highly critical in the climate studies^{1,16} and, moreover, is fraught with uncertainty. Figure 3 shows an example of transmission function calculation by direct method for overlapping absorption bands of H_2O and CO_2 , and Figure 4 gives the approximation error that can amount to 3-4%.

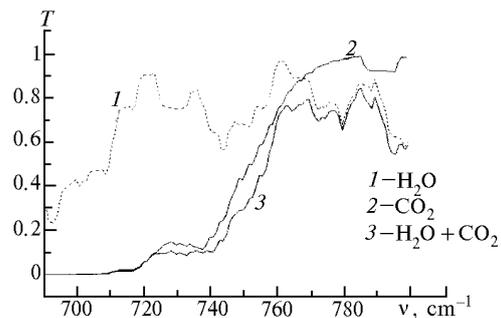


FIG. 3. Transmission spectrum of vertical atmospheric path 0-50 km. The spectral resolution is 10 cm^{-1} . LBL calculation by midlatitude summer meteorological model.

An interesting method of treating overlapping absorption bands of two gases has been suggested in Ref. 6. In essence, transmission function for a single gas can be considered as a transform of $f(k)$; therefore, for absorption of two gases a convolution-type expression

$$g(k) = \int_0^k g_1(k - k') g_2(k') dk' \tag{16}$$

is valid.

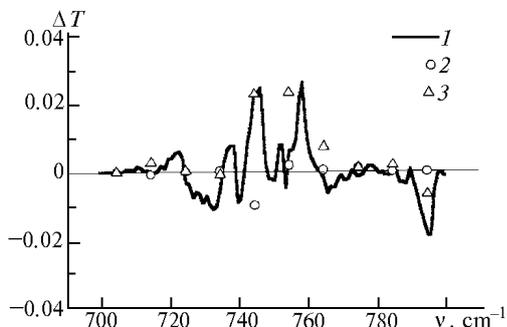


FIG. 4. Errors of using different approximations for treating overlapping H₂O and CO₂ absorption bands: the total transmission function as a product of H₂O and CO₂ transmission functions (1); midlatitude summer (2) and highlatitude winter (3) models.

On the one hand, this expression improves the above deficiency by not producing many terms due to exponential expansion of transmission function; but on the other hand, a detailed information on $g_1(k)$ and $g_2(k)$ is required now to evaluate integral (16).

We decided not to use the traditional method of treating overlapping absorption bands as the product of transmission functions. Our approach to this problem has been detailed elsewhere¹⁵; so only basic features are repeated below. For simplicity, we will consider a homogeneous atmospheric path. In the case of two absorbing gases, the transmission function can be represented as

$$T(U_1, U_2) = \frac{1}{\Delta\nu} \int_{\nu_1}^{\nu_2} \exp \{-K_1(\nu) U_1 - K_2(\nu) U_2\} d\nu. \tag{17}$$

In principle, a one-dimensional Laplace transform can be applied to Eq. (17) to produce an expression similar to Eq. (7), with a total optical depth given by $\tau(g) = k_1(g) U_1 + k_2(g) U_2$. Clearly, to calculate $\tau(g)$, the latter is to be invoked every time U_1 and U_2 change.

Our suggestion is that, when the spectra of different gases are partially correlated, the total transmission function might be represented as

$$T_A(U_1, U_2) = \int_0^1 \exp \{-k_1(g) U_1 - \varphi_2(g) U_2\} dg \tag{18}$$

with unknown function $\varphi_2(g)$, being subject to the condition

$$T_A(U_1 = 0, U_2) = \int_0^1 \exp \{-\varphi_2(g) U_2\} dg = \int_0^1 \exp \{-k_2(g) U_2\} dg \tag{19}$$

which makes relation (18) exact for either $U_1 = 0$ or $U_2 = 0$. This latter condition provides a relation between $\varphi_2(g)$ and $k_2(g)$, namely

$$k_2^{-1}(g) = g(k_2) = \int_0^1 W_\varphi(g) dg, \tag{20}$$

where

$$W_\varphi(g) = \begin{cases} 1, & \varphi(g) < k_2, \\ 0, & \varphi(g) > k_2. \end{cases} \tag{21}$$

Relations (20)–(21) do not provide a scheme of constructing $\varphi_2(g)$. So, we took a purely phenomenological path of constructing this unknown function. It was assumed that $\varphi_2(g)$ is a smooth, unimodal curve and can be derived from $k_2(g)$ by transforming the latter in accordance with condition (21). This transformation is feasible in view of the fact that integral transformation (19) admits an ambiguity. A typical view of $\varphi_2(g)$ appears in Fig. 5.

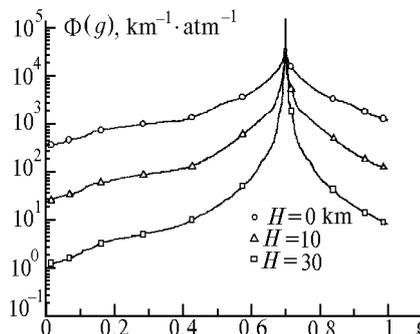


FIG. 5. Typical view of the function $\varphi_2(g)$.

We have found that, as a rule, transmission of the mixture is overestimated once the function peaks at $g_0 = 1$, and underestimated once $g_0 = 0$. Conversely, using unimodal curve to represent $\varphi_2(g)$, the approximation expression and exact calculation can be brought into much closer agreement by varying g_0 . More complex shapes of the function $\varphi_2(g)$ are possible with more expansion terms retained.

The position of the maximum is determined from the condition

$$\int_0^\infty \int_0^\infty [T_A(U_1, U_2) - T(U_1, U_2)]^2 dU_1 dU_2 = \delta \rightarrow \min. \tag{22}$$

Applying Gaussian quadratures to Eq. (17), the exponential series can be obtained

$$T_A(U_1, U_2) = \sum_{i=1}^n C_i \exp\{-k_1(g_i) U_1 - \varphi_2(g_i) U_2\}. \quad (23)$$

As numerical simulations have shown, ten expansion terms will be sufficient.

Figure 4 shows the error of transmission function calculation from formula (23) in comparison with the direct calculation,¹⁸ by using spectral line parameters from HITRAN-92 atlas^{19,20} for zonal-mean meteorological models.²¹ The position of the center of the function $\varphi_2(g)$ was determined for the meteorological conditions corresponding to the midlatitude model. Change of the meteorological conditions caused larger error, random in character and not exceeding the errors due to multiplication of transmission functions of individual gases. Subsequent averaging over wider spectral interval substantially reduces the error.

MAIN CONCLUSIONS

With the method presented here, a 10-term expansion can be successfully used to represent the transmission function with any spectral resolution.

A range of possible atmospheric meteorological conditions is accounted for by representing the absorption coefficient as a matrix $K(g_k, P_m, T_n)$, $k=1, 10$; $m=1, 20$; $n=1, 5$. Altitude integration is performed using a spline function.

In comparison with LBL technique, the error due to the present method does not exceed 1%, increasing slightly when different gases have considerably overlapping absorption bands. Subsequent averaging over a wider spectral interval reduces the error.

ACKNOWLEDGMENT

The work was partially supported by the Russian Foundation for Fundamental Research (under grants No. 96-05-64293, 96-15-98476).

REFERENCES

1. G.L. Stephens, *Monthly Weather Review* **112**, 826–867 (1984).
2. Y. Fouquart, in: *Physically-based Modeling and Simulation of Climate and Climatic Change*. Part 1, Shlesinger M.E., ed. (Kluwer Academic Publishers, 1988), pp. 223–283.
3. B.A. Fomin, "Effective line-by-line technique to compute radiation absorption in gases, B Preprint IAE-5658/1, Russian Research Center "Kurchatov Institute", Moscow (1993).
4. A.A. Mitsel' and K.M. Firsov, *J. Quant. Spectrosc. Radiat. Transfer* **54**, 549–557 (1995).
5. E.V. Rozanov, Yu.M. Timofeev, and A.N. Trotsenko, *Izv. Akad. Nauk SSSR, Fiz. Atmos. Okeana* **26**, No. 6, 602–606 (1990).
6. R. Goody, R. West, L. Chen, and D. Crisp, *J. Quant. Spectrosc. Radiat. Transfer* **42**, No. 6, 539–550 (1989).
7. S.D. Tvorogov, *Atmos. Oceanic Opt.* **10**, Nos. 4–5, 249–254 (1997).
8. W.-C. Wang and G.-Yu. Shi, *J. Quant. Spectrosc. Radiat. Transfer* **39**, No. 5, 387–397 (1988).
9. M. Chou and L. Kouvaris, *J. Geophys. Res.* **96**, No. D5, 9003–9012 (1991).
10. Y. Fouquart, B. Bonnel, and V. Ramaswamy, *J. Geophys. Res.* **96**, No. D5, 8955–8968 (1991).
11. M.D. Chou and A. Arking, *J. Atmos. Sci.* **38**, 798–807 (1981).
12. S.D. Tvorogov, *Atmos. Oceanic Opt.* **7**, No. 3, 165–171 (1994).
13. A. Lacis and V. Oinas, *J. Geophys. Res.* **96(D)**, No. 5, 9027 (1991).
14. K.M. Firsov and A.B. Smirnov, *Atmos. Oceanic Opt.* **8**, No. 8, 659–662 (1995).
15. K.M. Firsov and A.A. Mitsel', in: *Proc. of the XIIth International Symposium on High-Resolution Molecular Spectroscopy (SPIE)*, pp. 361–366.
16. V.Ya. Galin, "Formation of the thermal radiative fluxes in the atmospheric general circulation model, B Preprint No. 75, Department of Computational Mathematics, USSR Academy of Sci. (1984).
17. Ph. Rivere, A. Soufiani, and J. Taginet, *J. Quant. Spectrosc. Radiat. Transfer* **48**, No. 2, 187–203 (1992).
18. A.A. Mitsel', I.V. Ptashnik, K.M. Firsov, and B.A. Fomin, *Atmos. Oceanic Opt.* **8**, No. 10, 847–849 (1995).
19. L.S. Rothman, R.R. Gamache, A. Goldman, et al., *Appl. Opt.* **26**, 4058–4097 (1987).
20. L.S. Rothman, R.R. Gamache, R.H. Tipping, et al., *J. Quant. Spectrosc. Radiat. Transfer* **48**, 469–507 (1992).
21. V.E. Zuev and V.S. Komarov, *Statistical Models of Atmospheric Temperature and Gaseous Constituents (Gidrometeoizdat, Leningrad, 1986)*, 264 pp.