Optimization of the line-by-line algorithm for calculation of molecular absorption

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Received November 8, 2000

Four well-known algorithms for calculation of the Voigt profile [R.J. Wells, J. Quant. Spectrosc. Radiat. Transfer **62**, 29–48 (1999); M. Kuntz and M. Hopfner, J. Quant. Spectrosc. Radiat. Transfer **63**, 97–114 (1999); J. Humlicek, J. Quant. Spectrosc. Radiat. Transfer **27**, 437 (1982); and S.R. Draison, J. Quant. Spectrosc. Radiat. Transfer **16**, No. 7, 611–614 (1976)] are compared in the speed and accuracy. It is shown that the Draison's algorithm provides the best results. Simple estimating equations are given for optimization of the rule of transition from one grid to another in a multigrid algorithm [B.A. Fomin, "*Effective line-by-line technique to compute radiation absorption in gases*," Preprint IAE–5658/1 (Russian Research Center "Kurchatov Institute," Moscow, 1993); B.A. Fomin, J. Quant. Spectrosc. Radiat. Transfer **53**, 663–669 (1995)] for the line-by-line method.

Introduction

The line-by-line method for calculation of the absorption characteristics of a gaseous medium[1] is known as a reference one and used both for verification of various approximate transmission models and for direct simulation of radiative transfer in molecular absorbing media. In this connection, development of new highly efficient algorithms is an urgent problem being of considerable interest for specialists. In this paper, we compare several algorithms for calculation of the Voigt profile and describe further development of one of the most efficient algorithms for speeding up the line-by-line method – the so-called multigrid algorithm.[2,3]

Comparison of algorithms for calculation of the Voigt profile

Calculation of line profiles is the most computationally expensive part in calculating the integral transmittance. Choosing the highest-speed and, at the same time, most accurate algorithm for calculation of the Voigt profile, one can achieve significant speedup of the line-by-line program. In this paper, we consider four algorithms: Wells–99 (Ref. 4), Kuntz–99 (Ref. 5), Humlicek–82 (Ref. 6), and Draison–76 (Ref. 7).

The table compares these algorithms in the time consumed by each of them for calculation of the Voigt profile. The results are given both for the possible extreme values of x and y and for two actual conditions of calculation

$$V(x, y) = \frac{y}{\pi} \int_{-\infty}^{+\infty} \frac{\exp(-t^2)}{(x - t)^2 + y^2}\, dt,$$

where $x = \sqrt{\ln 2}\,(\nu - \nu_0)/\gamma_D$ and $y = \sqrt{\ln 2}\,\gamma_L/\gamma_D$ are the dimensionless parameters; $\nu - \nu_0$ is frequency detuning from the line center; γ_L and γ_D are, respectively, the Lorentz and Doppler line halfwidths at halfmaximum. The results for actual conditions were obtained for vertical paths of 0–10 and 0–100 km in the spectral region of 1000–1005 cm^{-1} for the gases H_2O, CO_2, and O_3.

Table. Time needed to different algorithms for computation of the Voigt profile, in rel. units

Computational conditions	Draison–76	Humlicek–82	Kuntz–99	Wells–99
$x = 0$; $y = 0.001$	19.0	16.0	19.1	20.7
$x = 0$; $y = 50$	4.2	7.1	4.2	8.8
$x = 50$; $y = 0.001$	3.5	8.9	4.4	13.1
$x = 50$; $y = 50$	3.5	8.0	4.3	8.8
Actual conditions:				
(0–10 km)	6.2	8.6	7.0	9.3
(0–100 km)	89.0	154.0	115.0	195.0

The table shows that it makes sense to combine the advantages of the Humlicek–82 algorithm in the range of small x and y with the advantages of the Kuntz–99 or Draison–76 algorithm in the range of large x and y. Under actual conditions, the Draison–76 and Kuntz–99 algorithms are likely the most time-saving. However, when using the Draison algorithm, it should be modified, because the initial algorithm does not allow simultaneous calculation at an array of values of the parameter x (Ref. 7).

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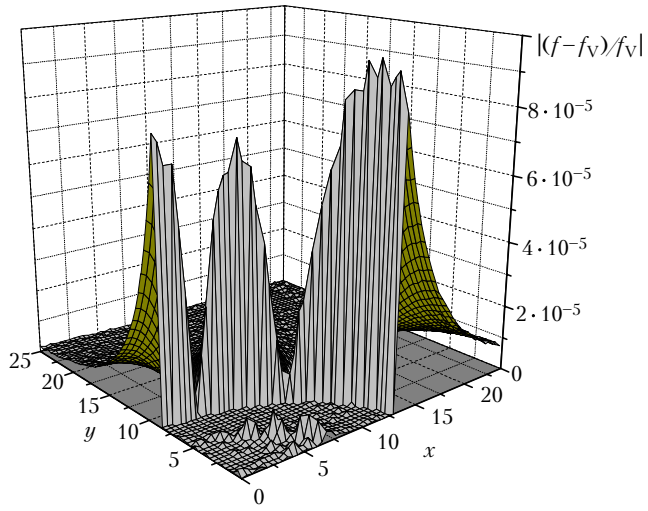

Fig. 1. Relative error of the Wells–99 algorithm (Ref. 4).

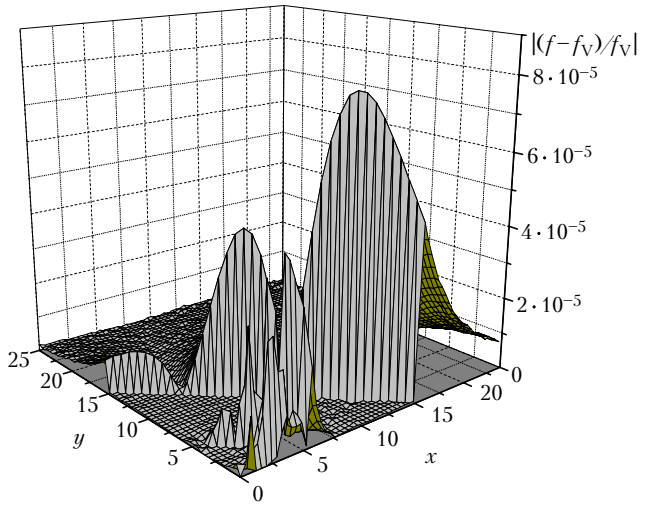

Fig. 2. Relative error of the Kuntz–99 algorithm (Ref. 5).

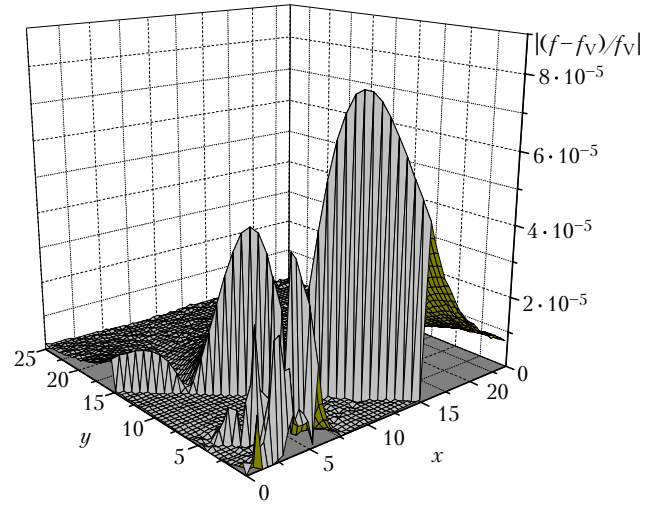

Fig. 3. Relative error of the Humlicek–82 algorithm (Ref. 6).

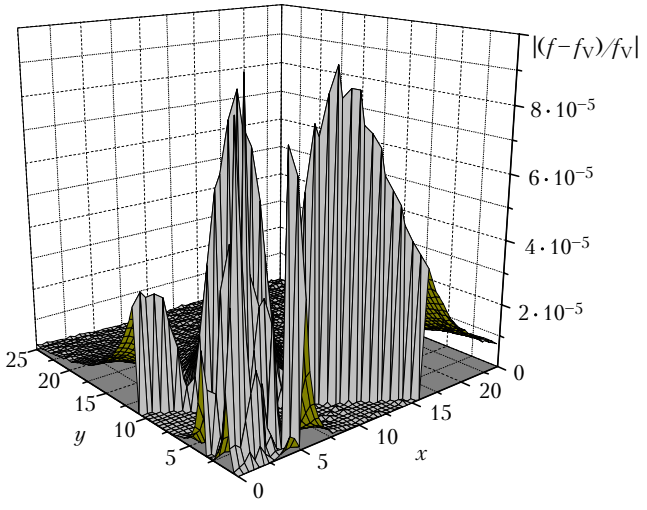

Fig. 4. Relative error of the Draison–76 algorithm (Ref. 7).

The results of comparison of the algorithms in the accuracy are shown in Figs. 1–4. The calculated results were compared with the results of exact numerical calculation of the Voigt profile f_V. The maximum error of the Draison–76 algorithm in our calculations was half as much as the error of the Schreier algorithm.[8] It is seen that the maximum errors of all the four algorithms in the range x, $y < 20$ differ insignificantly (no more than by 30%) and are sufficiently small for these algorithms could be used in the line-by-line calculations. Only in the range x, $y < 5$ the Wells algorithm has a marked advantage in the accuracy but loses in the computational time.

It is worth noting that the Kuntz–99 and Humlicek–82 algorithms insignificantly differ in accuracy.

Optimization of the frequency grid

When calculating the integral transmittance, one has to calculate the spectral transmittance T_ν at some frequency grid. The simplest grid is uniform. It allows the integral transmittance to be calculated with high accuracy, but the time needed for calculation is inversely proportional to the grid step.

As was mentioned above, calculation of line profiles is computationally expensive. Therefore, the efficiency of the line-by-line algorithms can be improved by optimizing (minimizing without loss in accuracy) the number of points at which the profile of each line is to be calculated. This is possible in principle, because the line profile becomes smoother far from the line center.

In this paper we consider a highly efficient, convenient, and illustrative multigrid method proposed by Fomin (Refs. 2 and 3) and used in Refs. 5 and 11. This method uses a set of uniform grids with doubling steps h_i:

$$h_l = h_0\, 2^l, \quad l = 0, \ldots, L;$$

$$\nu_j^{(l)} = \nu_{\text{in}} + h_l\, j, \quad j = 0, 1, \ldots,$$

where h_0 is the step of the finest grid (which is chosen based on the mean line halfwidth under given conditions and the needed accuracy); l is the grid number; L is the number of the coarsest grid; ν_{in} is the initial frequency of the computational region. One can see that eleven grids are enough to increase the step from 0.001 cm^{-1} (characteristic width of a line in the upper atmosphere) to 1 cm^{-1}, i.e., three orders of magnitude. The absorption coefficients are calculated at the grid nodes. The number of the grid, at which the contribution of a specific line is calculated, increases with the distance from the line center. In such an approach, the profile of each line is calculated independently of other lines. Figure 5 schematically illustrates the grid expansion of a line profile. This illustration is borrowed from Ref. 2.

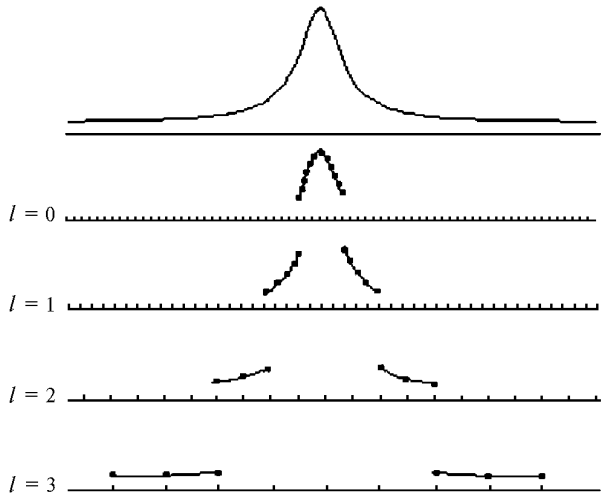

Fig. 5. Illustration of the multigrid algorithm for calculation of transmittance.[2]

Thus, the contribution of any line is summed separately at its own grid for every part of the profile.

Once all lines are considered, the recurrent procedure recalculates the contributions from coarse grids to finer ones. This procedure is based on a simple square (or linear) interpolation; it allows the sought absorption coefficient to be finally determined at the nodes of the finest grid. This procedure is executed only once and, as a rule, for the time negligibly short as compared to the complete computational time.

Implementation of the described multigrid algorithm minimizes the time needed for calculation of the spectral transmittance without loss in accuracy. The gain in time due to use of the multigrid algorithm can be more than an order of magnitude.[2,3]

The further development of this method is in optimization of the rule of transition from a coarse grid to a finer one. In Ref. 2, such a transition is carried out when there are less than three steps of the used grid from the current point to the line center. This rule gives an error no higher than 1% at square interpolation and the finest grid step $h_0 = \gamma_V/4$, where γ_V is the Voigt halfwidth. Disadvantages of this approach are fixed accuracy and independence of the transition coordinates on the halfwidth of a specific line. Another transition rule was proposed in Refs. 5 and 10. It is based on exact numerical determination of the maximum error in the square three-point interpolation of a profile. In this paper, we propose an algorithm based on the approximate but simple estimation of the maximum grid step providing the needed relative error in the square interpolation of the Voigt profile at a given distance from the line center. The transition to a coarse grid is carried out in the case that with the distance from the line center the step needed to achieve the required accuracy becomes larger than or equal to the grid step. This allows us to avoid calculations at unnecessary points.

In this paper, we use the approximation of the absorption coefficient for a line with the Voigt profile (this approximation was proposed in Ref. 12 and described in Ref. 8):

$$K(\tilde{x},\tilde{y},y)=\frac{S}{\gamma_D}\sqrt{\frac{\ln 2}{\pi}}V(0,y)\{[1-\tilde{y}]G(\tilde{x})+\tilde{y}L(\tilde{x})\}, \quad (1)$$

where $G(\tilde{x}) = \exp(-\ln 2\,\tilde{x}^2)$; $L(\tilde{x}) = 1/(1+\tilde{x}^2)$; $\tilde{x} = (\nu-\nu_0)/\gamma_V$; $\tilde{y} = \gamma_L/\gamma_V$; S is the line intensity.

Let us consider the case of square interpolation of an individual line at a grid with the step $\tilde{h} = \Delta\nu/\gamma_V$. The relative error δ of the square interpolation of the function $K(\tilde{x})$ at some point $\tilde{x}$ is described by the equation[9]:

$$\delta = \frac{\tilde{h}^3}{6K(\tilde{x})}\,q\,(q-1)\,(q-2)\,\mu_3, \quad (2)$$

where

$$\mu_3 = |K'''(\tilde{x})| = \Bigg| 12\,K(0,\,y)\times$$

$$\times\left\{\ln^2 2\cdot\tilde{x}\cdot\exp\,(-\ln 2\,\tilde{x}^2)(1-\tilde{y})(1-2/3\,\ln 2x^2)+\right.$$

$$\left.+\,2\,\tilde{x}\,\tilde{y}\,\frac{1-\tilde{x}^2}{(1+\tilde{x}^2)^4}\right|\Bigg\} \quad (3)$$

is the third derivative of the function $K(\tilde{x})$ at some intermediate point in the interval $[\tilde{x}_i;\,\tilde{x}_i+2\tilde{h}]$, $q = (\tilde{x}-\tilde{x}_i)/\tilde{h}$. Here $\tilde{x}_i$ and $\tilde{x}$ $(\tilde{x}-\tilde{x}_i \le 2\tilde{h})$ are the frequencies of the ith node point and the point of interpolation, respectively. Assuming that the third derivative and the function itself vary only slightly within the interval $[\tilde{x}_i;\,\tilde{x}_i+2\tilde{h}]$, we take the value of the third derivative at the point $\tilde{x}_i$ (i.e., $K'''(\tilde{x}_i)$) as its maximum value. Obviously, this assumption is true for the most part of the profile. This approximation can only slightly overestimate the value of the maximum error in the interval $[\tilde{x}_i;\,\tilde{x}_i+2\tilde{h}]$. Then let us find the maximum value of the product $q\,(q-1)\,(q-2)$. Differentiating it in terms of dq, we can find $\max[q(q-1)(q-2)] = 2/(3\sqrt{3})$ at $q_{max} = 1-\sqrt{1/3}$.

Based on these results and substituting Eq. (3) into Eq. (2), we derive the equation for the optimal (maximum) grid step $\tilde{h}_\delta$ providing the relative error δ at a given distance $\tilde{x}$ from the line center:

$$\tilde{h}_\delta = \frac{\sqrt{3}}{2} \times \left| (2\delta[(1 - \tilde{y}) \exp(-\ln 2\tilde{x}^2) + \tilde{y}/(1 + \tilde{x}^2)])/ \right.$$

$$/(\ln^2 2\tilde{x} \exp(-\ln 2\tilde{x}^2)(1 - \tilde{y}) (1 - \frac{2}{3} \ln 2\tilde{x}^2) +$$

$$\left. + 2\tilde{y}\tilde{x}(1 - \tilde{x}^2)/(1 + \tilde{x}^2)^4) \right|^{1/3}. \qquad (4)$$

When solving Eq. (4) for $\tilde{x}$ at given $\tilde{y}$ and δ, we can find the coordinates $\tilde{x}_l$ of transitions from fine grids to coarse ones for a given set of the grids $\tilde{h}_l$.

Figure 6 shows the grid step (expressed in halfwidths) providing the relative error of interpolation $\delta = 0.001$ as a function of the distance to the line center. The case $\tilde{y} \ll 1$ corresponds to prevalence of the Doppler broadening of an absorption line, and the case $\tilde{y} \sim 1$ corresponds to the Lorentz broadening. It is seen that at $\tilde{y} < 0.5$ the minimum optimal grid step providing the given accuracy of interpolation can be rather far from the line center – at a distance larger than 3 halfwidths. As the case of purely Lorentz broadening is approached, the position of the optimal grid step minimum approaches the distance ~0.36 $\gamma_V \approx 0.36\ \gamma_L$ from the line center.

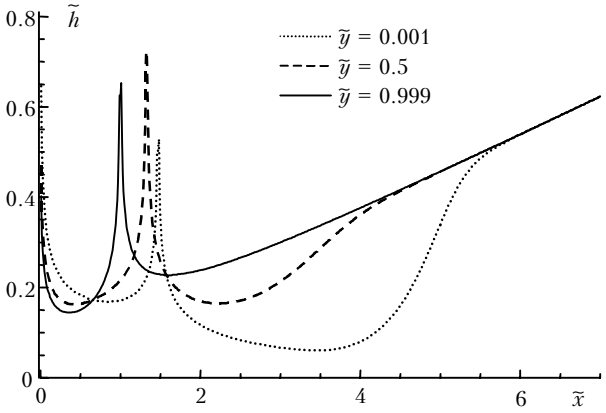

Fig. 6. Optimal grid step providing the relative error of the square interpolation $\delta = 0.001$ as a function of the distance to the line center for the Voigt profile at different $\tilde{y} = \gamma_L/\gamma_V$.

Peaks in Fig. 6 (and the symmetric peaks in the region of negative $\tilde{x}$ that are not shown in this figure) correspond to the zero of the third frequency derivative of the Voigt profile, i.e., profile inflection, and are due to the used approximation. Obviously, these peaks can be ignored.

The absorption coefficient $K(\nu)$ not always is the final sought parameter; it is often used for calculation of the optical thickness $T(\nu) = \exp\{-K(\nu) L\}$ (L is the path length), whose relative error δT is proportional to the absolute error of the absorption coefficient ($dT/dK = T L \Rightarrow \Delta T/T \equiv \delta T = \Delta K L$). Therefore, it is worth using the equation for the step providing a given absolute error Δ:

$$\Delta = \frac{\tilde{h}^3}{6} q (q - 1) (q - 2) \mu_3 ,$$

wherefrom we can obtain

$$\tilde{h}_\Delta = \frac{\sqrt{3}}{2} \times \left| (2\Delta)/(K_0[\ln^2 2\tilde{x} \exp\{-\ln 2\tilde{x}^2\}(1 - \tilde{y}) \times \right.$$

$$\left. \times (1 - \frac{2}{3} \ln 2\tilde{x}^2) + 2\tilde{y}\tilde{x}(1 - \tilde{x}^2)/(1 + \tilde{x}^2)^4) \right|^{1/3}, \qquad (5)$$

where K_0 is the absorption coefficient at the line center. It is equal to $S\sqrt{\ln 2/\pi}\, K(0, y)/\gamma_D$ for the Voigt profile. The plots of $\tilde{h}_\Delta(\tilde{x}, \tilde{y})$ for $\Delta/K_0 = 0.0001$ are shown in Fig. 7. One can see from the figure that the minimum of the optimal step is within $(0.4–0.7)\gamma_V$ from the line center as $\tilde{y}$ varies within wide limits (from 0.001 to 0.999).

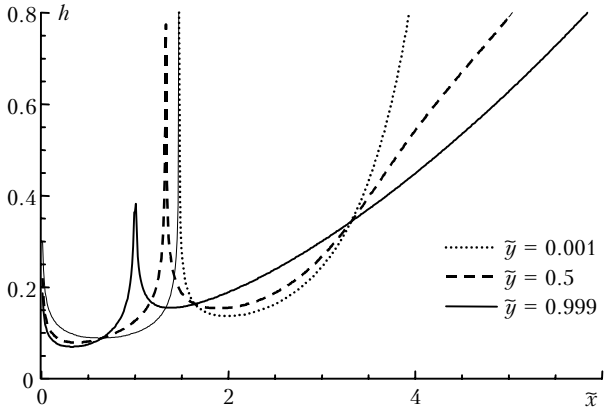

Fig. 7. Optimal grid step providing the absolute error of the square interpolation $\Delta = 10^{-4} K_0$ as a function of the distance to the line center for the Voigt profile at different $\tilde{y} = \gamma_L/\gamma_V$.

Conclusions

In this paper, we have compared several available algorithms for calculation of the Voigt profile. The best performance (in combination of two parameters: computational speed and accuracy) was demonstrated by the Draison algorithm.

The estimating equations for optimization of the rule of transition from one grid to another in the multigrid algorithm are obtained. The advantage of these equations is their simplicity, although they are insufficiently exact.

It should be noted that it is suffice to solve the equation like Eq. (4) (i.e., for the fixed relative error of interpolation) only once for all spectral lines of a given gas, because it weakly depends on $\sqrt{\ln 2}\ \gamma_L/\gamma_D$.

In the case of fixed absolute error of interpolation, the equation like Eq. (5) should be solved individually for every line (or for a set of lines with close values of

K_0). By this reason, the step of the finest grid (determined by the minimum value of the optimal step) in the case (4) is almost the same for all lines, whereas in the case (5), the parameters of the line having the maximum value of K_0 should be used for its calculation.

Acknowledgments

This work was partially supported by the Russian Foundation for Basic Research within the framework of the Project No. 00–07–90175.

References

1. H.J.P. Smith, D.J. Dube, M.E. Gardner, S.A. Clough, F.X. Kneizys, and L.S. Rothman, "*FASCOD – Fast Atmospheric Signature Code (Spectral Transmittance and Radiance)*," Rep. AFGL–TR–78–0081 (Air Force Geophys. Lab., Hanscom., Mass., USA, 1978).
2. B.A. Fomin, "*Effective line-by-line technique to compute radiation absorption in gases*," Preprint IAE–5658/1, Russian Research Center "Kurchatov Institute," Moscow (1993), 13 pp.
3. B.A. Fomin, J. Quant. Spectrosc. Radiat. Transfer **53**, 663–669 (1995).
4. R.J. Wells, J. Quant. Spectrosc. Radiat. Transfer **62**, 29–48 (1999).
5. M. Kuntz and M. Hopfner, J. Quant. Spectrosc. Radiat. Transfer **63**, 97–114 (1999).
6. J. Humlicek, J. Quant. Spectrosc. Radiat. Transfer **27**, 437 (1982).
7. S.R. Draison, J. Quant. Spectrosc. Radiat. Transfer **16**, No. 7, 611–614 (1976).
8. F. Schreier, J. Quant. Spectrosc. Radiat. Transfer **48**, Nos. 5/6, 743–762 (1992).
9. R.W. Hamming, *Numerical Methods for Scientist and Engineering* (Mc Graw-Hill Book Company, Inc., New York – San Francisco – Toronto – London, 1962).
10. L. Sparks, in: *Optical Remote Sensing of the Atmosphere*. Vol. 2. OSA Technical Digest Series (Optical Society of America, Washington, DC., 1995), pp. 68–70.
11. A.A. Mitsel', I.V. Ptashnik, K.M. Firsov, and B.A. Fomin, Atmos. Oceanic Opt. **8**, No. 10, 847–850 (1995).
12. E.E. Whiting, J. Quant. Spectrosc. Radiat. Transfer **8**, 1379 (1968).