Simple atmospheric transmittance calculation based on Fourier-transformed Voigt profile

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Abstract-- A method of line-by-line transmission calculation for a homogeneous atmospheric layer using the Fourier-transformed Voigt profile is presented. The method is based on a pure Voigt function with no approximation and an interference term which takes into account the line mixing effect. The method can be used to calculate transmittance considering each line shape under the effects of temperature and pressure using the line database with an arbitrary wave number range and resolution. To show that the method is feasible for practical model development, the calculated transmittance was compared with that obtained using a conventional model and a good consistency was observed.

1. Introduction

The line-by-line atmospheric absorption calculation generally requires line shapes derived by Voigt function calculation. The Voigt function is presented as an integral form, and the direct computation of the Voigt profiles involves a high computational cost for line-by-line calculation. The calculation of the

Voigt function becomes sufficiently rapid for a small number of lines upon using a proper approximation method such as Drayson's method[1] which partitions the x-y domain of the function into several regions and uses a polynomial for the approximation of each region. There are many variants of the partitioning /approximating method and newer ones are more sophisticated, for example, as summarized by Wells.[2]

Another approach is to use Fourier-transform methods for calculating absorption line shapes in the Fourier space. The Fourier-transform methods require higher computation cost than the approximation methods; however, the use of Fourier-transform methods gives rise to the possibility of avoiding the disadvantages caused by approximating the Voigt function. The calculational advantages of the Fourier-transform method, for example, that the overlap of line shapes can be represented as a simple sum in the Fourier space and that the mapping of the line shapes, defined by various line centers onto equally spaced wave number calculation points is not necessary, are still considerable.

When the atmospheric absorption line shape is represented as a pure Voigt profile, we can use the directly Fourier-transformed, not approximated, Voigt function. Armstrong[3] showed the expression of the Voigt function in the Fourier-transform style, and Karp[4] applied the Fourier-transformed Voigt function to the calculation of the line absorption coefficient. Kobayashi,[5] following Karp's method, introduced a new method which can considerably reduce the total number of calculations. However,

this study concerned only with the calculation of the Voigt profile.

Here, we demonstrate that the method is feasible for atmospheric applications, taking into account the molecular mass, optical path length, temperature, pressure, temperature/pressure-dependent line intensity, and also the interfered line shape caused by the line-mixing effect. The model should be evaluated using experimental data or atmospheric observation data; however, a preliminary consistency check with a conventional line-by-line model was performed.

2. Transmittance Calculation Using Fourier-Transformed Voigt Function

The optical depth τ for a homogeneous path is given by the product of the line intensity, the Voigt function, and the column density of the molecules using discrete Fourier transform. For multiple *j* lines with a total number of *w*, we obtain discrete Fourier-transform-style optical depth as the real part of the following equation using the Voigt profile calculation algorithm of Kobayashi:

$$\tau = \frac{1}{n^{1/2}} k_s \alpha_h \sum_{r=1}^{n} \sum_{j=1}^{w} \frac{1}{\nu_{0j}} a_{rj} I_j b_s \exp\left[2\pi i (r-1)(d-1)/n\right], \qquad (1)$$

where ν_{0j} is the line center of line j, I_j is the line intensity and b_s is the column molecular number density (molecule/m^2). The *d* is calculation step for the *f(t)* to make the numerical list of a_{rj} of length *n* for the *j*-th line and k_s is the scaling coefficient derived by Kobayashi when *f(t)* is defined as

$$f(t) = \exp\left[-y(t\nu) - (t\nu)^2/4\right] \exp\left(-it\nu\alpha_h\right)\nu, \qquad (2)$$

where ν is the line center of the *j*-th line normalized by ν_{max} which is the maximum wave number of the calculation range. In the practical case, length of the numerical list should be defined considering the

fast-Fourier-transform, and it can be adjusted using the method provided by Kobayashi.[5] In Eq.(2), y is the ratio of Lorentz to Doppler widths:

$$y = \frac{\alpha_L}{\alpha_D}(\ln 2)^{1/2}, \tag{3}$$

and the a_h is defined as

$$\alpha_h = \left(\frac{Mc^2}{2kT}\right)^{1/2}, \tag{4}$$

where M is the molecular weight (kg), and k, c, and T are the Boltzmann constant, speed of light, and temperature respectively.

Hence, we call the present method the line-by-line calculation using the Fourier-transformed Voigt function (L2FTV). The validation of the L2FTV should be performed by model accuracy analysis in comparison with atmospheric-observation data. In this study, however, we perform the method consistency check through comparison with an atmospheric transmission model. The FASCOD[6] was selected as the reference. Figure 1 shows an example of the results of the FASCOD and the L2FTV where temperature dependence of the line intensity was formulated following Rothman et al.[7] The dashed line represents the result from the FASCOD, and the solid line that from the L2FTV. The line plotted at the bottom of the figure is the difference between the results of the two models. Apparently, the differences at each end of the calculation band are caused by the effects of the high-intensity lines positioned in the outer range and are not considered in the L2FTV calculation. When excluding these differences, the figure shows a good agreement between the results of the FASCOD and the L2FTV.

The corresponding line peak values are identical when neglecting the very small computational error (discrepancy is less than 10^{-4}). There are still slight differences between the line shapes; however, considering that the L2FTV is based on the nonapproximated Voigt function, the discrepancy may be caused by the different implementations applied to the Voigt function.

3. Approximation Method of the Line Mixing Effect in the Fourier Space

Sometimes the line mixing effect is significant and should not be neglected in a certain wave number region in atmosphere, even if the pressure is 1 atm. or less.[8] Here, we follow Rosenkranz's line mixing formulation.[9] He showed a formula for the overlapping lines band shape under the first-order approximation of pressure and also assumed no first-order frequency shift of lines. When pressure P is constant, the band shape F is presented as

$$F = \sum_j \Phi_j d_j^2 \frac{P w_{jj} + (\nu - \nu_j) W_j}{(\nu - \nu_j)^2 + (P w_{jj})^2} \quad , \qquad (5)$$

where

$$W_j = 2P \sum_{k \neq j} \frac{d_k / d_j w_{kj}}{\nu_j - \nu_k} \quad . \qquad (6)$$

In Eq.(5), d_j is the amplitude of the jth line, Φ_j is the fractional population of the initial state associated

with the line, and w_{kj} is the transition rate matrix elements. Equation (5) can be regarded as a sum of two terms: the first term of the numerator, which shows the Lorentzian shapes, and the second term of the numerator, which represents the contribution of the line mixing effect. Then we can introduce the line mixing effect as compensation for the Lorentzian shapes which can be calculated by the method described above, using conventional line data. This method may be applicable when the pressure is relatively low and the valleys between lines are not negligible, such as in the case of the transmittance calculation between the ground and space.

Since the Voigt function is regarded as a convolution of the Lorentzian shape and the Doppler shape, we can replace the Lorentzian part with the modified Lorentzian which accompanies a compensation term, and can introduce a modified Voigt function. The L2FTV calculates each line shape using the Voigt function in the Fourier space, so we can obtain the line shape interfered by the line mixing effect, using the modified Voigt function. The Voigt function $K(x,y)$ is defined as

$$K(x,y) = \frac{y}{\pi}\int_{-\infty}^{\infty} \frac{\exp(-t^2)}{y^2 + (x-t)^2} dt \quad . \qquad (7)$$

First, considering the Rosenkranz formula, we introduce a function in which the numerator of the Lorentzian part is replaced with $y+W(x-t)$. This replacement means that the diagonal element of the transition rate matrix w_{jj} is represented as y which can be calculated from the line data taking into account pressure and temperature; then we can expect the pressure/temperature dependences of the compensation part to be of the second-order scale.

Here, we can derive the integral form for the modified Lorentzian shape function as

$$\frac{y + W(x-t)}{(x-t)^2 + y^2} = \int_0^\infty \exp(-yq)(W\sin((x-t)q) + \cos((x-t)q))dq \quad . \qquad (8)$$

Then applying Eq.(8) to Eq.(7) and integrating for q, we obtain the Fourier form of the modified Voigt function, then similar to Eq.(2), we can also find the following modified function $f(t)$:

$$f(t) = (1 + ik_m W)\exp\left[-y(t\nu) - (t\nu)^2/4\right]\exp(-it\nu\alpha_h)\nu \quad , \qquad (9)$$

where k_m is the scaling factor required for the numerical calculation in Fourier space, and should be defined in the future study. The obtained function $f(t)$ becomes simply the modified version of Eq.(2), and we find that the implementation of the line mixing effect does not disturb the simple and compact calculation kernel.

The transition rate matrix will be obtained through laboratory measurements or be given as the adjusted values fitted to the atmospheric measurements. In this paper, we do not discuss the parameters for line mixing, but verify that the introduced method is applicable by comparing it with the conventional transmittance model. Figure 2 shows the sample calculations for the CO_2 Q branch of the 618 cm^{-1} band. In this case, W_j for line j was given as -1 and scaling factor k_m was adjusted to minimize the residual of the two models, and given as 1.6. Apparently, the calculation with the line-mixing effect

approached the result of FASCOD calculation, however, the discrepancy with the FASCOD is still large. This discrepancy can be lowered by adjusting each W_j value, however, further study using laboratory/atmospheric measurement data will be required in the future.

4. Conclusions

A simple method for line-by-line calculation using the Fourier-transformed Voigt function is feasible for the atmospheric radiation/transmission model. The straightforward structure of the algorithm enabled simple line-by-line calculation program implementation and was easily adapted to the calculation of atmospheric transmittance. The presented method is expandable to the practical atmospheric model that simulates the atmosphere with subdivided layers in which temperature, pressure, and mixing ratio of each constituent are assumed to be constant in each layer. Total computation cost for the practical atmospheric transmittance calculation may be higher than the conventional line shape approximation model, however, the Fourier transform method is still viable for a future model, taking into account its simplicity of the algorithm.

References

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Figure Captions

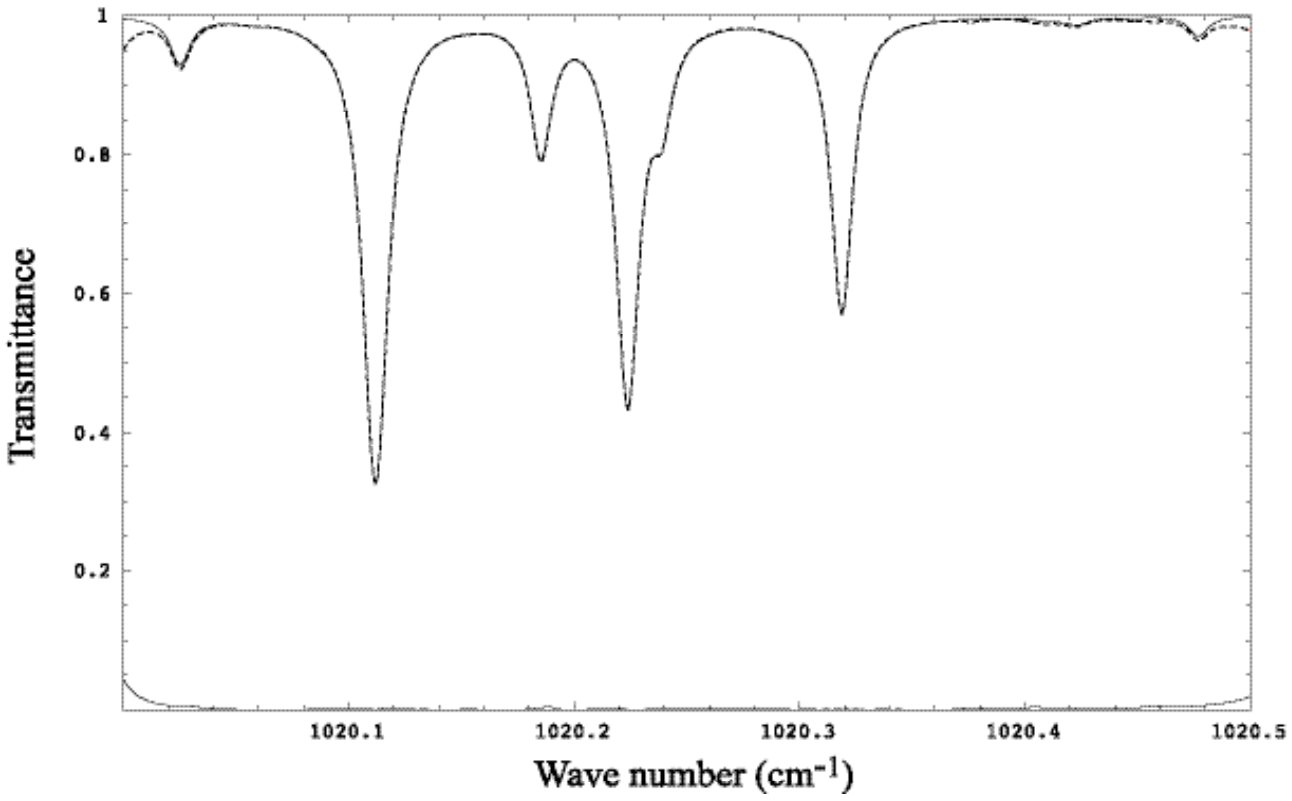

Fig. 1. Sample transmittance calculation using FASCOD version 3P (dashed line) and the L2FTV (solid line) for the wave number region 1020.0 to 1020.5 cm^{-1}.

The thin solid line at the bottom is the difference between the two calculations. The FASCOD calculation conditions are *P* of 55.29 hPa, T of 216.7 K (Z= 20 km of U.S. standard atmosphere 1976), and horizontal path of 1 km for O_3 only. In this case, the FASCOD parameter DV, the wave number spacing for the interpolated result, is set to 0 which induces 0.001314 cm^{-1} internally. The molecular density is 4.769 $x10^{12}$ molecules/cm^3. The scanning function is the rectangular convolution for the transmission, and the parameter SCAN is set to 0.0005 cm^{-1}. The minimum optical depth parameter DPTMIN is set to the default value, 2 x 10^{-4}. The L2FTV method parameters are ν_{max}=1021.5 cm^{-1}, ν_{min}=1018.95, *res*=0.1247 cm^{-1}, and Fourier-transform size *F*=2048. For the L2FTV calculation, 74-line data included in the target wave number range are used, taking into account the line intensity.

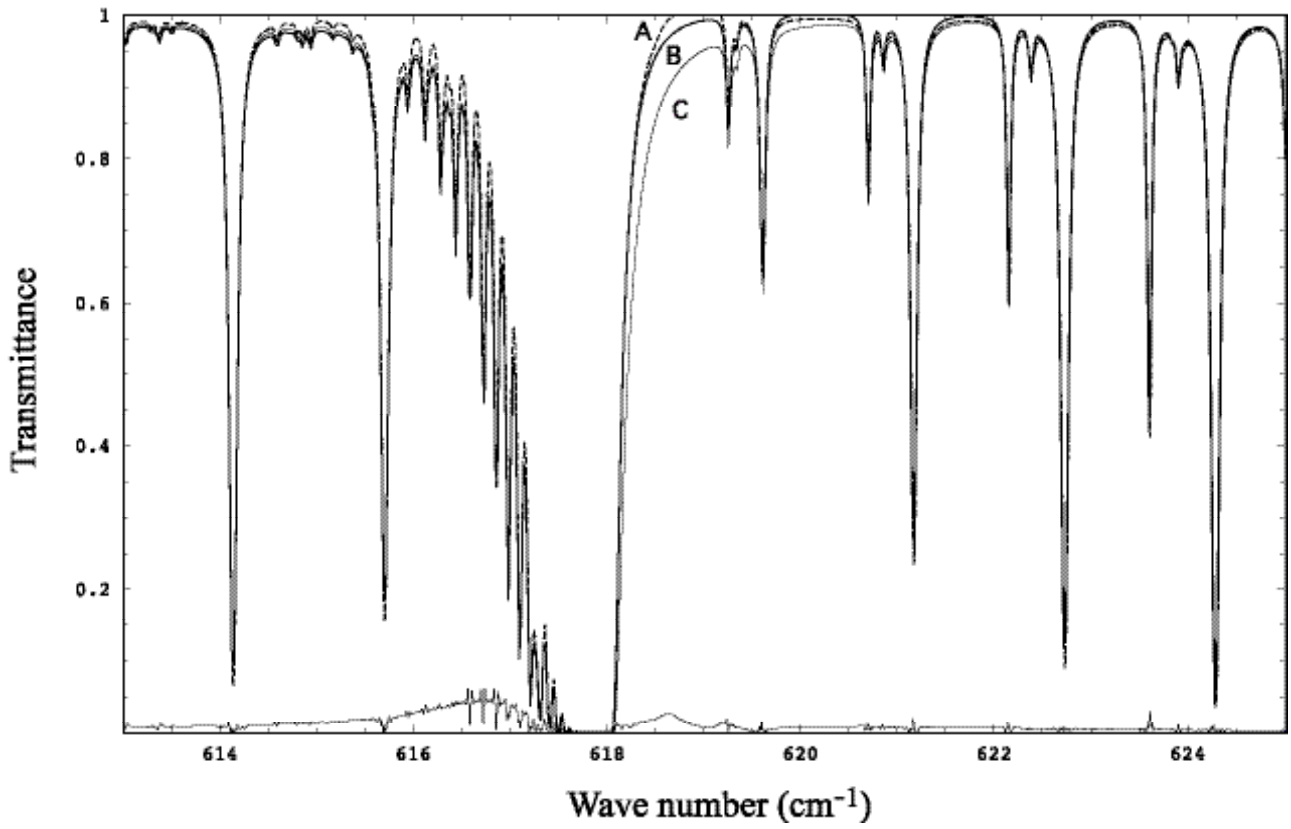

Fig. 2. Sample transmittance calculation including line mixing effect for a CO_2 Q branch using FASCODE3P (A: dashed line), the L2FTV (B: solid thick line), and the L2FTV without line-mixing

effect (C: solid thin line).

The thin solid line at the bottom is the difference between the two models with the line-mixing effect. The FASCOD calculation conditions are P=265 hPa, T=223.3 K, and CO_2 density= 3.011×10^{20} molecule/cm^2 for major isotope only. Other FASCOD parameters are equal to those in the case of Fig.1. The L2FTV method calculation conditions are res=0.01736 cm^{-1}, Fourier-transform size F=2048, and the scaling factor for the line mixing effect k_m heuristically given as 1.6. In the calculation process of FASCOD, small line shifts of about 0.006 cm^{-1} are given to this band, and the L2FTV is also adopted for this sample.