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Line-by-Line Calculation using Fourier-Transformed Voigt Function

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Abstract-- A line-by-line calculation algorithm in the Fourier space utilizing the Fourier-transformed Voigt function has been developed. The algorithm requires no approximation method for line shape calculation, and provides a straightforward model for the implementation of high-resolution radiation/transmission calculation with huge absorption lines for the modern computing environment.

1. INTRODUCTION

The line-by-line calculation for the radiation transfer model is required to perform a numerical evaluation of the atmospheric radiant observations using high-resolution spectrometer. The line-by-line method requires the line shapes which can be derived via Voigt function calculation. The Voigt function is presented as an integrated form, and the direct computation of the Voigt profiles involves a high computational cost. Many investigations were performed using the table-driven method or the polynomial-fitting-to-the-function method to reduce this computation cost. A widely known rapid computation method was described by Drayson.[1] His implementation of the Voigt profile computation is adequately rapid under the condition of a limited absolute accuracy of 4 decimal digits and is practical for transmittance calculations.

The recent radiance/transmittance calculation model for high-resolution and wide-band spectroscopy requires more efficiency and more flexibility for the line-by-line computation. The Voigt function computation method using, for example, Taylor-series expansion, is rapid enough for small number of lines. However, in the case of using a high-resolution Fourier transform spectrometer (FTS), the Voigt function calculation method such as Drayson's method involves substantial computation cost because of the huge number of lines. Since the conventional method, in general, is composed of complicated subparts that are internally controlled by the parameters of the Voigt function, it was difficult to develop an algorithm for the rapid Voigt function computation even when applying recent computation environments such as parallel computation approaches. For example, for the utilization of FTS to an atmospheric sensor from the space,[2] we attempted to develop the table-driven system using the precalculated transmittance without direct adaptation of the original Drayson's method. The table-driven method is rapid, however it becomes very large and stiff for the algorithm modifications.

Additional computation cost requirement factor originates in the line-by-line calculation in the wavenumber space which includes many randomly positioned lines. In the conventional method,

each line shape must be mapped in the wavenumber space according to its line center position, which is generally accompanied by the cutoff of the line shape wings. For example, for the application related to the FTS, the conventional method requires the convolution process for matching the instrument function or wavenumber resolution.

The expression of the Voigt function with the Fourier form was proposed in an old paper,[3] and the result was referred in the review on the mathematical properties of the Voigt function.[4] After the development of Cooley and Turkey's method for the fast Fourier transform (FFT), the Voigt function calculation using the Fourier transform method became practical. Karp, then, demonstrated that the Fourier transform method is computationally more efficient than the previous approaches.[5] However, Karp did not clarify the implementation of the method which basically requires a large number of computational points, and his method did not get followers. Many studies concerning the method for calculating Voigt profiles and the comparison of implementations have been continued, without adopting Fourier transform method.[6]

Recently, Abousahl et al compared the FFT for the Voigt profile with other algorithms.[7] However, their algorithm was based on the inverse Fourier transform of the convolution of Fourier-transformed Gaussian and Lorentzian functions considering the fact the Voigt function is the convolution of these two functions. This algorithm is simple, however, the computation of convolution involves a high computation cost.

2. PREPARATION OF FOURIER TRANSFORM EXPRESSION FOR THE VOIGT FUNCTION

The expression of the Voigt function using the Fourier transform style is introduced as follows.[4] The Vogit function K(x,y) is generally presented as

$$K(x,y) = \frac{y}{\pi}\int_{-\infty}^{+\infty}\frac{\exp(-q^2)}{y^2+(x-q)^2}\,dq\,, \tag{1}$$

where y is the ratio of the Lorentz-to-Doppler width

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

and x is the wavenumber scale normalized on the line center ν_0. According Reiche,[3] the integrand of Eq. (1) can be represented as follows, when y>0.

$$\frac{y}{y^2+(x-q)^2} = \int_0^{\infty}\exp(-y\,t)\cos[(x-q)\,t]\,dt \tag{3}$$

Applying Eq. (3) to Eq. (1), and carrying out the integration over *q,* we can obtain the Fourier transform of the Voigt function as

$$K(x,y) = \frac{1}{\pi^{1/2}} \int_0^\infty \exp(-yt - t^2/4) \cos xt \, dt \, . \tag{4}$$

In this paper, a new implementation path for the radiation transfer calculation model is described.

3. IMPLEMENTATION OF THE SPECTRAL CALCULATION USING FFT

Considering the characteristics of Fourier transformation and the Fourier coefficients, regarding the linearity of Fourier transform as also mentioned,[5] we can expect that the absorption coefficients for many atmospheric lines can be represented as a Fourier transform of the multiple sum of each term which is shown as the integrand of Eq. (4).

When applying Eq. (4) to the calculation of multiple lines, we can modify the term cos(xt) in the integrand of Eq. (4) to exp(-i ν^* t) for each line, where ν^* is the normalized wavenumber of each line center. For the wavenumber normalization, we introduce the maximum calculation wavenumber ν_{max} .

We must first consider the scale for x in the representation of the Vogit function K(x,y). The parameter x is represented as

$$x = \frac{\nu - \nu_0}{\alpha_D} (\ln 2)^{1/2} \, . \tag{6}$$

α_D is the Doppler half-width defined as

$$\alpha_D = \nu_0 \left(\frac{2kT \ln 2}{Mc^2} \right)^{1/2} , \tag{7}$$

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

$$x = \frac{\nu - \nu_0}{\nu_0} V(T,M) \, . \tag{8}$$

V is a nondimensional function of temperature and the specified molecular weight, and is represented as

$$V(T,M) = \left(\frac{Mc^2}{2kT} \right)^{1/2} \, . \tag{9}$$

In general, if the line-by-line calculation is carried out under constant temperature and pressure conditions, the function V can be treated as a constant V_{TM} in the Fourier transform.

Then we can obtain the integrand of Eq. (4) for the absorption lines indexed with j,

$$f(t) = \sum_j \exp[-y_j(t\nu_j) - (t\nu_j)^2/4] \exp[-it\nu_j V_{TM}] \nu_j \quad , \tag{10}$$

where ν_j is a line center normalized with ν_{max} as $\nu_j = \nu / \nu_{max}$.

There are several conventions for the computational implementation for the Fourier transform. We adopted the Fourier transform function b_s of a_r defined as

$$\frac{1}{\pi^{1/2}} \sum_{r=1}^{n} a_r \exp[2\pi i (r-1)(s-1)/n] \quad . \tag{11}$$

In this case, the numerical list a_r of length n is produced from the function $f(t)$. Considering that the discrete Fourier transform (DFT) may be applied to the function having a period of 2π, a_r becomes a numerical list calculated using $f(t)$ for t from 0 to P with the step s. Each of these parameters is defined as

$$P = 2\pi(r_s - 1/V_{TM}) \quad , \tag{12}$$

$$s = 2\pi/V_{TM} \quad . \tag{13}$$

The length n is defined as

$$n = V_{TM}\, r_s - 1 \, , \tag{14}$$

where r_S is the scale adjustment parameter for the number n. Obviously, r_S defines the wave-number resolution of the results. In a common case, the parameter r_S would be used to adjust n to 2^m for the convenience of FFT.

Finally, we can produce the line-by-line calculation model as the real part of

$$\frac{1}{\pi^{1/2}} k_s \sum_{r=1}^{n} a_r \exp[2\pi i (r-1)(s-1)/n] , \tag{15}$$

where k_S is the scaling coefficient which can be shown as

$$k_s = 2(\pi r_s / V_{TM})^{1/2} \quad . \tag{16}$$

Figure 1 shows a sample of the list a_r to be Fourier transformed. The calculation parameters are the same as those shown in the following section. We can see the analogies between the relations of the interferogram obtained by FTS and the spectrum calculated from the interferogram in this figure, and easily expect the method to define the wavenumber resolution and the application defining the instrument function.

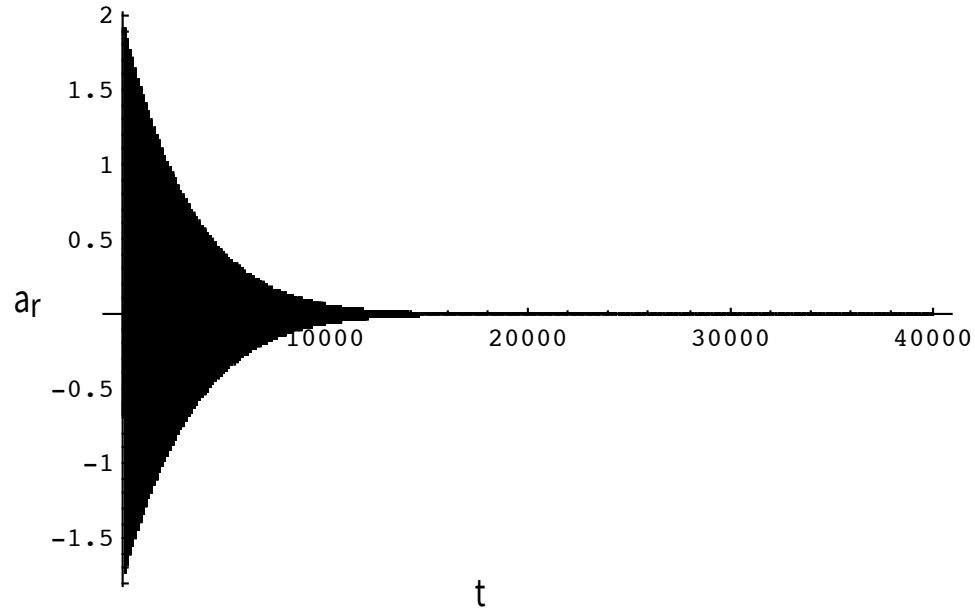


Fig. 1. The numerical list of a_r to be Fourier transformed, which represents the sum of absorption lines in the Fourier space and is corresponding to an interferogram of the FTS.

4. NUMERICAL EVALUATION OF THE METHOD

In atmosphere, V_{TM} becomes a relatively large number, according to Eq. (9). When T=300 K, V_{TM} becomes 5.6946*10^5 for H_2O. This condition requires a large computation size for the FFT. The FFT computation size close to 2^{19} is not very large for the modern computing environment, however, a smaller size may be better. In order to reduce the size, we can introduce the Fourier transform computation scale l, where l=1, 2, 3, ..., m. Using this scale, we can reduce the total calculation number to halve, one third, or more, and Eqs. (13) and (16) are modified as

$$s = 2l\pi / V_{TM} \quad , \tag{17}$$

$$k_s = 2\left(l\pi r_s / K_{TM}\right)^{1/2} \quad . \tag{18}$$

When we introduce the scale l, the line-by-line calculation presented by Eq. (15) yields the result in the scope of a band from $\nu_{max} - \nu_{max}/l$ to ν_{max} .

To evaluate Eq. (15), the original Voigt function defined using Eq. (1) was numerically integrated with the machine precision of 20 decimal digits and an accuracy of 10 digits. Figure 2 shows the result for two sample lines, 1,550 cm^{-1} and 1,520 cm^{-1} with V_{TM}=500,000 and for each y=1 and 2, where the sample size of the Fourier transform is 40,000. As expected, replacing the integrals in Eq. (4) by a sum over a finite equation of Eq. (15) could introduce an aliasing error. To reduce this aliasing error, we should consider the relation between the calculation range of the band mentioned above and position of the lines at each end of the line cluster. Each end-line position must be such that the wing of the line is small enough at the end of the calculation range compared to the model accuracy requirement. Also, there is a well-known truncation error induced due to replacing the infinite integrals in Eq. (4) by a sum over a finite representation of Eq. (15).

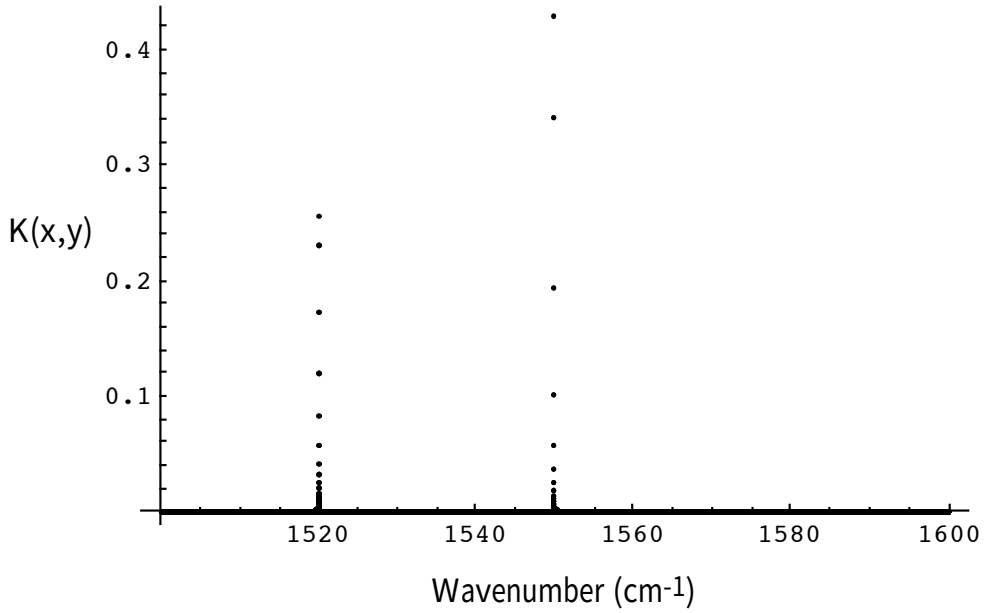
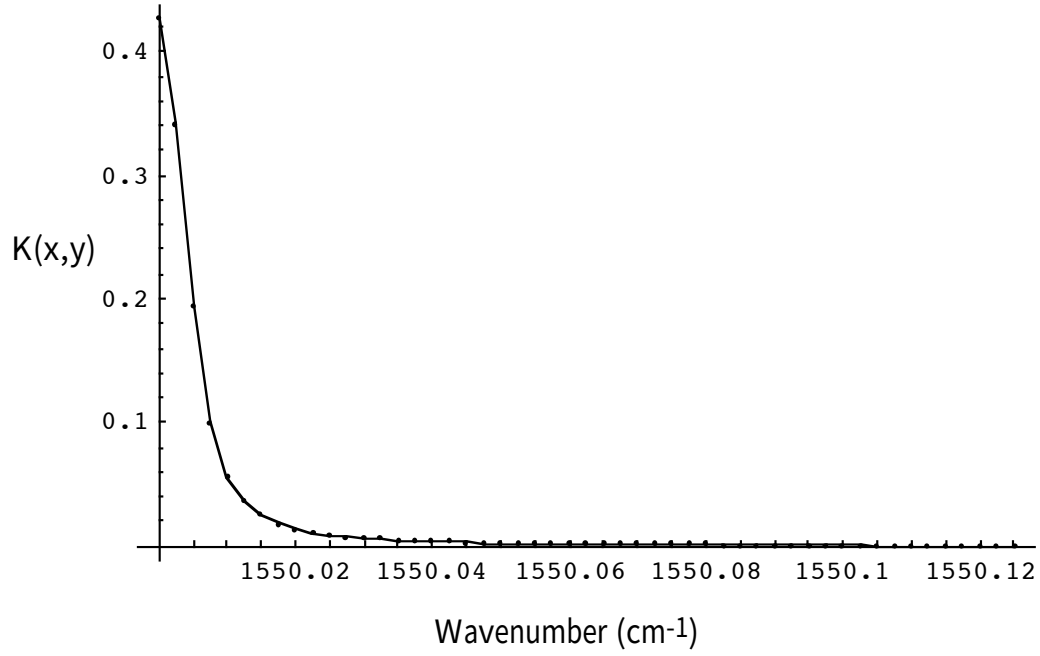


Fig. 2. The result of line-by-line calculation for two example lines, where the numerical calculation was performed for the wavenumber range from 1500 cm^{-1} to 1600 cm^{-1} and the Fourier sample size of 40000.

Figure 3 shows the comparison of the lines between the result of the Fourier-transformed Voigt function represented by dots and the result of numerical integration of Eq. (1) represented by the solid line. The numerical integration for Eq. (1) was performed with an accuracy of 10 decimal digits. The upper figure is for the line centered at 1550 cm^{-1} and the maximum difference between the two results was 0.000109. The lower panel shows the same result of the comparison for the line centered at 1520 cm^{-1}, and the maximum difference between the two was also 0.000109, as expected.



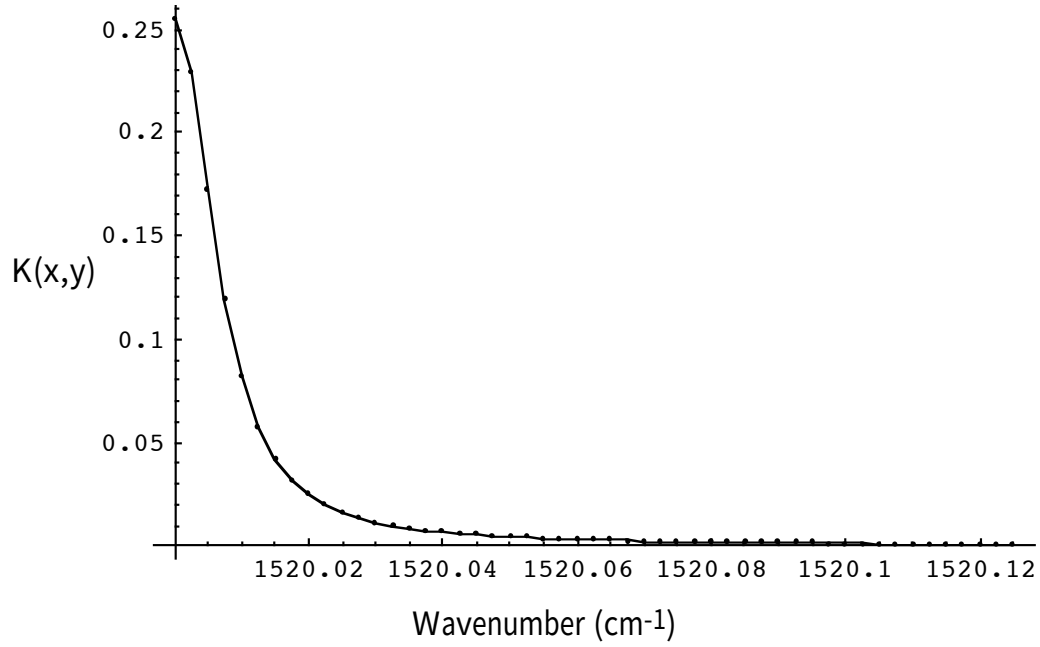


Fig. 3. Numerically evaluated results of the Fourier transform method, where dots represent the results obtained using this method and solid lines were obtained from the direct numerical integration of Eq. (1). The upper figure shows the close-up of the line centered at 1550 cm^{-1} and the lower figure shows the line centered at 1520 cm^{-1}.

As shown, we can achieve the line-by-line calculation using DFT within an accuracy of 4 decimal digits, and the difference can be further reduced because the implementation of the Fourier-transformed Voigt function itself is not approximated using such a polynomial, but is related only to the size of the DFT (or FFT) samples and with the accuracy of the internal floating point number representation of each computer. The practical approach should be adopted for the reduction of errors introduced by the finite Fourier transform operation when we implement a radiative transfer model applying this algorithm.

5. CONCLUSIONS

A line-by-line calculation algorithm was presented utilizing Fourier transform. Because the line summation is performed in the Fourier space, arbitrary wavenumber resolution can be obtained easily, and neither the line-shape cutoff at the wing part nor the mapping procedure of each different centered line shape to the wavenumber space in the conventional method are required. Since the developed method was analytically introduced from the definition of the Voigt function, the developed algorithm is independent of the approximation methods included in the conventional method. The straightforward structure produced from the developed algorithm can adapt well to a modern computation environment in high-speed line-by-line calculation.

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