# －A simplifying method for the transmittance calculation based on a Fourier-transformed Voigt function considering the instrument function

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**Abstract**
A line-by-line transmission calculation for a homogeneous atmospheric layer based on a pure Voigt function with no approximation can be performed using the Fourier-transformed Voigt profile. This method also includes an interference term that takes into account the line mixing effect. The method can be used to calculate transmittance/radiance considering each line shape under the effects of temperature and pressure using the line database with an arbitrary wave number range and resolution. This method adopts line-by-line calculation in the Fourier space, then considering the instrument function, we can reduce total calculation cost to use this method for practical applications. Evaluation was performed comparing this method with a conventional atmospheric transmittance calculation model.

## 1. Introduction

Recently, Kobayashi [1] showed an algorithm to calculate the Fourier transformed Voigt function directory, and indicated a way of the simple line-by-line calculation method. When the Voigt function is represented with Fourier form, it is easily expected the line-by-line calculation becomes simple because all the lines are simply summed in the Fourier space. An arbitrary wave number resolution can be obtained by this method and neither the line-wing part cutoff nor the mapping procedure of each different centered line shape to the wavenumber space are required. Also, Kobayashi [2] made the comparison between the widely using model (FASCOD) and his model and showed that results of two models are identical.

In general, practical atmospheric transmission calculations involves the instrument function because the atmospheric transmission observations are carried out by the instrument which restricted by the instrument function, in this case, the response of the instrument in wavenumber space, such as amplitude response and wavenumber resolution. This paper shows the path to reduce the calculation cost of the line-by-line model using Fourier transformed Voigt function considering the practical transmittance calculation always associates the convolution of instrument function.

## 2. Numerical Expression of the Voigt Profile Using the Discrete Fourier Transform

Armstrong[3] showed the expression of the Voigt function K(x,y) with the Fourier-transform style as

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

where y is the ratio of Lorentz to Doppler widths. As Karp[4] showed, the integrand of Eq. (1) for the multiple absorption lines is represented as

$$f(t) = \sum \exp\{-y(t\nu) - (t\nu)^2/4\}\exp(-it\nu\alpha_h)\nu \quad , \tag{2}$$

where for each line j, $\nu_j$ is the line center. Eq. (2) is basically equal to the Karp's conclusion, but Kobayashi[1] introduced νmax to normalize the line center as $\nu_j = \nu0_j/\nu_{max}$ . Introducing the wavenumber calculation maximum, we can reduce the total calculation number, and perform the line-by-line calculation on the arbitrary band range from $\nu_{min} = \nu_{max} - \nu_{max}/l$ to $\nu_{max}$ where $l$ is the Fourier transform computation scale ($l$ =1,2, ... m) . We call this method L2FTV (line-by-line calculation using Fourier transformed Voigt function).

Figure 1 shows an example of the results of the FASCOD and the L2FTV. The corresponding line peak values are identical when neglecting very small computational error (discrepancy is less than $10^{-4}$.

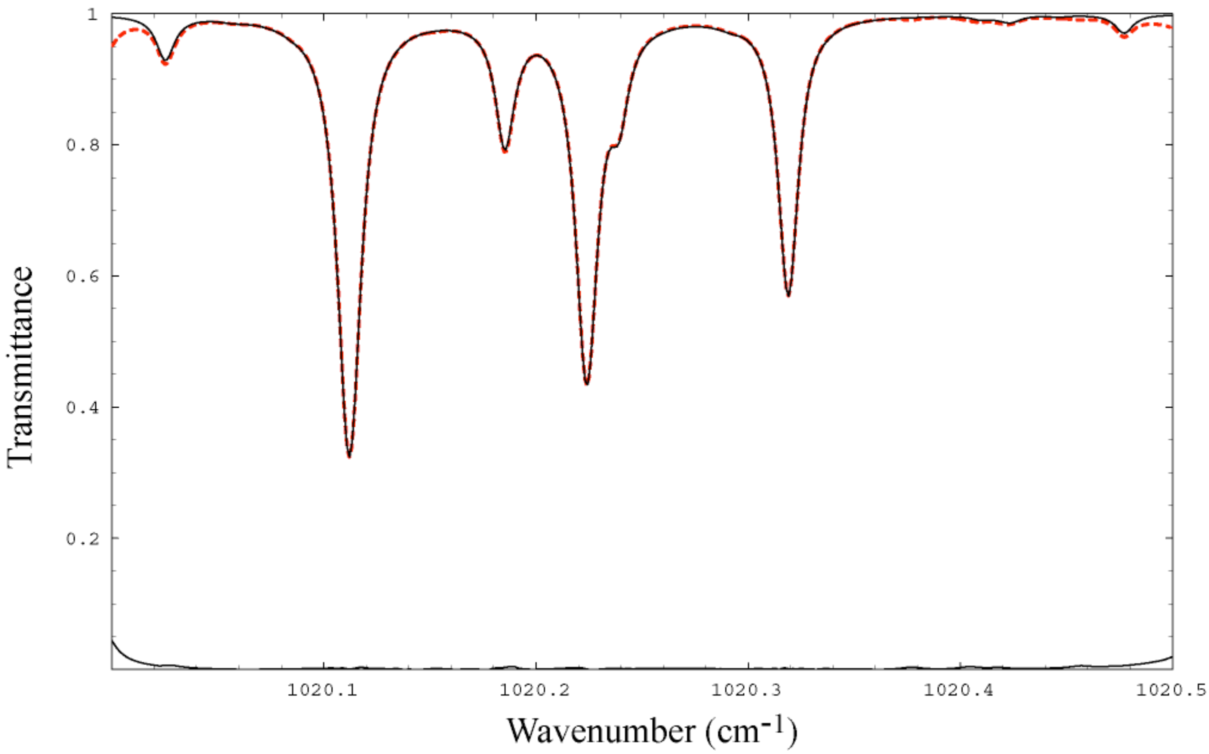

Fig. 1. Sample transmittance calculation using FASCOD version 3P (dashed line) and the L2FTV (solid line) for the wavenumber region 1020.0 to 1020.5 $cm^{-1}$.

The thin solid line at the bottom is the difference between the two models, defined as the root of the squared difference. The FASCOD calculation conditions are P: 55.29 hPa, T: 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 wavenumber 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 model parameters are scale l=400, $\nu_{max}$=1021.5 $cm^{-1}$, $\nu_{min}$=1018.95, res=0.1247 $cm^{-1}$, and Fourier-transform size F=2048. For the L2FTV calculation, 74-line data included in the target wavenumber range are used taking into account of the line intensity. The temperature dependency of the line intensity was calculated following Rothman and Gamache.

**3. L2FTV calculation cost saving considering instrument function**

The L2FTV calculation cost saving is performed by apodizing the optical depth in the Fourier space. In the Fourier space this apodization is accomplished by zero filling which introduces the calculation cost reduction. The focusing point is that the convolution of the instrument function is applied to the transmittance and the L2FTV calculation cost saving is performed by apodizing the optical depth in the Fourier space. Because the transmittance is obtained applying the exponential function to the optical depth, even if using a same instrument-apodizing function, there is a difference between the instrument function applied transmittance and the same instrument applied transmittance but using a optical depth derived by the calculation cost saving. The evaluation steps are followings; (1) define the reference transmittance spectrum obtained from the L2FTV applying appropriate instrument function, (2) confirm the first step comparing FASCOD produced transmittance applied same instrument function, (3) apply weak (which means small effect for the resolution response) apodizing function (rectangular function) onto the optical depth derived by the L2FTV in the Fourier space, (4) apply stronger apodizing function, (5) evaluate critical strength of the apodizing function. Figure 2 shows this evaluation process.

We can estimate the relationship between the masking function and the instrument function as follows. When we observe the actual atmosphere radiance using a spectrometer such as FTS, observed spectrum $S_{fts}$ is represented using blackbody radiation Br, atmospheric transmittance Tr and the instrument function f*as,

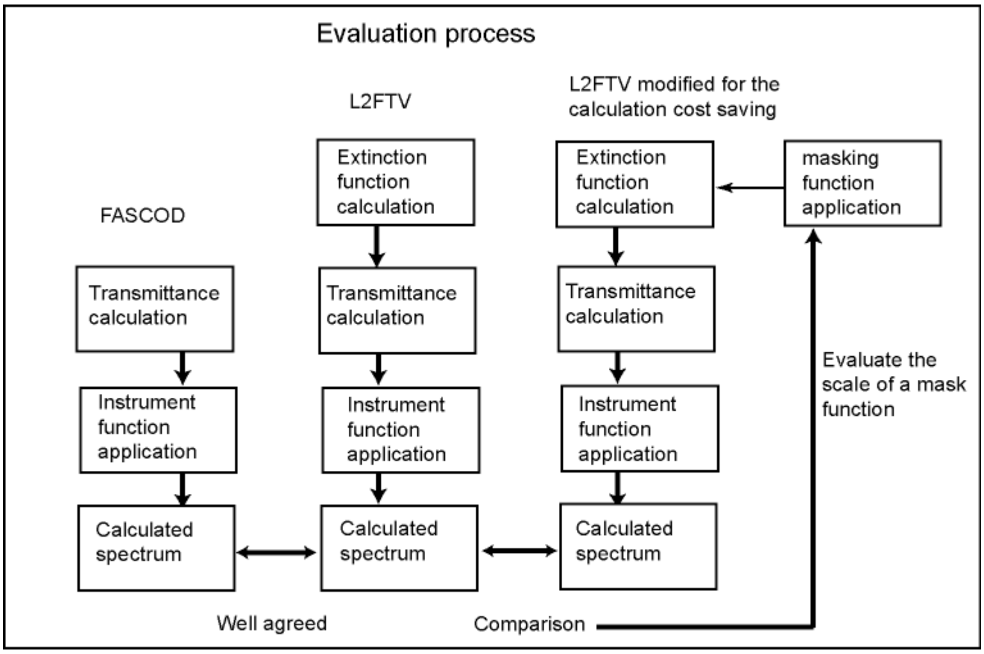


Fig. 2. The evaluation process of calculation cost saving method considering the instrument function.

A conventional line by line calculation code, such as FASCOD, can calculate the transmittance spectrum applying an instrument function to simulate a spectrometer such as the FTS. On the L2FTV model, calculation cost saving is performed applying a masking function onto the extinction calculation process. An evaluation for the tradeoff between the strength of the masking function and the error of the resulted spectrum was performed.

$$S_{fts}=f^{*}\otimes(Br\cdot Tr) \quad (3)$$

where Br variation in wavenumber is relatively small considering the resolution of actual FTS application, and Tr=exp(-r k*) then we obtain ignoring constant r,

$$S_{fts}=f^{*}\otimes exp(-k^{*}) \quad (4).$$

In L2FTV calculation cost saving process, calculated spectrum $S_m$ is represented as,

$$S_m=exp(-f'^{*}\otimes k^{*}) \quad (5)$$

where f'* is the masking function for the extinction function calculation. We can represent these relations using Fourier transformation F when each of k, f, f' is Fourier transformed form of k*, f*, f'*,

$$S_{fts}=F\{f\cdot F^{*}(exp(-k^{*}))\} \quad (6)$$

$$S_m=exp(-F\{f'\cdot k\})$$

Then applying the series expansion around 0, these equations become

$$S_m=1-F\{f'\cdot k\}+F\{f'\cdot k\}2/2-F\{f'\cdot k\}3/6+O \quad (7)$$

$$S_{fts}=F\{f\cdot F^{*}(1-k^{*}+k^{*}2/2-k^{*}3/6+O)\} \quad (8)$$

Executing Fourier transform of inner part of Eq.8, we obtain

$$S_{fts}=F\{f\cdot d\}-F\{f\cdot k\}+\{f\cdot F^{*}(k^{*}2/2)\}-\{f\cdot F^{*}(k^{*}3/6)\}+O \quad (9).$$

Comparing Eq.7 and 9 from the standing point of the effect strength of the masking function f' and the instrument function f, we found the second term is same, and in the third term of Eq.7, the masking function f' has quadratic form, however the instrument function f has linear form in Eq.9. So, we can estimate that the masking function affect strongly to the spectrum comparing the effect of the instrument function.

in this evaluation, we use the Norton-Beer[4] instrument function, and the rectangular mask function. First, we apply the Norton-Beer instrument function to the L2FTV spectrum to confirm that is equal to the FASCOD provided spectrum as shown in Fig.1. Hence, we use the effective instrument/mask function width that is defined as the relative size where function becomes 0 considering calculation scale, which is, in the L2FTV, the Fourier transform size.

Figure 3 shows the original L2FTV calculation and the instrument function applied low resolution transmittance spectrum. Figure 4 shows the R.M.S error between the original spectrum and rectangular mask function applied transmittance when a reference instrument function effective width is 0.121. The figure shows that the mask function worked well for the reduction of the calculation cost when its effective size is relatively equal or larger than that of the instrument function.

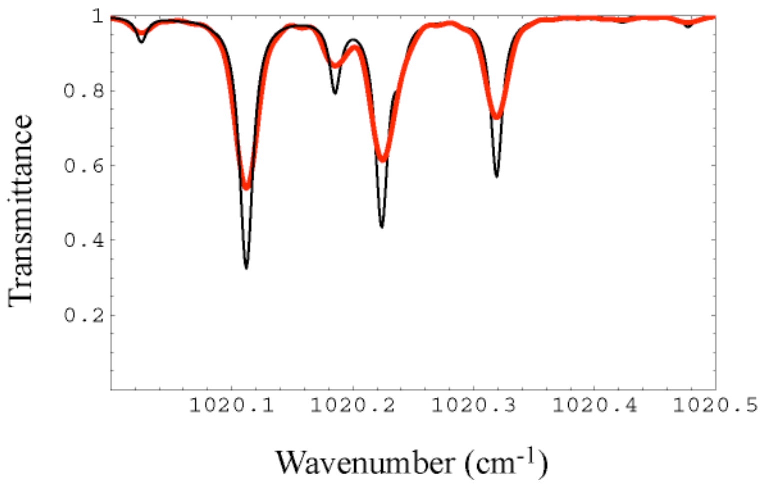


Fig. 3. An effect of the instrument function.
Thin solid line is the original L2FTV provided spectrum, and bold one is a spectrum applied the Norton-Beer instrument function.

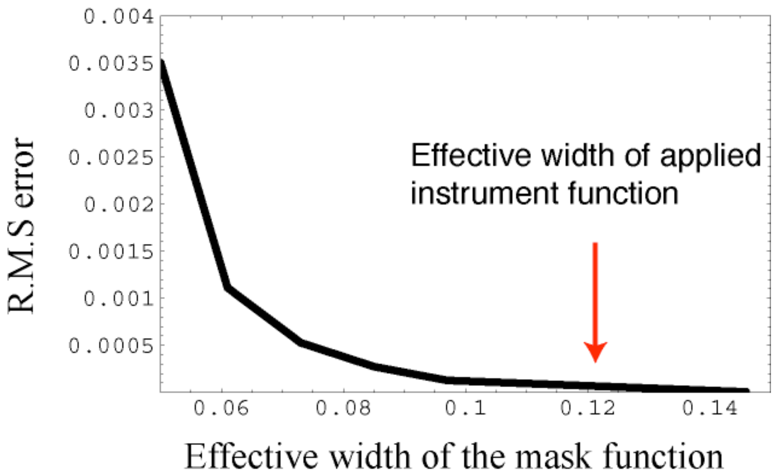


Fig. 4. The effect of the mask function
Wider mask function reduces rms error of re-produced spectrum, however, comparatively equal width to the instrument function gives small and acceptable error.

**4. Conclusion**

The developed calculation cost saving method was evaluated and it is confirmed that the rectangular calculation mask can reduce the total calculation cost. Applying this method, the L2FTV line by line calculation cost can be reduced to the comparable level of the conventional line by line model, keeping its simplicity and exactness produced by the analytical representation of Voigt profile.

**References**

1. H. Kobayashi, JQSRT 62, 477 (1999).
2. H. Kobayashi, Appl. Optics, 41, 33, (2002).
3. B.H. Armstrong, JQSRT 7, 61 (1967).
4. A. H. Karp, JQSRT 20, 379 (1978).
5. R.H. Norton and R. Beer, J. Opt. Soc. Am.66, 259 (1976).