

CORRESPONDENCE

Reply

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ABSTRACT

In response to a comment on their previous note about the Voigt line profile, here the authors clarify relevant statements and numeric algorithms in the original note.

In Huang and Yung (2004, hereafter HY04) we described a mistake commonly found in several textbooks regarding the Voigt line profile. Five years after the original note was published, Schreier (2009; see also the associated corrigendum; these are hereafter jointly referred to as S09) had several comments on it.¹ Below we clarify a couple of issues regarding these comments.

1) We agree with the comments about the half-widths in S09. In all atmospheric radiation textbooks (or chapters about atmospheric radiation in atmospheric science textbooks) that we have noticed, the common notations are α_L for the half-width of Lorentz broadening and α_D for the e -folding half-width of the Doppler broadening. Most textbooks (e.g., Goody and Yung 1989; Liou 2002; López-Puertas and Taylor 2001) simply refer them as the Lorentz width and Doppler width, respectively. The terms “Lorentz width” and “Doppler width” are also commonly used in other fields of optics to refer the half-width and e -folding half-width, respectively. Examples of

recently published textbooks include one book in laser spectroscopy (Demtröder 2008) and two books about quantum optics (Grynberg et al. 2010; Demtröder 2010). Thus, even though the half-width and e -folding half-width are two different concepts, it is a convention to denote them with similar symbols (i.e., α_L and α_D). HY04 assumed that this convention had been widely used and had been well aware of by the community and therefore did not explicitly clarify that α_D is the e -folding half-width.

2) About “ambiguous specifications of the Voigt profile”: if there were no context, we would agree with what was stated in the abstract of S09, “there is no unique corresponding Voigt profile,” since the word “corresponding” can be interpreted in different ways as S09 elaborated. However, in HY04, we first presented Fig. 3.2 in *Radiative Transfer in the Atmosphere and Ocean* by Thomas and Stamnes (1999) as Fig. 1 in HY04 and it defined the context. The caption of this figure clearly stated that “ $\Delta\nu$ is the Doppler width α_D for both Doppler broadening and Voigt broadening and is the Lorentz width α_L for Lorentz broadening. $\alpha = \alpha_L/\alpha_D = 1$ was used for the Voigt profile.” These descriptions clearly defined $\alpha_L = \alpha_D = \Delta\nu$ for the Lorentz and Doppler profiles as well as the corresponding Voigt profile being the convolution of such two profiles. These descriptions left no ambiguity. The corresponding Voigt profile within this context, is what we plotted in Fig. 2 of HY04, which is also identical to the green dashed line

¹ The e-mail address provided in HY04 for correspondence was discontinued shortly after Dr. Huang graduated in 2004. As a result, both authors were not notified for the submission of S09; hence no response was made then.

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(labeled as Voigt: $\alpha_L = \alpha_D = 1$) in Fig. 2 of S09. HY04 was aware of the possible ambiguity of the wording and its potential to cause confusion. This was why HY04 acknowledged in the very first paragraph that a similar figure with different figure caption [i.e., Fig. 3.11 in Andrews (2000)] was correctly plotted.

- 3) S09 commented about the numerical integration that HY04 used in calculating “the Voigt profile by numerical integration of Eq. (1) (in HY04) from $y = -200$ to $y = 200$ using the trapezoidal rule with interval $\Delta y = 10^{-4}$.” S09 argued that “[calculating this integral] by numerical quadrature (Trapez, Gauss-Hermite, etc.) cannot be recommended in general and is only justified numerically for $y \geq 1$.” What has been used in HY04 is a composite trapezoidal rule (otherwise, there would have been no need to specify a $\Delta y = 10^{-4}$), not the simple trapezoid rule. Specifically, for a given x , the Eq. (1) of HY04 was evaluated as

$$\begin{aligned}
 f(x) &\approx \frac{\alpha_L}{\alpha_D^2} \frac{1}{\pi^{3/2}} \frac{\Delta y}{2} \sum_{i=0}^{N-1} [g(x; y_i) + g(x; y_{i+1})] \\
 &= \frac{\alpha_L}{\alpha_D^2} \frac{1}{\pi^{3/2}} \Delta y \left[\frac{1}{2} g(x; y_0) + \frac{1}{2} g(x; y_N) \right. \\
 &\quad \left. + \sum_{i=1}^{N-1} g(x; y_i) \right], \tag{1}
 \end{aligned}$$

where $g(x; y) = e^{-y^2} / [(x - y)^2 + (\alpha_L / \alpha_D)^2]$, $y_i = y_0 + i\Delta y$, and the starting and end points of integration are y_0 and y_N , respectively. Other symbols were the same as those defined in HY04.

For any given x , from $y = -\infty$ to $y = +\infty$, $g(x; y)$ is a smooth curve that monotonically increases from zero to its single maximum and then monotonically decreases toward zero. Therefore, it can be well approximated by a composite trapezoidal integration as long as the step size is small enough. As shown in standard numerical analysis textbooks, the accuracy of composite trapezoidal integration scales as Δy^2 . We chose $y_0 = -200$, $y_N = 200$, and $\Delta y = 10^{-4}$ after testing the convergence numerically. For example, if we chose a new set of $y_0 = -2000$, $y_N = 2000$, and

$\Delta y = 10^{-5}$, the relative difference in $f(x)$ between two sets of numerical integration is only about 10^{-13} or even smaller (for the Voigt profiles discussed in HY04 and a wide range of $x \in [-100, +100]$).

- 4) Humlicek (1982) is an efficient algorithm to compute the Voigt profile and is still widely cited and used in remote sensing applications and radiative transfer modeling. HY04 used it together with the aforementioned brutal-force numerical integration to cross-validate the results. There are other efficient and accurate algorithms as described in S09. However, Humlicek (1982) is accurate enough for the purpose of HY04 and it is not the objective of HY04 to examine different algorithms on computing the Voigt profile.
- 5) As for comments for visualization, we believe that the graphical presentations in HY04 were adequate and clear enough. Alternative visualization is merely an individual preference.

REFERENCES

Andrews, D. G., Ed., 2000: Atmospheric radiation. *An Introduction to Atmospheric Physics*, Cambridge University Press, 55–96.

Demtröder, W., 2008: *Basic Principles*. Vol. 1, *Laser Spectroscopy*, Springer, 457 pp.

—, 2010: *Atoms, Molecules and Photons: An Introduction to Atomic, Molecular, and Quantum Physics*. 2nd ed. Springer, 589 pp.

Goody, R. M., and Y. L. Yung, 1989: *Atmospheric Radiation: Theoretical Basis*. 2nd ed. Oxford University Press, 544 pp.

Grynberg, G., and Coauthors, 2010: *Introduction to Quantum Optics: From the Semi-Classical Approach to Quantized Light*. Cambridge University Press, 665 pp.

Huang, X. L., and Y. L. Yung, 2004: A common misunderstanding about the Voigt line profile. *J. Atmos. Sci.*, **61**, 1630–1632.

Humlicek, J., 1982: Optimized computation of the Voigt and complex probability functions. *J. Quant. Spectrosc. Radiat. Transfer*, **27**, 437–444.

Liou, K. N., 2002: *An Introduction to Atmospheric Radiation*. 2nd ed. Academic Press, 583 pp.

López-Puertas, M., and F. W. Taylor, 2001: *Non-LTE Radiative Transfer in the Atmosphere*. World Scientific, 450 pp.

Schreier, F., 2009: Comments on “A common misunderstanding about the Voigt line profile.” *J. Atmos. Sci.*, **66**, 1860–1864; Corrigendum, **66**, 3744–3745.

Thomas, G. E., and K. Stamnes, Eds., 1999: Basic scattering processes. *Radiative Transfer in the Atmosphere and Ocean*, Cambridge University Press, 56–83.