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Technical Note: A novel parameterization of the transmissivity due to ozone absorption in the *k*-distribution method and correlated-*k* approximation of Kato et al. (1999) over the UV band

W. Wandji Nyamsi[1], A. Arola[2], P. Blanc[1], A. V. Lindfors[2], V. Cesnulyte[2,3], M. R. A. Pitkänen[2,3], and L. Wald[1]

[1]MINES ParisTech, PSL Research University, O.I.E. – Centre Observation, Impacts, Energy, Sophia Antipolis, France
[2]Finnish Meteorological Institute, Yliopistonranta 1 F, Kuopio, Finland
[3]Department of Applied Physics, University of Eastern Finland, Kuopio, Finland

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Correspondence to: W. Wandji Nyamsi (william.wandji@mines-paristech.fr)

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Abstract

The *k*-distribution method and the correlated-*k* approximation of Kato et al. (1999) is a computationally efficient approach originally designed for calculations of the broadband solar radiation at ground level by dividing the solar spectrum in 32 specific spectral bands from 240 to 4606 nm. Compared to a spectrally-resolved computation, its performance in the UV band appears to be inaccurate, especially in the spectral intervals #3 [283, 307] nm and #4 [307, 328] nm because of inaccuracy in modelling the transmissivity due to ozone absorption. Numerical simulations presented in this paper indicate that a single effective ozone cross section is insufficient to accurately represent the transmissivity over each spectral interval. A novel parameterization of the transmissivity using more quadrature points yields maximum error of respectively 0.0006 and 0.0041 for interval #3 and #4. How to practically implement this new parameterization in a radiative transfer model is discussed for the case of libRadtran.

1 Introduction

Radiative Transfer Models (RTM) are often used to provide estimates of the UV irradiance. One of the difficulties in the computation lies in taking into account the gaseous absorption cross sections that are highly wavelength dependent (Molina and Molina, 1986). For instance, the ozone cross section changes by more than two orders of magnitude over the UV band [280, 400] nm. The best estimate of the UV irradiance is made by a spectrally-resolved calculation of the radiative transfer for each wavelength followed by integration over the UV band. However, such spectrally detailed calculations are computationally expensive. Therefore, several methods have been proposed to reduce the number of calculations. Among them, are the *k*-distribution method and the correlated-*k* approximation proposed by Kato et al. (1999). It is originally designed for providing a good estimate of the total surface solar irradiance by using 32 specific spectral intervals across the solar spectrum from 240 to 4606 nm. Hereafter, these

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spectral intervals are abbreviated in KB. The Kato et al. method is implemented in several RTMs and is a very efficient way to speed up computations of the total surface solar irradiance. Its performance over the UV band is not very accurate when compared to detailed spectral calculations made with libRadtran (Mayer et al., 2005) or SMARTS (Gueymard, 1995).

For a spectral interval $\Delta\lambda$ where λ is the wavelength, let $I_{0\Delta\lambda}$ and $I_{\Delta\lambda}$ denote respectively the irradiance on a horizontal plane at the top of atmosphere and at surface, the spectral clearness index $\mathrm{KT}_{\Delta\lambda}$, also known as spectral global transmissivity of the atmosphere, or spectral atmospheric transmittance, is defined as:

$$\mathrm{KT}_{\Delta\lambda} = \frac{I_{\Delta\lambda}}{I_{0\Delta\lambda}} \quad (1)$$

Wandji Nyamsi et al. (2014) compared $\mathrm{KT}_{\Delta\lambda}$ obtained by the correlated-k approach against that obtained by spectrally resolved computations using libRadtran and SMARTS, both for clear-sky and cloudy conditions for a set of realistic atmospheric and cloud coverage states, and for each KB. They found that the Kato et al. method underestimates transmissivity in KB #3 [283, 307] nm and #4 [307, 328] nm covering the UV range by respectively –90 and –17 % in relative value and exhibits relative root mean square error of 132 and 16 % in clear-sky conditions. Similar relative errors are observed for cloudy conditions.

The underestimation for these two bands can be explained by the fact that Kato et al. (1999) assume that the ozone cross section at the center wavelength in each interval represents the absorption over the whole interval. The ozone cross sections were taken from WMO (1985). Actually, the ozone cross section is strongly dependent on the wavelength in the UV region (Molina and Molina, 1986). Both KB #3 and #4 in the UV range are large for considering only a single value of ozone cross section.

In order to improve the potential of Kato et al. method for estimating narrow band UV irradiances, in particular for the KBs #3 and #4, a new parameterization is proposed for the transmissivity due to the sole ozone absorption. Then, for each spectral interval,

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an assessment of the performance of the new parameterization in representing this transmissivity is made for a wide range of realistic cases against detailed spectral calculations. Finally, a short section describes how to implement this parameterization in the practical case of the RTM libRadtran.

2 Transmissivity due to ozone absorption

The average transmissivity $T_{O_3\Delta\lambda}$ due to the sole ozone absorption for $\Delta\lambda$ can be defined by Eq. (2).

$$T_{O_3\Delta\lambda} = \frac{1}{I_{0\Delta\lambda}} \int_{\Delta\lambda} I_{0\lambda} e^{-k_\lambda \frac{u}{\mu_0}} d\lambda \,. \tag{2}$$

where $I_{0\lambda}$ is the spectral irradiance at the top of the atmosphere on a horizontal plane, k_λ the ozone cross section at λ, u the amount of ozone in the atmospheric column and μ_0 the cosine of the solar zenith angle.

A technique widely used for computing $T_{O_3\Delta\lambda}$ is based on a discrete sum of selected exponential functions (Wiscombe and Evans, 1977):

$$T^n_{O_3\Delta\lambda} = \sum_{i=1}^{n} a_i e^{-k_i u/\mu_0} \,. \tag{3}$$

where $\{k_i\}$ are the effective ozone cross sections and $\{a_i\}$ are the weighting coefficients obeying $\sum_{i=1}^{n} a_i = 1$.

In the Kato et al. method, only one exponential function ($n = 1$) is used for each KB to estimate the average transmissivity $T_{O_{3KB}}$:

$$T_{O_{3KB}} = e^{-k_{KB} \frac{u}{\mu_0}} \,. \tag{4}$$

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Kato et al. (1999) have chosen the ozone cross section at the central wavelength for each KB #3 or KB #4 for a temperature of 203 K: $k_{\mathrm{KB3}} = 5.84965 \times 10^{-19}\,\mathrm{cm}^2$ and $k_{\mathrm{KB4}} = 4.32825 \times 10^{-20}\,\mathrm{cm}^2$.

3 Effective ozone cross section

Is there a single effective ozone cross section that may represent the absorption over the whole interval? In that case, this effective cross section k_{eff} is determined for each KB from the combination of Eqs. (2) and (3) with $n = 1$:

$$T_{\mathrm{O_{3eff}}} = e^{-k_{\mathrm{eff}}\frac{u}{\mu_0}} = \frac{1}{I_{0\Delta\lambda}} \int\limits_{\Delta\lambda} I_{0\lambda} e^{-k_\lambda \frac{u}{\mu_0}} \mathrm{d}\lambda \,. \tag{5}$$

This equation may be rewritten

$$k_{\mathrm{eff}} \frac{u}{\mu_0} = \ln \frac{1}{I_{0\Delta\lambda}} \int\limits_{\Delta\lambda} I_{0\lambda} e^{-k_\lambda \frac{u}{\mu_0}} \mathrm{d}\lambda \,. \tag{6}$$

Several simulations are made to study this hypothesis. The ozone cross sections are those from Molina and Molina (1986) at 226, 263 and 298 K, and the top-of-atmosphere solar spectrum of Gueymard (2004) is used. The ozone cross sections at 203 K are obtained by linear extrapolation for each wavelength (Fig. 1). Samples of 10 000 pairs (μ_0, u) were generated by a Monte-Carlo technique. The random selection of the solar zenith angles follows a uniform distribution in [0°, 80°]. Similarly to what was done by Lefevre et al. (2013) and Oumbe et al. (2014), u is computed in Dobson unit as:

$$u = 300\beta + 100 \tag{7}$$

where β follows the beta distribution with A parameter = 2, and B parameter = 2.

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The 10 000 simulations yield a set X of $\left(\frac{u}{\mu_0}\right)$ and a set Y of values $\ln \frac{1}{I_{0\Delta\lambda}} \int_{\Delta\lambda} I_{0\lambda} e^{-k_\lambda \frac{u}{\mu_0}} d\lambda$.

Equation (6) is then

$$k_{\text{eff}} X = Y \tag{8}$$

and k_{eff} can be found by least-square fitting technique. For the KB #3 and #4, the values obtained are respectively $k_{\text{eff3}} = 2.29 \times 10^{-19}\,\text{cm}^2$ and $k_{\text{eff4}} = 2.65 \times 10^{-20}\,\text{cm}^2$. The average transmissivity $T_{O_{3\text{eff}}}$ with the effective ozone cross section is then computed by Eq. (5).

Estimated transmissivities $T_{O_{3\text{KB}}}$ and $T_{O_{3\text{eff}}}$ computed with Eqs. (4) and (5) using a second set of 10 000 pairs (μ_0, u) randomly selected are compared to the reference transmissivity $T_{O_3\Delta\lambda}$computed with Eq. (2) for each KB (Fig. 2). In KB #3, $T_{O_{3\text{KB}}}$ (red line) strongly underestimates $T_{O_3\Delta\lambda}$ meaning that the single ozone cross section adopted by Kato et al. is too large. On the contrary, $T_{O_{3\text{eff}}}$ (blue line) exhibits a large overestimation meaning that the efficient ozone cross section k_{eff} is too low. That may be explained by the fact that the solar radiation at the short wavelengths is completely absorbed and therefore becomes somewhat unimportant for the effective ozone cross sections. In this interval, the ozone cross section is strongly variable as shown in Fig. 1. Since k_{eff} is the optimal value reducing as much as possible the discrepancy between $T_{O_{3\text{eff}}}$ and $T_{O_3\Delta\lambda}$, it may be concluded that a single effective ozone cross section may not accurately represent the absorption over the whole KB #3.

In KB #4, $T_{O_{3\text{KB}}}$ (red line) noticeably underestimates $T_{O_3\Delta\lambda}$ meaning that the single ozone cross section adopted by Kato et al. is too large. $T_{O_{3\text{eff}}}$ is closer to $T_{O_3\Delta\lambda}$ though it exhibits underestimation when $T_{O_3\Delta\lambda} < 0.47$ and overestimation when $T_{O_3\Delta\lambda} > 0.47$. Like previously stated, it may be concluded that a single effective ozone cross section may not accurately represent the absorption over the whole KB #4.

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4 New parameterization

The new parameterization $T_{O_{3new}}$ for computing $T_{O_3\Delta\lambda}$ consists in using Eq. (3) with n greater than 1 but as small as possible to decrease the number of calculations while retaining a sufficient accuracy. n can be seen as the number of sub-interval $\delta\lambda_i$ included in $\Delta\lambda$ for which effective ozone cross section and weighting coefficients can be defined. The greater the n, the greater the number of calculations, the more accurate the modelling of $T_{O_3\Delta\lambda}$.

One solution is obtained by setting n to 4 and adopting equal weights for the sub-intervals for both KB #3 and #4. It comes:

$$T_{O_{3new}} = \sum_{i=1}^{4} 0.25 e^{-k_i u/\mu_0}, \quad (9)$$

where k_i is the effective ozone cross section for each of the four sub-intervals. Using a third set of 10 000 randomly selected pairs (μ_0, u), from which $T_{O_3\Delta\lambda}$ is computed (Eq. 2), the optimal set of four k_i minimizing the discrepancy between $T_{O_3\Delta\lambda}$ and $T_{O_{3new}}$ is obtained by the algorithm of Levenberg–Marquardt. Table 1 gives for each KB, the sub-intervals and their corresponding effective ozone cross section k_i, weight a_i for computing $T_{O_{3new}}$. The advantage is that such parameterization is defined once for all.

Reference transmissivity $T_{O_3\Delta\lambda}$ and estimated transmissivity $T_{O_{3new}}$ are computed with respectively Eqs. (2) and (9) using a fourth set of 10 000 pairs (μ_0, u) randomly selected and are compared to each other for each KB (Fig. 3). $T_{O_{3KB}}$ (red line) is also reported in Fig. 3. The difference between $T_{O_{3KB}}$ and $T_{O_{3new}}$ is striking. In each KB, $T_{O_{3new}}$ is almost equal to $T_{O_3\Delta\lambda}$ in all cases. While the mean value for $T_{O_3\Delta\lambda}$ is respectively 0.0314 for KB #3 and 0.6360 for KB #4 for this data set, the maximum error in absolute value in transmissivity is respectively 0.0006 and 0.0041.

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5 Practical implementation in radiative transfer model: the case of libRadtran

The file *o3.dat* in libRadtran depicts ozone absorption. In the corresponding file, a header of seven lines describes the meanings of the following three columns. The first column contains the number of the spectral interval: KB #1 to 32. The second one gives the number of quadrature points in each KB; the value is 1 in UV bands. The third column can be either the value of the single ozone cross section in each wavelength interval expressed in cm^2 or –1 when the number of quadrature point is greater than one. In this last case, libRadtran refers to netcdf file *cross_section.table._O3.noKB.cdf* – where *noKB* is the number of the KB – that contains the weight, the effective ozone cross section dependent of temperature and pressure.

Including the new parameterization needs two actions. Firstly, for KB #3 and KB #4, set the second column to 4 and the third column to –1. Secondly, create two netcdf files named *cross_section.table._O3.03.cdf* and *cross_section.table._O3.04.cdf* containing for each interval their corresponding weight and effective cross sections given in Table 1.

6 Conclusions

The present paper has shown the inadequacy of parameterization of the transmissivity due to the sole ozone absorption based on a single ozone cross section for the bands KB #3 [283, 307] nm and KB #4 [307, 328] nm in the *k*-distribution method and correlated-*k* approximation of Kato et al. (1999). A novel parameterization using more quadrature points better represents the transmissivity with maximum error of respectively 0.0006 and 0.0041 for interval KB #3 and #4. This opens the way for more accurate estimates of the irradiance at surface in the UV range, and possibly in narrower spectral bands such as UV-A and UV-B.

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Table 1. Sub-intervals, effective ozone absorption coefficient and weight in each wavelength interval for computing $T_{O_{3new}}$.

Interval $\Delta\lambda$, nm	Sub-interval $\delta\lambda_i$, nm	Effective ozone cross section k_i (10^{-19} cm^2)	Weight a_i
KB #3	283–292	11.360	0.250
283–307	292–294	8.551	0.250
	294–301	3.877	0.250
	301–307	1.775	0.250
KB #4	307–311	0.938	0.250
307–328	311–321	0.350	0.250
	321–323	0.153	0.250
	323–328	0.076	0.250

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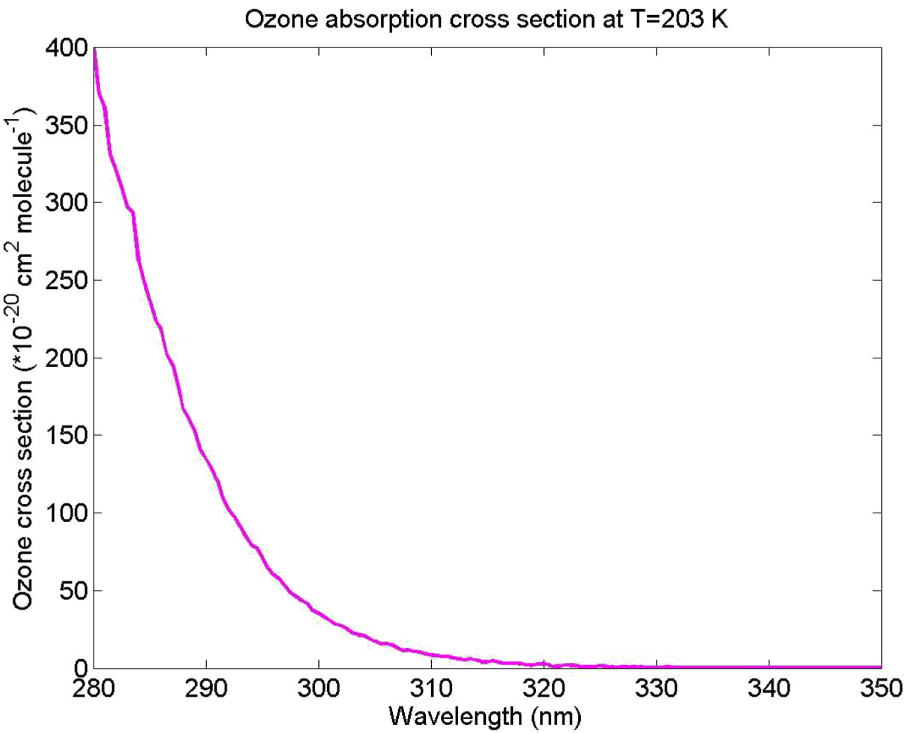

Figure 1. Ozone cross sections at 203 K as a function of the wavelength.

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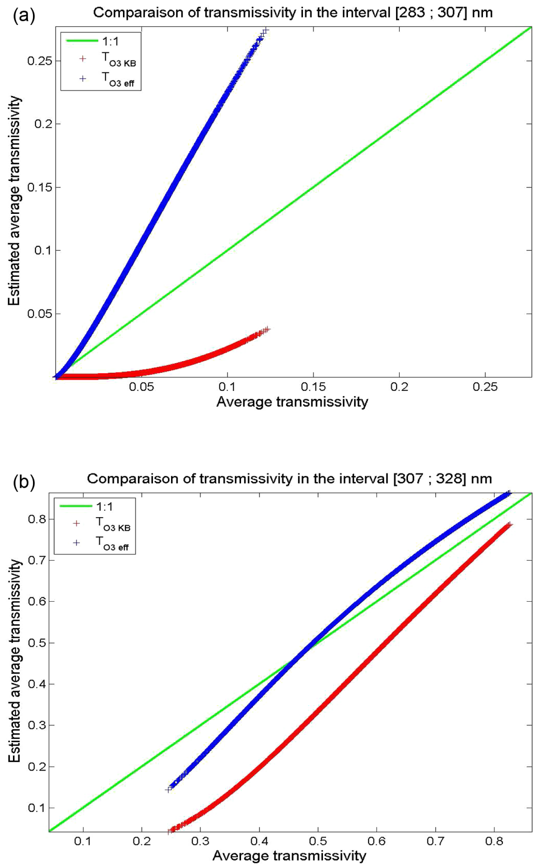

Figure 2. Scatterplot between average transmissivity $T_{O_3\Delta\lambda}$ and the estimated $T_{O_{3KB}}$ (red line) and $T_{O_{3eff}}$ (blue line) for **(a)** KB #3 [283, 307] nm; **(b)** KB #4 [307, 328] nm.

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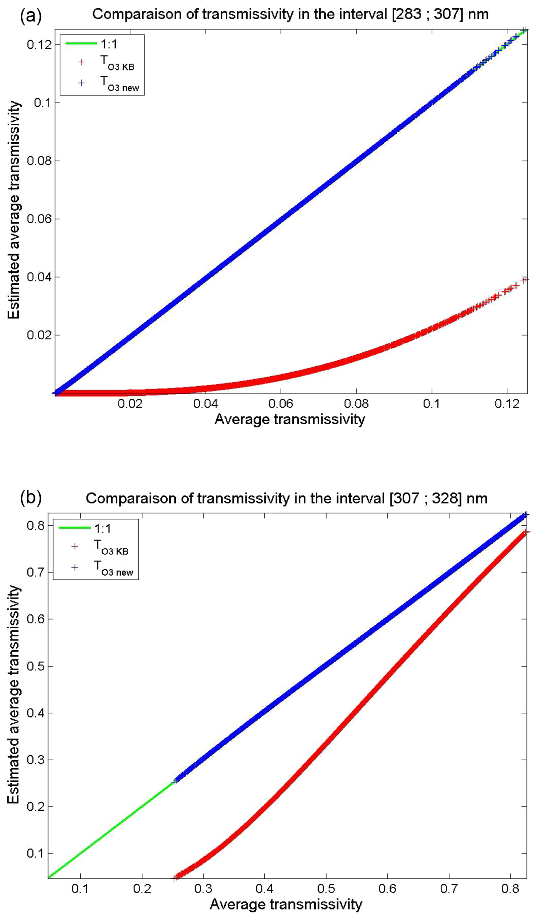

Figure 3. Scatterplot between average transmissivity $T_{O_{3\Delta\lambda}}$ and the estimated $T_{O_{3KB}}$ (red line) and $T_{O_{3new}}$ (blue line) for **(a)** KB #3 [283, 307] nm; **(b)** KB #4 [307, 328] nm.