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Published in:

RADIATION PROCESSES IN THE ATMOSPHERE AND OCEAN

DOI:

[10.1063/1.4975567](https://doi.org/10.1063/1.4975567)

Published: 01/01/2017

Document Version

Publisher's PDF, also known as Version of record

Please cite the original version:

Kärhä, P., Vaskuri, A., Gröbner, J., Egli, L., & Ikonen, E. (2017). Monte Carlo analysis of uncertainty of total atmospheric ozone derived from measured spectra. In *RADIATION PROCESSES IN THE ATMOSPHERE AND OCEAN: International Radiation Symposium (IRC/IAMAS) - Radiation Processes in the Atmosphere and Ocean [110005]* (AIP Conference Proceedings; Vol. 1810). American Institute of Physics.
<https://doi.org/10.1063/1.4975567>

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Cite as: AIP Conference Proceedings **1810**, 110005 (2017); <https://doi.org/10.1063/1.4975567>
Published Online: 22 February 2017

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Monte Carlo Analysis of Uncertainty of Total Atmospheric Ozone Derived from Measured Spectra

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Abstract. We present a Monte Carlo based model to study effects that possible correlations in spectral irradiance data may have on the derived total ozone column values. Correlations may produce systematic errors in the spectral irradiance which behave differently from uncorrelated data. The effects are demonstrated by analyzing the data of one day's measurements.

INTRODUCTION

Monte Carlo (MC) analysis is a convenient method to derive uncertainties of quantities in cases where analytical calculation is complicated. In MC analysis, input quantities are varied within their uncertainties and the resulting deviations in the derived quantities give their uncertainties.

With spectrally derived quantities, where the quantity is calculated from a measured spectrum using e.g. integration or recursive analysis, MC analysis can be carried out by varying the measured spectral irradiance values. However, this approach may be problematic because of correlations in the data. The uncertainties of the spectral data may hide systematic wavelength dependent errors e.g. due to interpolation of data, wavelength shifts, geometrical factors, or systematic errors in the standard lamps. Guide to the Expression of Uncertainty in Measurement [1] presents ways to take correlation in data into account. However, if the correlations are unknown, these methods cannot be used.

With unknown correlations, assumptions need to be made. The most typical assumption is that the data are not correlated. This may lead into underestimated uncertainties, because spectrally varying systematic errors often produce larger deviations than wavelength independent noise-like variations.

Kärhä *et al.* have recently proposed a method to study measurement errors that unknown correlations may introduce in derived quantities and applied this to study uncertainties of the correlated color temperature [2]. Spectral error functions with varying order of complexity are formed and used to find maximum errors that the uncertainties permit. In this paper, we test the method [2] to study uncertainties of the total atmospheric ozone determined from spectral measurements of direct solar UV irradiance [3].

MATERIALS AND METHODS

Deriving ozone from measured spectrum

Huber *et al.* have presented a method for deriving total ozone column values (*TOC*) from high resolution spectral measurements of direct solar UV irradiance [3]. In our analysis, we consider measurements in the spectral range $\lambda = [295, 340]$ nm with wavelength interval $\Delta\lambda = 0.5$ nm. *TOC* is determined by fitting model calculations to the measured spectra.

Spectral irradiance $E(\lambda)$ measured at Earth level can be calculated from the extraterrestrial irradiance $E_{Ext}(\lambda)$ by

$$E(\lambda) = E_{Ext}(\lambda) \cdot e^{-\tau(\lambda) \cdot m}, \quad (1)$$

where m is the relative air mass and $\tau(\lambda)$ is the optical depth of the atmosphere. $\tau(\lambda)$ consists of factors such as the ozone absorption cross section $\alpha_{O_3}(\lambda)$, the total ozone column TOC , the Rayleigh scattering optical depth $d_{Rayleigh}(\lambda)$ and the aerosol optical depth $d_{aod}(\lambda)$.

In the analysis, TOC and the aerosol optical depth are varied to minimize the differences between the measured and the modeled irradiance values using least squares fitting. Convolution is accounted for by convoluting the extraterrestrial data with the instrument's slit function.

FIGURE 1. Examples of error functions produced using Eq. (3). White Gaussian noise has been added to the lowest figure to demonstrate that at the Nyquist criterion, correlation is lost, and the function resembles noise.

Model for studying effects of possible correlations

The model is based on orthogonal base functions formed as a series of Sines,

$$E(\lambda) = \begin{cases} f_i(\lambda) = \sqrt{2} \sin \left[i \left(2\pi \frac{\lambda - \lambda_1}{\lambda_2 - \lambda_1} \right) + \phi_i \right] \\ f_0(\lambda) = 1 \end{cases}, \quad (2)$$

which all have variances $\sigma^2 = 1$. Wavelength limits $\lambda_1 = 295$ nm and $\lambda_2 = 340$ nm may be varied e.g. in the case of noisy data. Phase terms ϕ_i vary the locations of sign changes within the wavelength range. The phase shift of each base function is uniformly distributed.

An error function is formed by combining the $N + 1$ first terms with varying weights,

$$\delta(\lambda) = \sum_{i=0}^N \gamma_i f_i(\lambda). \quad (3)$$

The weights γ_i are chosen randomly from the surface of an $N + 1$ dimensional sphere to keep variance at 1. Figure 1 shows three examples of error functions with three different values of N . The spectral irradiance data are disturbed as

$$E_e(\lambda) = [1 + \delta(\lambda) u_c(\lambda)]E(\lambda), \quad (4)$$

and the resulting $E_e(\lambda)$ are used to calculate TOC . The results are repeated to calculate standard deviations, and the order of complexity N is varied to see how different waveforms affect the uncertainties.

RESULTS AND DISCUSSION

The method was applied on spectra measured in Mauna Loa, USA on Nov 30, 2001 at 6:14 – 18:54. The analyzed TOC was ~ 264 DU. Figure 2 presents uncertainties at noon (12:20) analyzed for three uncertainty levels in spectral irradiance, $u_c(k=1) = 1\%$, 2.5% , and 5% . The maximum uncertainty is found at $N = 1$ indicating that a simple slope-like error would produce the highest uncertainty. The first term, $N = 0$, indicates that fully correlated data, where all wavelengths have the same error, produces very small errors in TOC . The last data point at $N = 45$, which is the Nyquist limit for the analysis, gives an uncertainty in the case assuming no correlations. The black solid lines demonstrate that the analysis method is scalable. Values obtained with $u_c = 1\%$ can thus be used as sensitivities and scaled with the actual uncertainty. For a typical expanded uncertainty value $U(k=2) = 5\%$, we can see that the resulting uncertainty in TOC is $U_{TOC} = 0.3\%$ assuming full correlation, $U_{TOC} = 0.8\%$ assuming no correlation, and $U_{TOC} = 2.75\%$ assuming the worst possible correlation. These values give practical limits for the uncertainty. Assuming that the correlation is equally distributed among the three cases would yield $U_{TOC} = 1.3\%$ (3.4 DU).

FIGURE 2. Uncertainties of TOC at noon as a function of the order of complexity N at three different levels of uncertainty in spectral irradiance indicated with symbols in the figure legend. The black solid lines obtained by multiplying the 1% uncertainties indicate scalability of the model.

Figure 3 presents the uncertainties of TOC analyzed throughout the day assuming $u_c(k=1) = 2.5\%$ for the spectral irradiance. Sensitivity of the TOC uncertainty on uncertainty in irradiance is highest at Noon and lowest in the evening and morning. On the other hand, uncertainties of spectral irradiance are also higher in the evening and morning due to lower signal levels, which the model does not yet take into account.

FIGURE 3. Uncertainties of *TOC* during the day at various order of complexity levels *N* indicated in the figure legend.

CONCLUSIONS

We have demonstrated that the uncertainty of *TOC* derived from direct solar UV spectral irradiance measurements may be seriously affected by possible spectrally varying systematic wavelength dependent errors that unknown correlations may well produce within the uncertainties. We have also presented a model that can be used to study the limits of these errors. The presented model only takes into account uncertainty of the spectral irradiance. In practice, also factors such as the extraterrestrial irradiance $E_{Ext}(\lambda)$, the air mass m , the ozone absorption cross section $\alpha_{O_3}(\lambda)$, and the aerosol optical depth $d_{aod}(\lambda)$ have uncertainties that should be accounted for. Some of these factors are located in the exponent of Eq. 1 and thus require separate analysis.

ACKNOWLEDGMENTS

This work has been supported by the European Metrology Research Programme (EMRP) within the joint research project ENV59 “Traceability for atmospheric total column ozone” (ATMOZ). The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union. Tomi Pulli is acknowledged for fruitful discussions on the mathematics.

REFERENCES

1. JCGM 101:2008, Evaluation of measurement data — Guide to the expression of uncertainty in measurement (Joint Committee for Guides in Metrology JCGM, 2008), 120 p.
2. P. Kärh, A. Vaskuri, H. Mntynen, N. Mikkonen, and E. Ikonen, “Method for estimating effects of unknown correlations in spectral irradiance data on uncertainties of spectrally integrated colorimetric quantities,” (submitted).
3. M. Huber, M. Blumthaler, W. Ambach, and J. Staehelin, “Total atmospheric ozone determined from spectral measurements of direct solar UV irradiance,” *Geophys. Res. Lett.* **22**, 53–56 (1995).