Aalto University
School of Electrical
Engineering

pmod wrc

Model for simulating uncertainties of TOC of spectral measurements applied to measurements at Izaña field campaign

Petri Kärhä[1], Anna Vaskuri[1], Julian Gröbner[2], Luca Egli[2], and Erkki Ikonen[1]

1. Aalto University School of Electrical Engineering, Espoo, Finland
2. PMOD / WRC, Davos, Switzerland

Introduction

- Total Ozone Column TOC can be determined from the ground-based spectral measurements of direct solar UV irradiance between 290–350 nm [1].
- The spectral data may hide systematic wavelength dependent errors due to correlations [2], which may lead into underestimated *U*(TOC) values.
- We have developed a Monte Carlo -based model to estimate uncertainties of the derived TOC values in presence of correlations.

1. M. Huber et al., “Total atmospheric ozone determined from spectral measurements of direct UV irradiance,” *Geophys. Res. Lett.* **22**, 1995.
2. P. Kärhä et al., “Method for estimating effects of unknown correlations in spectral irradiance data on uncertainties of spectrally integrated colorimetric quantities,” (submitted).

Atmospheric model for TOC

- The relationship between the measured spectral irradiance $E(\lambda)$ and extra-terrestrial solar spectrum $E_{ext}(\lambda)$ can be defined as [1]

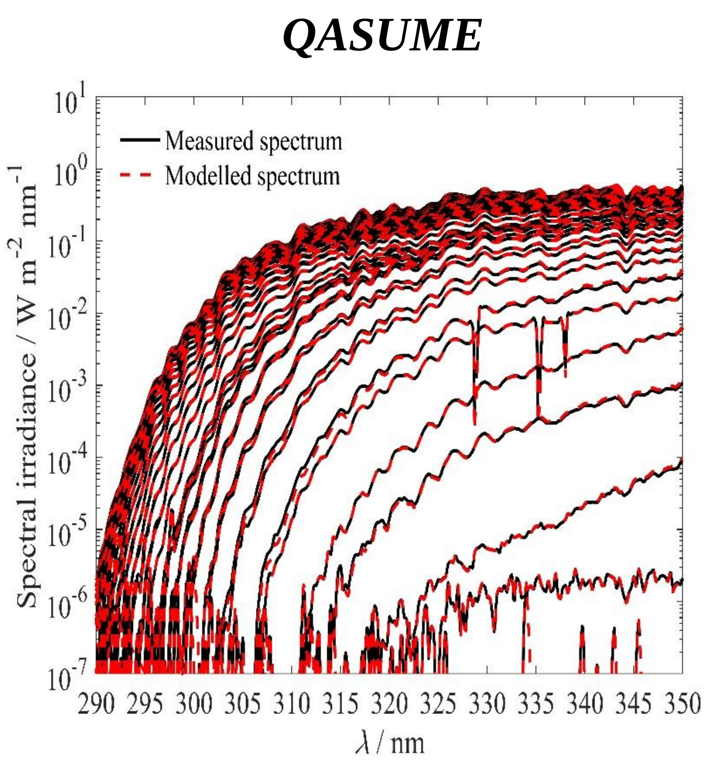
$$E(\lambda) = E_{\mathrm{ext}}(\lambda) \cdot e^{-\left[\alpha_{\mathrm{O_3}}(\lambda) \cdot TOC + d_{\mathrm{R}}(\lambda) + d_{\mathrm{AOD}}(\lambda)\right] \cdot m},$$

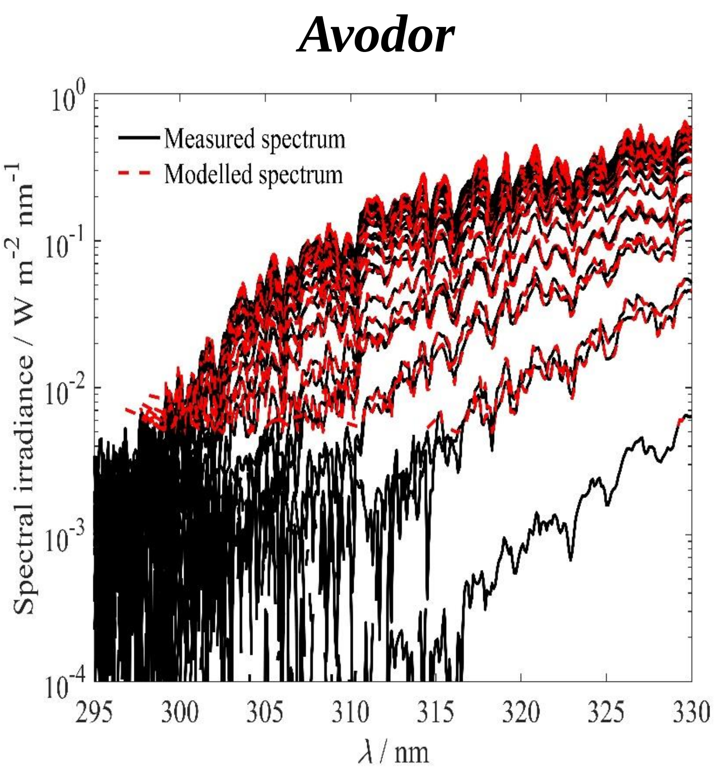
- where $\alpha_{O3}(\lambda)$ is the ozone absorption cross section, $d_R(\lambda)$ is the Rayleigh scattering optical depth, and m is the relative air mass. The aerosol optical depth is approximated as

$$d_{\mathrm{AOD}}(\lambda) = \beta \lambda^{-\alpha},$$

- where $\alpha \approx 1.4$ is the Ångström coefficient and β is a scaling factor (fitting parameters *TOC* and β).

Examples of fitting atmospheric model to the ground-based solar UV spectra.

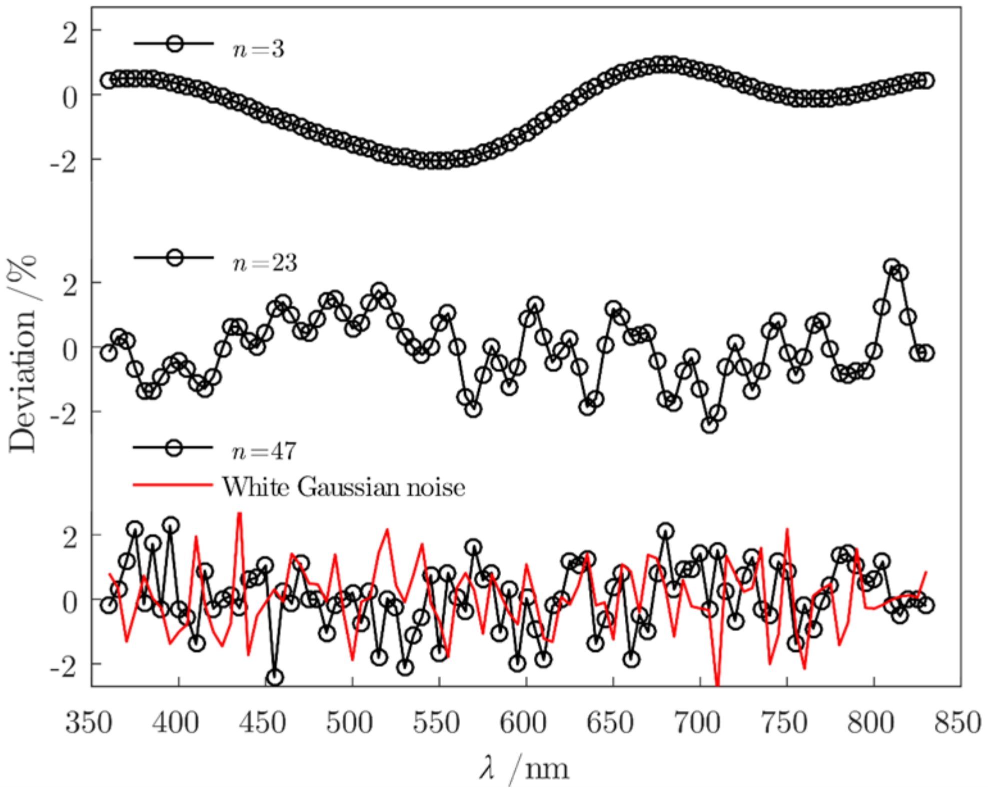




- Fittings carried out over wavelength regions with signal levels exceeding threshold noise floors (10^{-7} / $5x10^{-3}$). Least sq. fitting for logarithmic data.

Correlations in measurement data

- Uncertainty of spectral irradiance typically includes:
  - Noise
  - Uncertainty of standard lamp
  - Transfer uncertainties of calibrations
  - Residuals of corrections
  - Interpolation errors
- Uncertainties may hide spectrally varying errors, correlations
- Typically it is assumed that spectral irradiance data are uncorrelated, noise
- Correlated data behave differently in integrations or models
- Correlation matrix needed (if available). If not, correlations need to be estimated.



Uncertainty estimation

- Systematic deviations contained within uncertainties are reproduced using cumulative Fourier series with sinusoidal base functions f_i, where index i depicts the order of complexity of the deviation [2].
- f_0 depicts full correlation.
- $f_0 + f_1 + \ldots + f_N$ depicts random spectral deviation.
- $f_0 + f_1$ depicts unfavourable correlations, we found in Ref. [3] that slope type errors produce largest errors in *TOC*.
- User must have some knowledge to decide, which components to include.

3. P. Kärhä *et al.*, "Monte Carlo Analysis of Uncertainty of Total Atmospheric Ozone Derived from Measured Spectra," *AIP Conf. Proc.* **1810**, 2017.

Method for analyzing possible correlations

- Orthogonal base functions formed as a series of Sines with $\sigma = 1$, limits λ_1 and λ_2 depend on application.

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

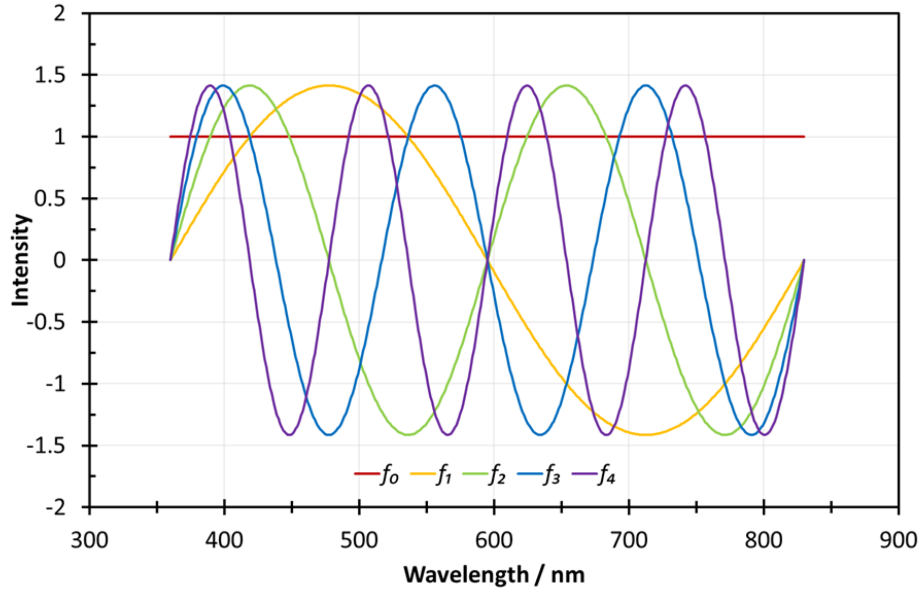
- An error function is formed by combining N+1 first terms with varying weights

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

- Weights γ_i are chosen randomly from the surface of N+1 dimensional sphere to keep variance 1.
- Data are disturbed as

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

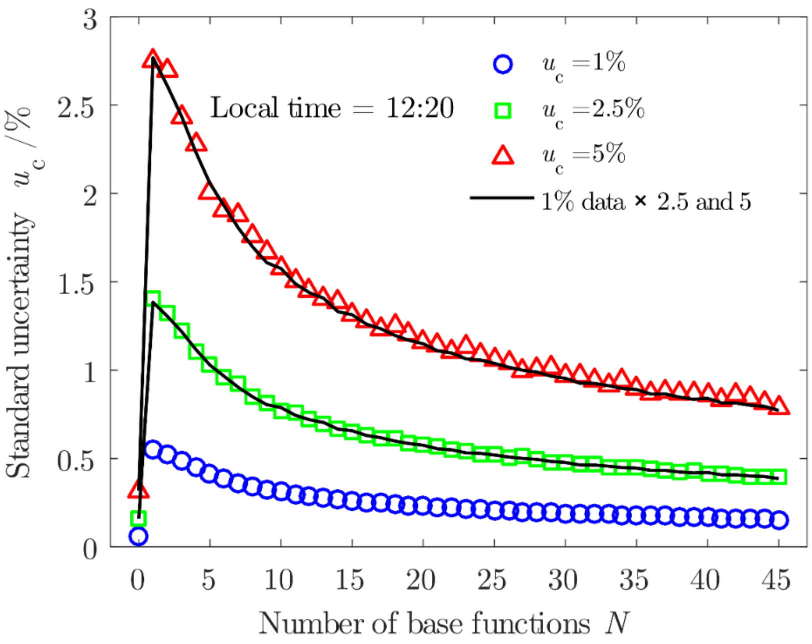
and used to calculate desired results *CCT* or *TOC*.
- Results are repeated to calculate standard deviations and N is varied.



$$P = \{\gamma_0, \gamma_1, \dots, \gamma_N\} = \left\{\frac{Y_0}{\sqrt{Y_0^2+Y_1^2+\dots+Y_N^2}}, \frac{Y_1}{\sqrt{Y_0^2+Y_1^2+\dots+Y_N^2}}, \dots, \frac{Y_N}{\sqrt{Y_0^2+Y_1^2+\dots+Y_N^2}}\right\}$$

Uncertainty of *TOC* at noon

- Spectra measured in Mauna Loa, USA on Nov 30, 2001, 6:14 – 18:54 analyzed.
- *TOC* was ~264 DU.
- Uncertainties at noon (12:20) analyzed for three uncertainties u_c (k = 1) = 1%, 2.5%, 5%
  - Maximum uncertainty at N = 1. Obviously a slope produces highest uncertainty.
  - Full correlation produces negligible uncertainty
  - Nyquist criterion (N=45) gives uncertainty assuming no correlations.
- For U (k = 2) = 5%, U_{FC} = 0.3%, U_{NC} = 0.8%, U_{UC} = 2.75%
- Assuming average of the three yields U = 1.3% (3.4 DU)



Uncertainty budget at local noon TOC = 279.3 ± 7.4 DU (k = 2)

Source of uncertainty	Standard uncertainty $E(\lambda)$ %	$\tau(\lambda) \cdot m$ %	Full	Correlation Unfavourable Fraction	Random	$u(TOC)$ DU
Measurement						
Standard lamp	1.0		1/3	1/3	1/3	0.51
Interpolation	0.2		0	1	0	0.35
Distance in calibration	0.2		1	0	0	0.25
Ageing of lamp	0.5		0	1	0	0.88
Drift of spectroradiometer	0.2		0	1	0	0.35
Linearity	0.3		0	1	0	0.53
Alignment	0.2		1	0	0	0.25
Other	0.2		1/3	1/3	1/3	0.10
Uncertainties related to $E(\lambda)$						
Extraterrestrial spectrum	2.3		1/6	2/3	1/6	2.14
Slit convolution	0.0					0.00
Wavelength shift due to air	0.0					0.00
Uncertainties related to $\tau(\lambda) \cdot m$						
Air mass (O_3 layer altitude of 7.9%)		0.025		(a)		0.02
Reference O_3 cross-section		1.0	1/3	1/3	1/3	1.30
Temperature of O_3 cross-section at -45 ± 15 °C		6.0		(b)		2.41
Aerosol optical depth (std. mean of the fit)		0.1	0	0	1	0.01
Rayleigh scattering optical depth		0.1	1/3	1/3	1/3	0.03

(a) Air mass varies as a function of ozone layer height.
(b) O_3 cross-section varies as a function of temperature.

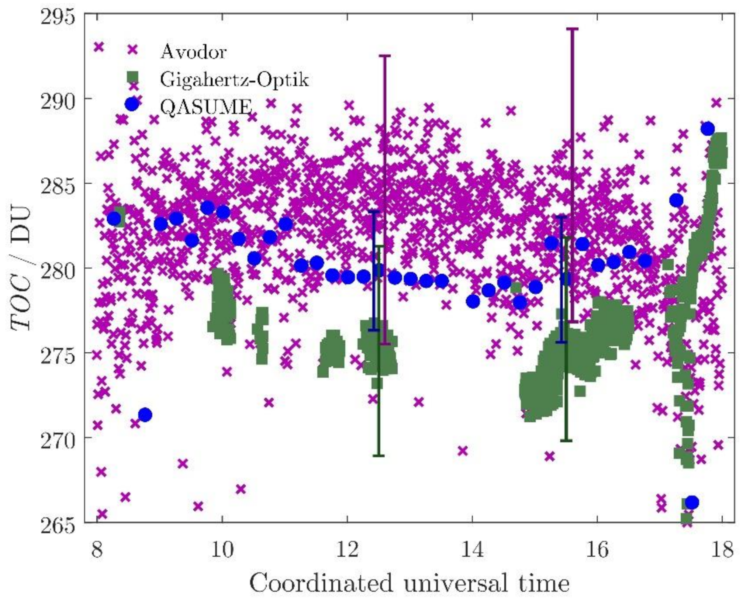
Application to Izana data

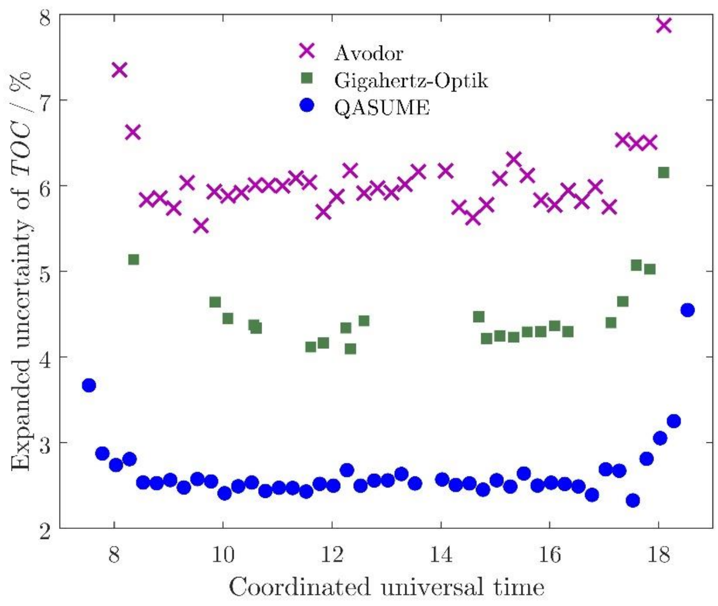
- Comparison of *TOC* derived from three spectral data sets (QASUME [4], Gigahertz-Optik [5], and Avodor) measured at Izaña, Tenerife Sept. 17, 2016.
- The measurement uncertainties were ~0.5% (unknown correlation), ~1.0% (unknown correlation), and ~2.5% (unfavourable correlation), respectively.
- Avodor correlations were considered worse because of noisy spectra, no straylight correction, and due to the distortion by the cut-off wavelength of 340 nm of the solar blind filter.
- Better results by fitting on logarithmic scale and by limiting the short wavelength range by the noise floor (10^{-7} for QASUME, $5 \cdot 10^{-3}$ for spectrographs).
- The model could be improved by adding stray light correction for array spectrometers and modelling vertical profiles for *TOC*, Rayleigh scattering and aerosols.

4. G. Hülsen *et al.*, "Traceability of solar UV measurements using the QASUME reference spectroradiometer," *Appl. Optics* **55**, 2016.

5. R. Zuber *et al.*, "A high dynamic stray light corrected array spectroradiometer for complex measurements in the UV spectral range," *NEWRAD 2017*, Tokyo, Japan, 2017.

Results and uncertainties





- On left, derived total ozone columns with k = 1 uncertainty bars for QASUME (290 – 350 nm, noise floor of 10^{-7}), Gigahertz-Optik (295 – 350 nm, noise floor of $5 \cdot 10^{-3}$), and Avodor (295 – 330 nm, noise floor of $5 \cdot 10^{-3}$). On right, the corresponding relative expanded uncertainties.

Discussion

- Major sources of uncertainty (k = 1)
  - Measurement of spectrum ~1 DU
  - Extraterrestrial spectrum ~2.1 DU
  - Reference O3 cross-section ~1.3 DU
  - Temperature of O3 cross-section ~2.4 DU
- Total uncertainties at noon (TOC = 280 DU) of the order of (k = 2)
  - QASUME 2.5 % / 7 DU
  - Gigahertz-Optik 4.3 % / 12 DU
  - Avodor 6 % / 17 DU
- Wavelength region used has an effect on values. We used noiseless data above threshold. Should rather weighting with $1/U^2$ be used?
- Uncertainties significantly larger than agreement of the 3 instruments. Many possible sources of error are the same in all devices.

EMRP ENV59 ATMOZ "Traceability for atmospheric total column ozone"

EMRP
European Metrology Research Programme
Programme of EURAMET
The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union
The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union
EURAMET