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School of Electrical Engineering

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Model for simulating uncertainties of TOC from multispectral measurements

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

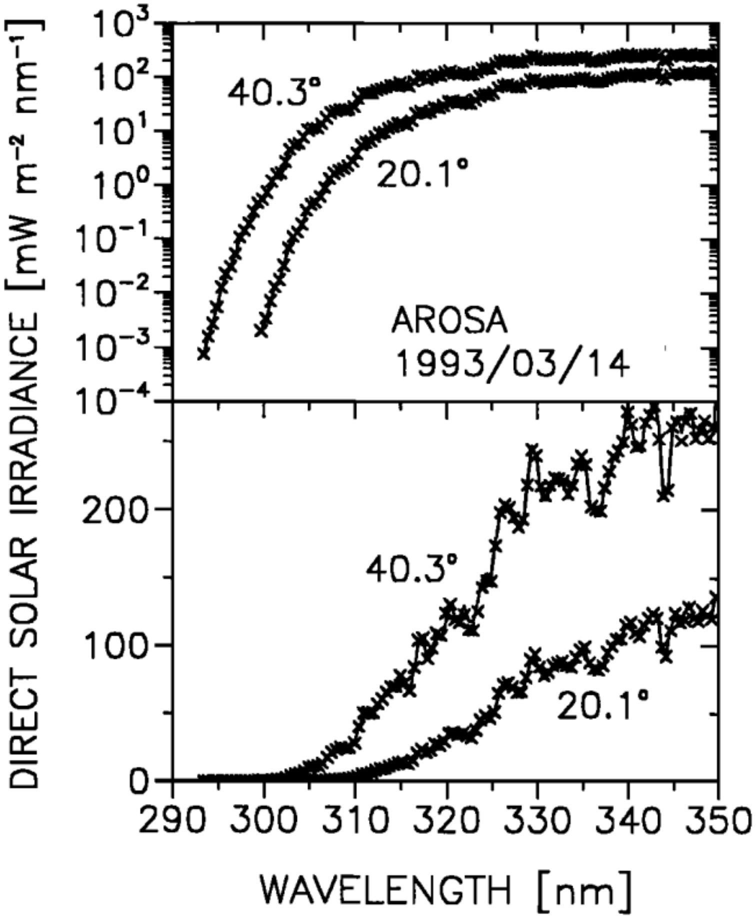
1. Aalto University School of Electrical Engineering, Espoo, Finland
2. PMOD / WRC, Davos, Switzerland

Contents

- Deriving ozone from measured spectrum
- Correlations in the measurement data
- MC-based method for analyzing correlation
- Uncertainty of correlated color temperature *CCT* of a lamp
- Uncertainty of total ozone column *TOC*

Deriving ozone from measured spectrum

- High resolution spectral measurements of direct solar UV irradiance
- λ = [290, 350] nm, $\Delta\lambda$ = 0.5 nm
- Total atmospheric ozone amount determined by fitting model calculations to the measured spectra
- M. Huber, M. Blumthaler, and W. Ambach, "Total atmospheric ozone determined from spectral measurements of direct solar UV irradiance," *Geophys. Res. Lett.* **22**, 53-56 (1995).

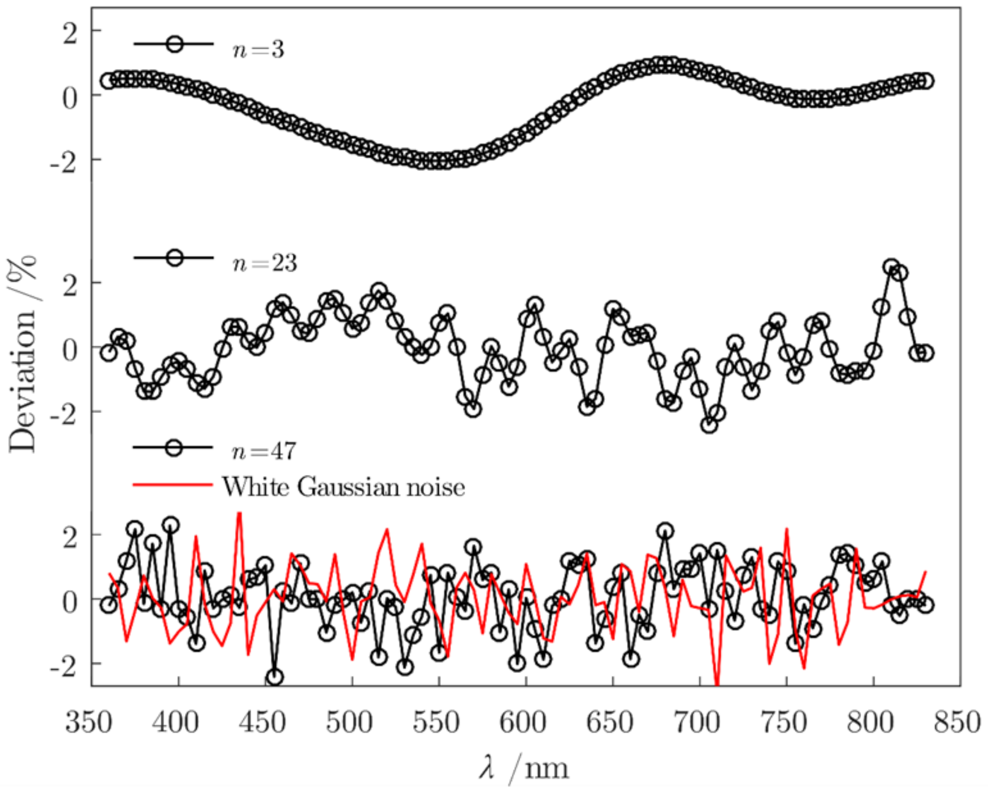


Model calculation

- Extraterrestrial solar spectrum $E_{Ext}(\lambda)$ used as starting point
- Effect of atmosphere is modeled as
- $E(\lambda) = E_{Ext}(\lambda) \cdot e^{-\tau(\lambda) \cdot m}$, where
- $\tau(\lambda) = \alpha_{O_3}(\lambda) \cdot TOC + d_{Rayleigh}(\lambda) + d_{aod}(\lambda)$
  - m is the relative air mass
  - $\tau(\lambda)$ is the optical depth of the atmosphere
  - $\alpha_{O_3}(\lambda)$ is the ozone absorption cross section
  - TOC is the total ozone column
  - $d_{Rayleigh}(\lambda)$ is the Rayleigh scattering optical depth
  - $d_{aod}(\lambda) = \beta \cdot \lambda^{-1.4}$ is the aerosol optical depth, λ in μm.
- In the analysis, TOC and β are varied to minimize difference between measured and modeled irradiances using least squares fitting
- Convolution accounted for.
- Simplified model to speed up calculations.

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 due to 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.



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

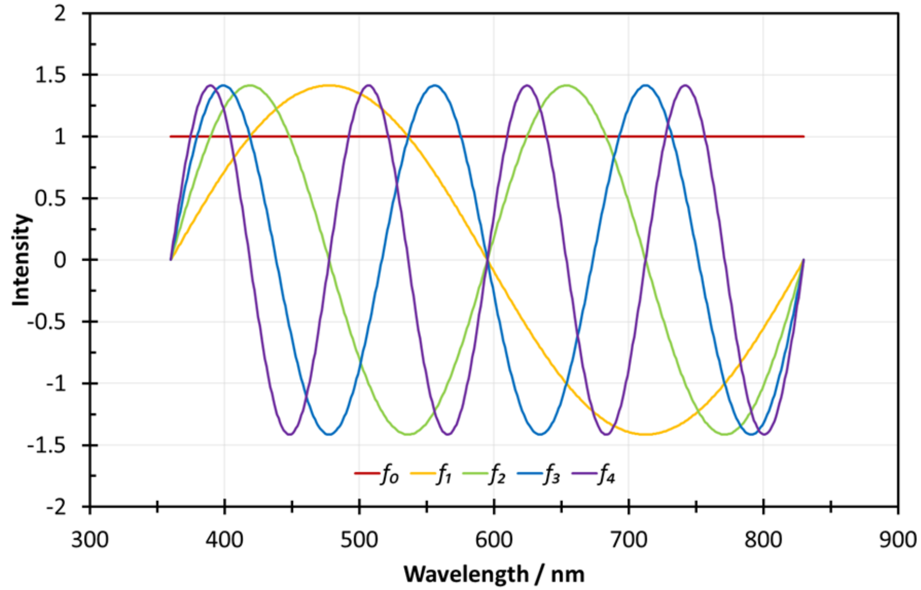
$$\delta(\lambda) = \sum_{i=0}^{N} \gamma_i f_i(\lambda)$$

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

$$E_\mathrm{e}(\lambda) = [1 + \delta(\lambda)\, u_\mathrm{c}(\lambda)]E(\lambda)$$

and used to calculate desired results *CCT* or *TOC*.

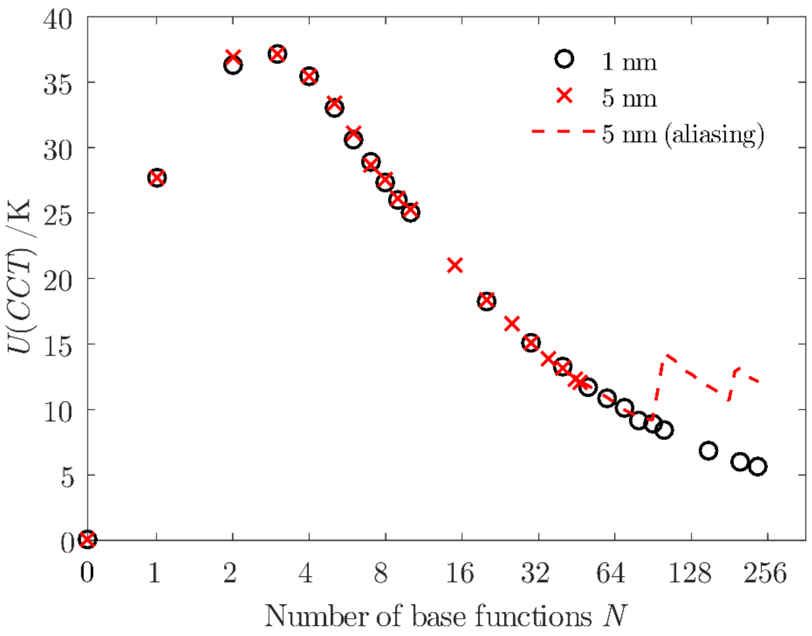
- Results are repeated to calculate standard deviations and *N* is varied.



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

Correlated color temperature *CCT* = 2856 K of a lamp

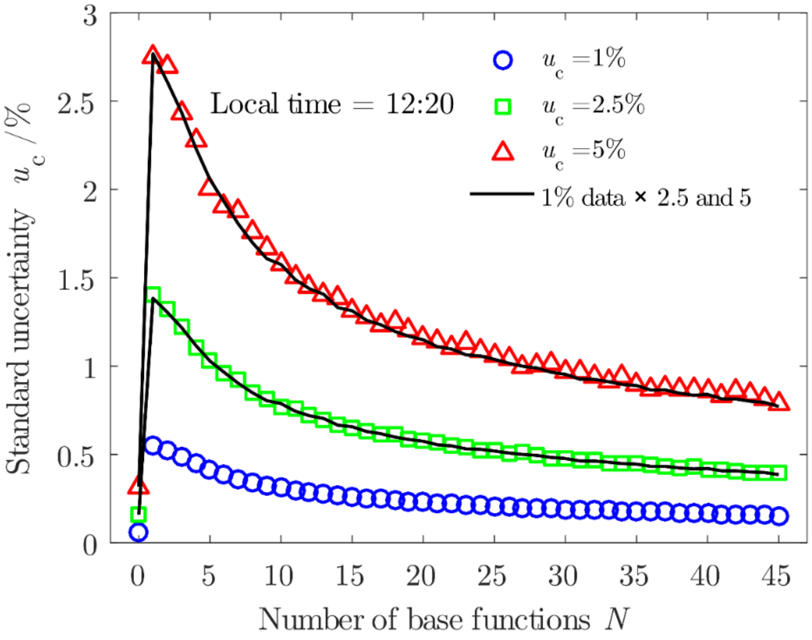
- *CCT* is the temperature of a Planckian radiator whose color coordinates (*u*, *v*) are closest to the color coordinates of the lamp.
- Assuming 1% standard uncertainty at each wavelength.
- Obtained graph gives three important values
  - Uncertainty with full correlation $N = 0$, $U_{FC} = 0$, in the case of *CCT*
  - Uncertainty with no correlation at Nyquist criterion $N = 235$, $U_{NC} = 5.6$ K
  - Uncertainty with unfavorable correlation $N = 3$, $U_{UC} = 37.2$ K. Worst case with 6 sign change within wavelength range.
- Unambiguous value can not be derived if correlations are unknown. One possibility to use average of the three values $U = 14$ K.



P. Kärhä, A. Vaskuri, H. Mäntynen, N. Mikkonen, and E Ikonen, "Method for estimating effects of unknown correlations in spectral irradiance data on uncertainties of spectrally integrated colorimetric quantities" (submitted).

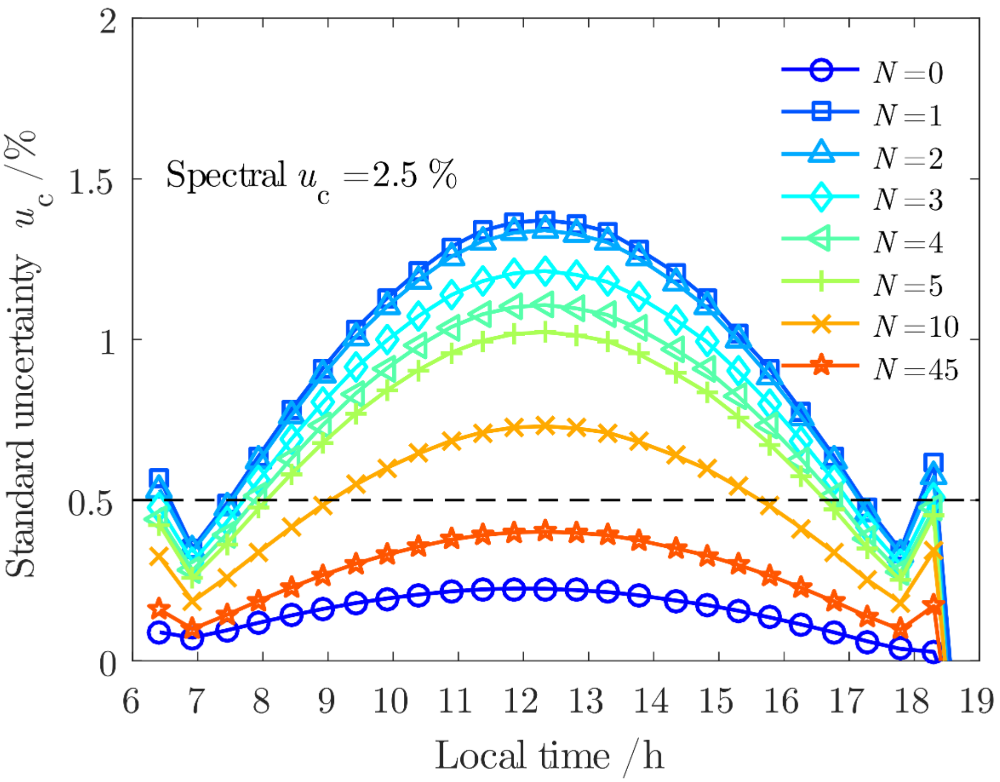
Uncertainty of *TOC* at noon

- 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.
  - Process is linear and scalable! Data can be used as sensitivities when analyzing uncertainties.
- For U (k = 2) = 5%, U_{FC} = 0.3%, U_{NC} = 0.8%, U_{UC} = 2.75%
- Assuming again average of the three yields U = 1.3% (3.4 DU)



Uncertainty of TOC during the day

- Uncertainties of *TOC* analyzed throughout the day assuming u_c (k = 1) = 2.5%.
- Sensitivity of O_3 uncertainty on uncertainty in irradiance is highest at Noon and lowest in the evening and morning due to length of the air mass.
- On the other hand, uncertainties of spectral irradiance are also higher in the evening and morning due to lower signal levels.



Conclusions

- In order to calculate uncertainties of quantities derived from spectra (*CCT*, *TOC*), uncertainty of spectral irradiance is not enough. Correlation data is needed as well.
- Correlation may decrease but also increase the uncertainties of derived quantities.
- We have presented a Monte Carlo based method for studying effects that possible correlations have on uncertainties of quantities derived from spectra. Can be used if correlation data is not available.
- Gives three useable values: Uncertainty assuming full correlation, Uncertainty assuming no correlations, and Uncertainty assuming an unfavorable case of correlations. The three values give limits within which the uncertainty must reside.
- *TOC* is most sensitive to a slope-type of error in spectral irradiance, whereas *CCT* suffers mostly from an error with 6 sign changes within the wavelength range of interest.

EMRP ENV59 ATMOZ "Traceability for atmospheric total column ozone"

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