Model for simulating uncertainties of TOC from multispectral measurements

Petri Kärhä¹, Anna Vaskuri¹, Nikke Mikkonen¹, Julian Gröbner², Luca Egli², and Erkki Ikonen¹

1. Aalto University School of Electrical Engineering, Espoo, Finland
2. PMOD / WRC, Davos, Switzerland
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Deriving ozone from measured spectrum

- High resolution spectral measurements of direct solar UV irradiance
  - $\lambda = [290, 350]$ nm, $\Delta \lambda = 0.5$ nm
- Total atmospheric ozone amount determined by fitting model calculations to the measured spectra
Model calculation

- Extraterrestrial solar spectrum $E_{Ext}(\lambda)$ used as starting point
- Effect of atmosphere is modeled as
  
  $$E(\lambda) = E_{Ext}(\lambda) \cdot e^{-\tau(\lambda)m},$$
  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, $\lambda$ in $\mu$m.

- In the analysis, $TOC$ and $\beta$ 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 $\lambda_1$ and $\lambda_2$ depend on application.
  \[
  \begin{align*}
  f_i(\lambda) &= \sqrt{2} \sin \left[ i \left( 2\pi \frac{\lambda - \lambda_1}{\lambda_2 - \lambda_1} \right) + \phi_i \right] \\
  f_0(\lambda) &= 1
  \end{align*}
  \]
- 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 $\gamma_i$ 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.

\[
P = \{ Y_0, Y_1, \ldots, Y_N \} = \left\{ \frac{Y_0}{\sqrt{Y_0^2 + Y_1^2 + \cdots + Y_N^2}}, \frac{Y_1}{\sqrt{Y_0^2 + Y_1^2 + \cdots + Y_N^2}}, \ldots, \frac{Y_N}{\sqrt{Y_0^2 + Y_1^2 + \cdots + Y_N^2}} \right\}
\]
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.

Uncertainty of \( TOC \) at noon

- Spectra measured in Mauna Loa, USA on Nov 30, 2001, 6:14 – 18:54 analyzed.
- \( TOC \) was \( \sim 264 \) 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.