A simulation tool to model ozone retrieval uncertainties of Brewer and Dobson instruments

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and

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(“ATMOZ Uncertainty Team”)

The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union
Project ATMOZ

Main objective:
A traceable and harmonized global total column ozone network within 1%

5 Workpackages (WP):

• **WP 1:** Radiometric characterization of Dobson, Brewer & Array spectrordiometers
• **WP 2:** Development of array-based solar UV spectroradiometers
• **WP 3:**
  - Improved and consistent *ozone absorption cross-sections*
  - Validation of high resolution *extraterrestrial solar reference spectra*
  - **Comprehensive uncertainty budget** incorporating instrumental and atmospheric uncertainties
• **WP 4:** Creating Impact /Dissemination (Publications, Workshops, Campaigns, Training Commercialization)
• **WP 5:** Management (PMOD/WRC)
Comprehensive Uncertainty Budget

**Radiometry**

**Atmospheric Model**

**Measurement**

Uncertainty of measurement: $\pm$

**Total Column Retrieval Method**

Uncertainty of model: $\pm$

**$O_3$ Value**

Uncertainty of $O_3$ value

Direct sun measurement:
- 4 Wavelengths: (Dobson/Brewer)
- Full spectrum: Array spectroradiometer

**Beer-Lambert Law**

$$I_\lambda = I_\lambda^0 e^{-\tau_\lambda m}$$
Comprehensive Uncertainty Budget

**Radiometry**

**Measurement**

Uncertainty of measurement: +

- noise of the measurement
- wavelength uncertainty
- uncertainty of calibration
- bandpass uncertainty
- temperature gradients
- dead-time effect / linearity
- ND filter

**Atmospheric Model**

**Total Column Retrieval Method**

Uncertainty of model:

- selected wavelengths (Brewer/Dobsons)
- selected cross-section
- selected atmospheric temperature
- extraterrestrial spectrum
- airmass uncertainty (atmospheric profile)
- rayleigh airmass uncertainty
- AOD / SO₂

**O₃ Value**

Uncertainty of O₃ value
Sensitivity on Parameters

Sensitivity Analysis:

- Investigate **single contributions to overall uncertainty** budget
- Find the **most important parameter affecting** the overall budget
- Potential for **improvement** of measurement and/or retrieval.
- Calculate the **overall uncertainty budget**.

A software tool is needed for simulation the effect on different parameters

<table>
<thead>
<tr>
<th>Uncertainty of <strong>measurement</strong>:</th>
<th>Uncertainty of <strong>model</strong>:</th>
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<td>noise of the measurement</td>
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**Dependencies** between measurement uncertainties and model uncertainties
Procedure of Simulation

1. Generating spectrum (PMOD-model) between 300 – 360 nm with known parameters and 49 atmospheric conditions 7 ozone x 7 airmass

\[ I_\lambda = I_\lambda^0 e^{-\tau_\lambda m} \]

FWHM as small as possible (=0.01 nm, ET)!
Procedure of Simulation

1. Generating spectrum (PMOD-model) between 300 – 360 nm with known parameters and 49 atmospheric conditions 7 ozone x 7 airmass

\[ I_\lambda = I_\lambda^0 e^{-\tau_\lambda m} \]

FWHM as small as possible (=0.01 nm, ET)!
2. Define retrieval method: **Double ratio technique** (Dobsons and Brewers)

\[ I_\lambda = I_\lambda^0 e^{-\tau_\lambda m} \]

Beer-Lambert Law

\[ \log I_i = \log I_i^0 - \tau_i^R m_R - \alpha_{i, O_3}^0 X m_{O_3} - \tau_i^{aod} m_{aod} \]

\( m_R, m_{O_3}, \) and \( m_{aod} \) are different airmasses due to different respective heights of the ozone, air and particle molecules within the different atmospheric profiles.

\( I_i^0 = \) Extraterrestrial Spectrum, \( i = \) wavelength-index

<table>
<thead>
<tr>
<th>( i ) (slit)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda )-Brewer (nm)</td>
<td>310.1</td>
<td>313.5</td>
<td>316.8</td>
<td>320</td>
</tr>
<tr>
<td>( \lambda )-Dobson (nm)</td>
<td>305.51</td>
<td>317.62</td>
<td>325.08</td>
<td>339.97</td>
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Dobson Slits - D064

Dobsons D064 (DWD) and D083 (NOAA) characterized for wavelength and bandpass at PTB Braunschweig with tuneable laser facilities (Saulius Nevas)

- Dobson: Peak 325 nm
- D064 A-S3: Peak 325.08 nm
- D083 A-S3: Peak 325.1 nm
- D083 A-S3 (1993): Peak 325.12 nm
Dobson Slits - D064

Dobsons D064 (DWD) and D083 (NOAA) characterized for wavelength and bandpass at PTB Braunschweig with tuneable laser facilities (Saulius Nevas)

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<tr>
<th>Slit</th>
<th>Peak (nm)</th>
<th>FWHM (nm)</th>
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<th>FWHM (nm)</th>
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<tr>
<td>A-S2</td>
<td>305.51</td>
<td>1.03</td>
<td>305.46</td>
<td>1.05</td>
<td>305.52</td>
<td>0.99</td>
</tr>
<tr>
<td>C-S2</td>
<td>311.50</td>
<td>1.08</td>
<td>311.47</td>
<td>1.09</td>
<td>311.46</td>
<td>1.04</td>
</tr>
<tr>
<td>D-S2</td>
<td>317.62</td>
<td>1.27</td>
<td>317.58</td>
<td>1.24</td>
<td>317.51</td>
<td>1.17</td>
</tr>
<tr>
<td>A-S3</td>
<td>325.08</td>
<td>3.56</td>
<td>325.10</td>
<td>3.56</td>
<td>325.02</td>
<td>3.46</td>
</tr>
<tr>
<td>C-S3</td>
<td>332.44</td>
<td>3.81</td>
<td>332.47</td>
<td>3.81</td>
<td>332.40</td>
<td>3.73</td>
</tr>
<tr>
<td>D-S3</td>
<td>339.97</td>
<td>4.06</td>
<td>334.00</td>
<td>4.12</td>
<td>339.90</td>
<td>4.01</td>
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</table>
Procedure of Simulation

«Double ratio» / «weighted ratio» technique (Dobsons and Brewers): combining all four wavelengths

\[ F = F_0 - \Delta \tau^R m_R - \Delta \alpha^{O3} X m_{O_3} - \Delta \tau^{aod} m_{aod} \]

where

\[ \Delta \tau^R = \sum_i W_i \tau_i^R ; \quad \Delta \alpha^{O3} = \sum_i W_i \alpha_i^{O3} \]

\( W_i(Dobsons) = (+1, -1, +1, -1) \) and \( W_i(Brewers) = (+1, -0.5, -2.2, +1.7) \), with \( \sum_i W_i = 0 \).

\[ \Delta \tau^{aod} = \sum_i W_i \tau_i^{aod} \approx 0 \]

\[ F = F_0 - \Delta \tau^R m_R - \Delta \alpha^{O3} X m_{O_3} \]

\[ TOC = X = \frac{F_0 - F - \Delta \tau^R m_R}{\Delta \alpha^{O3} m_{O_3}} \]
Procedure of Simulation

«Double ratio» / «weighted ratio» technique (Dobsons and Brewers):
combining all four wavelengths

\[ F = F_0 - \Delta\tau^R m_R - \Delta\alpha^O_3 X m_{O_3} - \Delta\tau^{aod} m_{aod} \]

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calculating integral over the slits
Procedure of Simulation

3. Random variation of uncertain parameters

\[ TOC = X = \frac{F_0 - F - \Delta \tau^R m_R}{\Delta \alpha^O_3 m_{O_3}} \]

Uncertainty of measurement:
- noise of the measurement
- wavelength uncertainty
- uncertainty of calibration
- bandpass uncertainty
- temperature gradients
- dead-time effect / linearity
- ND filter

Uncertainty of model:
- selected wavelengths (Brewer/Dobson)
- selected cross-section
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- extraterrestrial spectrum
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Procedure of Simulation

3. Random variation of uncertain parameters

\[ TOC = X = \frac{F_0 - F - \Delta \tau R m_R}{\Delta \alpha O_3 m_{O_3}} \]

\[ \equiv \text{Uncertainty of } O_3 \text{ value} \]

4. Making 100 runs with random variation, for all 49 atmospheric conditions

5. Comparison (ratio) between input ozone (no variation) and retrieved ozone

Uncertainty = standard deviation of all ratios
First Result: No Variation

Dobson: 0.14% - 0.3 % (systematic)
Brewer: 0.02% - 0.1% (systematic)

Simulation works.
First Result: Array SRM

FWHM of generated spectrum: 0.5 nm (not 0.01nm), sampling resolution: 0.2 nm

Dobson: 0.5% - 0.7 % (systematic)

Brewer: -6.4% - 5.6% (systematic)

Retrieval does not work for spectra of array spectroradiometer. Systematic bias can be eliminated by Langley calibration.
Variation of wavelength shift

Variation of wavelength-shift of input spectrum: ±0.025 / (±0.0035) nm

Dobson: 0.05% - 0.35%

Brewer: 0.05% - 0.5%
Variation of wavelength shift

Variation of wavelength-shift of input spectrum: ±0.025 / (±0.0035) nm

**Dobson:** 0.05% - 0.35%

**Brewer:** 0.5% - 3.5%
Result: Stratospheric Temperature


Dobson: 1.2% - 1.4%  
Brewer: 0.7% - 0.9%
Result: Stratospheric Temperature

Variation of stratospheric temperature (retrieval): 213K – 243K: «Bremen»

Dobson: 0.6% - 0.7%

Brewer: 0.27% - 0.32%
## Summary Sensitivity

Averaged uncertainty of **Ozone** over all atmospheric conditions:

<table>
<thead>
<tr>
<th></th>
<th>Dobsons</th>
<th>Brewer</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength <strong>±0.025 nm</strong></td>
<td>0.1%</td>
<td>0.9%</td>
<td></td>
</tr>
<tr>
<td>Noise of detector /Calibration /ND filter Deadtime /linearity/ Instr. Temperature <strong>±0.1%</strong></td>
<td>0.06%</td>
<td>0.4%</td>
<td>linear</td>
</tr>
<tr>
<td>Strat. Temp Bass-Paur: <strong>213K-243 K</strong></td>
<td>1.2%</td>
<td>0.8%</td>
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<tr>
<td>Strat. Temp Bremen: <strong>213K-243 K</strong></td>
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<td></td>
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<tr>
<td>Cross-Section Bass-Paur: <strong>±5%</strong></td>
<td>1.2%</td>
<td>2.4%</td>
<td></td>
</tr>
<tr>
<td>Extraterrestrial : <strong>±5%</strong></td>
<td>0%</td>
<td>0%</td>
<td>Uncertainty from Langley?</td>
</tr>
<tr>
<td>Ozone Air Mass Variation</td>
<td>linear</td>
<td>linear</td>
<td>Uncertainty of air mass need to be investigated</td>
</tr>
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<td>AOD / SO2</td>
<td>?</td>
<td>?</td>
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</table>
Variation of all Parameters

Variation of **uncertain input** and **model parameters**:
Wavelength ±0.025 nm; Calib: ±0.1%; Bass-Paur, Temp. 213-243K, Variation of cross section ±5%

**Dobson**: 1.5% - 1.9% = 1.7%

**Brewer**: 4.4% - 5.8% = 4.6%
## Summary Sensitivity

«Uncertainty reduction» by convention (identical cross-sections, ET etc.)

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«Harmonized instrument network»
## Summary Sensitivity

«Uncertainty reduction» by convention (identical cross-sections, ET etc.)

### Discussion / Decision

#### SAG Ozone

Scientific Steering Committee ATMOZ

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Uncertainty of air mass need to be investigated

Uncertainty from Langley?

«Harmonized instrument network»
Variation of all Parameters

Variation of **parameters**, which cannot be determined by convention
Wavelength ±0.025 nm; Calib: ±0.1%; Bremen, Temp. 213-243K

**Dobson:** 0.6% - 0.75% = 0.7%

**Brewer:** 0.5% - 3.5% = 1.1%
Conclusions

- **Dobson** show generally a lower uncertainty budget than **Brewers**
- Reducing **wavelength and calibration uncertainty** is crucial for Brewers
- **Brewers** show a less sensitivity to stratospheric temperature variation than Dobsons
- “**Bremen**” cross section is less sensitive to stratospheric temperature variations
Conclusions

• Uncertainties of signal at each individual slit is essential and may be composed of:
  – Calibration
  – Intensity of sun (airmass)
  – ND filters
  – Dead time / linearity
  – Temperature gradients of instruments

The impact of these effects on the uncertainty of the signal should be investigated individually to obtain one general uncertainty of signal.
Outlook

- Uncertainty of **Langley plot calibration** need to be quantified
- Stratospheric **temperature should be known** to reduce uncertainty
- Working on **method to retrieve stratospheric temperature** from direct sun measurements
- The software will be used to **determine the overall uncertainty** from Dobson / Brewer and array spectroradiometer measurements

<table>
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<tr>
<th>Array SRM</th>
<th>NEI=0.1mW</th>
<th>NEI=0.01mW</th>
<th>Remark</th>
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</thead>
<tbody>
<tr>
<td>Wavelength ±0.05 nm</td>
<td>1% (Full Spec.)</td>
<td>0.6% (Full Spec.)</td>
<td>Depending on FWHM</td>
</tr>
<tr>
<td></td>
<td>1.5% (Multi Double Ratio)</td>
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</tr>
<tr>
<td>Calibration ±5%</td>
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Remark: ±0.05 nm = 1% (Full Spec.) 1.5% (Multi Double Ratio)
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Outlook

- Uncertainty of **Langley plot calibration** need to be quantified
- Stratospheric **temperature should be known** to reduce uncertainty
- Working on **method to retrieve stratospheric temperature** from direct sun measurements
- The software will be used to **determine the overall uncertainty** from Dobson / Brewer and array spectroradiometer measurements, in combination with other approaches.

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**Next Talk: Petri Kärhä**
Array Spectroradiometer (full spectrum)

Automatic detection of cut-on wavelength

[Diagram showing generated UV spectra with 350 DU ozone, with different lines and markers indicating modelled and modified spectra, as well as cut-on wavelengths for different air masses.]
Cut-On Wavelength

Variation: ALL, NEI=1mW

Variation: ALL, NEI=0.1mW

Variation: ALL, NEI=0.01mW

Variation: ALL, NEI=0.001mW

Ozone (DU)

Air Mass
Variation of all Parameters

Variation of **all uncertain input** and **model parameters** (500 runs):
Bass-Paur crosssection / consistent networks

NEI=0.1mW: **1.5% - 2.5% / 0.8%-2.2%**
NEI=0.01mW: **1.8% - 3.8% (Double ratio)**

NEI=0.01mW: **1.3% - 1.9% / 0.7%-1.3%**
NEI=0.01mW: **1.6% - 3% (Double ratio)**
Conclusions

Overall uncertainty of ozone retrieval by multispectral measurements depends mainly on:

- **NEI = Noise equivalent Irradiance** => impact on selection of usable wavelength range
- Wavelength uncertainty
- Atmospheric conditions (mainly air-mass)
- Air-mass determination

Less contributions for the overall uncertainty are from:

- Selected X-sections; Variations of X-section => **convention to select one specific X-section** (recommendation: “Bremen X-section => new generation in ATMOZ)
- Variation of extraterrestrial spectrum => **convention to select one specific ET** (new measurements and validation in ATMOZ)
- Random Variation of input spectrum
- Stratospheric Temperature => **retrieving stratospheric temperature** (on-going research)
- Bandpass (except in combination with wavelength shift)
- Resolution (small impact on random variation)
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