Ozone Sonde Data Quality Assessment (O3S-DQA)

Resolving Inhomogenities in Long Term Ozone Sounding Records and Assessing Their Uncertainties

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(2) NOAA/GMD, Boulder, USA

SI2N at Quadrennial Ozone Symposium
10 September 2016, Edinburgh, UK
What Is An Ozone Sounding?

Electrochemical ozone sensor converts sampled ozone flow into electrical current:

- In aqueous KI-solution Ozone is converted into Iodine (I₂) molecules
- In electrochemical cell Iodine is converted at Pt-Cathode into Iodide-ions by uptake of two electrons per ozone molecule, which generates an electrical current in external circuit
Ozone Soundings: Role in Atmospheric Research

- **Ozone climatologies and trends** on regional and global scales (WMO/GAW-Network): *Long term changes*
- **Validation of satellite and other vertical profiling techniques** (e.g. CCVal, SI2N): *O3S are the back bone of remote sensing techniques*
- **Process studies** (e.g. MATCH, and many more ........)
- **Tracer for mapping atmospheric dynamics** for weather forecasting (e.g. ECMWF) or identification origin of air masses (moist convection versus large scale subsidence)
- Ozone as chemical component for **air quality forecastings**
Long Term Ozone Measurements
(Source: SI2N/Harris et al.)

Many records
- Umkehr: 50 years
- Sondes: 40 years
- Satellite: 30 years
- NDACC: 20 years

Independent

Correlative

Last 10 years?

O3S provide a-priori profiles for remote sensing techniques like Satellites, but also ground based Microwave and FTIR techniques)
Global O3S-Records: State of the Art

Four types of ozone sondes:
1. ECC (Electrochemical Concentration Cell) (nowadays 90% fly ECC)
2. BM (Brewer Mast: original) (since 1970: specially elder stations)
3. KC 79/96 (Japanese network: long term records since 1970’s)
4. IMD (BM-type produced and flown by Indian Meteorological Department): ??

Ozone sounding records:
- a) Short term: 5-10 years (Validation)
- b) Middle term: 10-25 years (after 1985) (Validation + Trends)
- c) Long term: 25-40 years (since 1970’s) (Validation + Trends)

Inhomogenities in long term O3S-records:
Due to changes of instruments or operating procedures
O3S-DQA: Where are we nowadays?

Comparison AURA-MLS versus OzoneSonde from Daan Hubert et al., AMT, 2016

Ozone sondes have presently relative uncertainty ±(5-10-20)% (incl. bias)

Targeting for:
Relative uncertainty better than ±5%, no bias, and traceable to one reference
O3S-DQA: Lessons we learned from Ozone Sondes (i.e. ECC's)

- From Design, Components and Type all ECC sondes look the same
- So everything should be fine and nothing to worry about

But:

Small changes of instrument or operating procedures or changing manufacturers can have large impact on data quality (e.g. JOSIE & BESOS)

Warning:

Cautious with regard to any changes

(Hint: the devil is always hiding himself in the details)
Controversy ECC-sondes since Mid 1990’s: Two Manufacturers and 3 Different Sensing Solution Types

<table>
<thead>
<tr>
<th>Manufacturer</th>
<th>Model Type</th>
<th>Years Manufactured.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Science Pump</td>
<td>SPC-6A</td>
<td>1995- present</td>
</tr>
<tr>
<td>EN-SCI</td>
<td>ENSCI-Z</td>
<td>1997 – present</td>
</tr>
</tbody>
</table>

Note: Since 2011 EN-SCI be taken over by DMT, Boulder, USA

<table>
<thead>
<tr>
<th>Sensing Solution Type (SST)</th>
<th>KI [g/L]</th>
<th>P_H-Buffer</th>
<th>KBr [g/L]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>NaH₂PO₄.H₂O</td>
<td>Na₂HPO₄.12H₂O</td>
</tr>
<tr>
<td>SST1.0: 1.0% KI &amp; full buffer (a)</td>
<td>10</td>
<td>1.250</td>
<td>5.0</td>
</tr>
<tr>
<td>SST0.5: 0.5% KI &amp; half buffer (b)</td>
<td>5</td>
<td>0.625</td>
<td>2.5</td>
</tr>
<tr>
<td>SST2.0: 2.0% KI &amp; no buffer (c)</td>
<td>20</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
JOSIE 2000 & BESOS 2004:
Comparison SPC-6A & ENSCI-Z @ Different Sensing Solutions
SST1.0 (1.0%KI, Full Buffer), SST0.5 (0.5%KI, Half Buffer), SST2.0 (2.0%KI, No Buffer)
[Data processed after Komhyr 1986, IB0 (PO2), No Total O3 Normalization]

Each sonde type (ENSCI or SPC):
- SST1.0 ≈ 5% larger than SST0.5
- SST0.5 ≈ 5% larger than SST2.0
- SST1.0 ≈ 10% larger than SST2.0

For each Sensing Solution Type
(SST1.0, SST0.5, and SST2.0):
- ENSCI 5-10% higher than SPC
- Precision about 3-6%
ASOPOS: Status 2010
(Assessment for Standard Operating Procedures for Ozone Sondes)

- ASOPOS-Report: QA/QC and SOP ‘s for O3S (GAW-report#201)
- Recommendations on use of sensing solution type (SST):
  - SPC6A: 1.0% KI, full buffer (SST1.0)
  - ENSCI: 0.5% KI, half buffer (SST0.5)
  
  Note: These two SST’s very close agreement with OPM (Ozone Photo Meter) at WCCOS

- Standardization of SOP ‘s leads to the best precision of 3-5 %
- Non uniformity in ozone sonde types or operating procedures can introduce “inhomogenenities” in sonde data records of each of the stations or between different stations of 5-20 %
- Need for transfer functions to homogenize sonde data records
- After homogenization accuracy can be better than 5-10 %

Sources: JOSIE [Smit et al., J.Geophys.Res., 2007]
BESOS [Deshler et al., J.Geophys.Res., 2008]
Transfer Functions Different SST's

Stuebi/Deshler et al., in preparation

Derived from dual soundings, JOSIE & BESOS campaigns:

<table>
<thead>
<tr>
<th>Equation</th>
<th>$Y$ dependent</th>
<th>Ratio</th>
<th>$X$ independent</th>
<th>Pressure</th>
<th>$O_3$-sonde or SST</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eq.7A</td>
<td>SST 0.5%</td>
<td>0.96</td>
<td>SST 1.0%</td>
<td>$P \geq 30$ hPa</td>
<td>Both SPC &amp; ENSCI</td>
</tr>
<tr>
<td>Eq.7B</td>
<td>SST 0.5%</td>
<td>0.90+0.041*log$_{10}$(p)</td>
<td>SST 1.0%</td>
<td>$P &lt; 30$ hPa</td>
<td>Both SPC &amp; ENSCI</td>
</tr>
<tr>
<td>Eq.7C</td>
<td>SPC</td>
<td>0.96</td>
<td>ENSCI</td>
<td>$P \geq 30$ hPa</td>
<td>0.5% &amp; 1.0%</td>
</tr>
<tr>
<td>Eq.7D</td>
<td>SPC</td>
<td>0.764+0.133*log$_{10}$(p)</td>
<td>ENSCI</td>
<td>$P &lt; 30$ hPa</td>
<td>0.5% &amp; 1.0%</td>
</tr>
<tr>
<td>Eq.7E</td>
<td>SPC-1.0%</td>
<td>1.01</td>
<td>ENSCI-0.5%</td>
<td>$P &gt; 0$</td>
<td></td>
</tr>
</tbody>
</table>

3. November 2016

Smit: O3S-DQA (Ozone Sonde Data Quality Assessment)
Quadrennial Ozone Symposium, 05-09 September 2016, Edinburgh, UK
O3S-DQA Homogenisation: Objectives

“Ozone Sonde Data Quality Assessment (O3S-DQA)” activity started in 2011 has following three major objectives:

1. Homogenization of a selected ozone sonde data set with the goal to reduce uncertainty from 10-20% down to 5-10% (focus on SST-transfer functions, but also other instrumental aspects)

2. Documentation of the homogenization process and the quality of ozonesonde measurements including quantification of the uncertainty of each ozone sonde measurement

3. Storage of additional raw data of O3S and the overall uncertainty of each O3S-measurement
Estimation

Overall Uncertainty $P_{O3}$

$$P_{O3} = 0.043085 \cdot \frac{T_P}{(\eta_C \cdot \Phi_P)} \cdot (I_M - I_B)$$

Assumption in O3S-DQA:
After all corrections have been done to resolve the different inhomogenities (bias effects) in the long term O3S-records all remaining individual uncertainties are random and following Gaussian statistics, then applying Gaussian law of error propagation can be applied:

$$\frac{\Delta P_{O3}}{P_{O3}} = \sqrt{\left(\frac{(\Delta I_M)^2 + (\Delta I_B)^2}{(I_M - I_B)^2}\right) + \left(\frac{(\Delta \eta_C)^2}{\eta_C}\right) + \left(\frac{(\Delta \Phi_P)^2}{\Phi_P}\right) + \left(\frac{(\Delta T_P)^2}{T_P}\right)}$$
1. **In Time (O3-trends @ individual stations)**
   
   Each station will homogenize his O3S-record individually
   
   a. Following guidelines prescribed by O3S-DQA panel
   b. Using transfer functions based on dual soundings & JOSIE 2009
   c. Coaching by O3S-DQA-expert.

2. **In Space (Validation: e.g. satellites )**
   
   All individual O3S station records using JOSIE 2009 based transfer functions to refer the homogenized O3S to one standard (OPM= UV-Photometer @ WCCOS-JOSIE, Juelich, Germany)

3. **Testing on Consistency**
   
   a. Comparison with other O3 profiling instrument @ O3S-site
   b. Troposphere-UTLS: MOZAIC-O3
   c. Satellites: e.g. Daan Huberts approach (AMT, 2016)
   d. Stratosphere: MATCH-approach
Guidelines for reprocessing O3S records:

1. Different sensing solutions and sonde type: Transfer functions
2. Uniform background current corrections (Ib2)
3. Pump flowrate: humidity correction
4. Uniform pump flow efficiency correction at lower pressures
5. Pump temperature scaled on piston temp. (internal-, external-, box-)
6. ECC: No total ozone normalization factor applied
7. Residual ozone columns from satellite climatologies (McPeters et al. tables)
8. Quantification of expected uncertainties & Documentation as meta data
9. Coaching by O3S-DQA-expert
Preparatory Work I:
Collection of Meta Data
A. “Table Log Book O3S-Station Data”
B. “Time Series O3S-Parameters”

Preparatory Work II:
Prepare Station Specific Guidelines To Process Long Term O3S Data

Reprocessing O3S-Data

Validation O3S-Data
A. Internal & External Consistency
B. Quantify Uncertainty PO3

Submission O3S-Data
SPARC Assessment
O3-Trend Use

Documentation
A. Data Processing
B. Uncertainty PO3
**O3S-DQA: Total Ozone Normalisation Before and After Homogenization of EC-Network**

**Tropospheric changes:** increases of up to 5% after 1979; up to 20% before 1980 (Brewer-Mast sondes), reducing with altitude.

**Stratospheric changes:** decreases of up to 4% before 1980 at 25 km, smaller decreases above and below. Increases of ~1% in 1980s, ~2-3% in 1990s; little change in 2000s.

<table>
<thead>
<tr>
<th></th>
<th>Mean K</th>
<th>Std Dev</th>
<th>Trend in K</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>BM data</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Original</td>
<td>1.27</td>
<td>0.303</td>
<td>2.7%/decade</td>
</tr>
<tr>
<td>Renormalized</td>
<td>1.20</td>
<td>0.198</td>
<td></td>
</tr>
<tr>
<td>Response correction</td>
<td>1.03</td>
<td>0.179</td>
<td>2.2%/decade</td>
</tr>
<tr>
<td><strong>ECC data</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Original</td>
<td>0.97</td>
<td>0.101</td>
<td>-2.6 +/- 0.6 %/decade</td>
</tr>
<tr>
<td>All corrections</td>
<td>0.99</td>
<td>0.087</td>
<td>0.6 +/- 0.5 %/decade</td>
</tr>
</tbody>
</table>
O3S-DQA: Uncertainty Budget

Edmonton 1972-1978

Edmonton 1980-1989

Edmonton 1990-1999

Edmonton 2000-2009

Source: Tarasick et al., AMT, 2016

Blue: Overall Uncertainty

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O3S-DQA: O3 Trends Before & After

Source: Tarasick et al., AMT, 2016

O3S-DQA: Status of Re-processing

→ September 2016: Total of 28 Stations records have been re-processed, 2 papers published

Goal for Summer 2017:
A. 40 Stations being homogenised (Re-processed data incl. RAW-Data, Overall Uncertainty, Documentation).
B. First Analysis on Validation → Evaluation can start
C. Key papers ready for publications: about 7
D. Provide homogenised data set to UNEP-Ozone Assessment 2018

QOS 2016: Posters on Re-processing O3S Data:
P194 Roeland van Malderen et al.: Uccle (B) & De Bilt (NL)
P273 Chance Sterling et al.: NOAA-Network
P274 Jacquie Witte et al.: SHADOZ-Network

A.) **ASOPOS-Report** (GAW report#201): Activity finished by 2009

B.) **JOSIE 2009/2010**: Addressing QA Manufacturing and Re-used sondes and Transfer functions different SST's traceable to OPM (UV-Photometer of WCCOS)

C.) **O3SEM-2009** (January 2009 @ Jülich, Germany): All facets of ozone soundings

D.) **Homogenisation long term O3S records-Part I (2011-2017)**: Will be finished by Mid of 2017 to take part in UNEP O3 Depletion Assessment 2018

   - O3S-Reprocessing Workshops in context of SI2N:
     i. NOAA/Boulder October 2011: Kick-Off
     ii. GSFC/Greenbelt April 2012: Transfer Functions
     iii. QOS/Toronto September 2012: Report on “Guidelines for Homogenisation of Long Term O3S Data Records,”
     iv. **O3SEM-2016** (September 2016, Edinburgh, UK):
         a. Outstanding instrumental issues
         b. Mid term review of Reprocessing for homogenisation O3S-records
         c. JOSIE-SHADOZ preparation

E.) **JOSIE 2017/2018**:

   I. JOSIE 2017 = **JOSIE-SHADOZ**: Addressing tropical profiling capabilities
   II. JOSIE 2018: New research on outstanding instrumental issues
   III. Laboratory & Field experiments addressing outstanding instrumental issues
Very important QA/QC factor to achieve the best data quality starts at the launch site:

(1) Good quality of preparation equipment, which is well maintained

(2) Well trained and motivated sonde operator

(3) Good & regular communication between scientist & sonde operator

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Extra Slides
O3S-DQA: Internal Data Server @ Juelich

Upload:
• Non-homogenized data: Old WOUDC or old NDACC-data format
• New Homogenized data: New WOUDC or New NDACC-data format
  ➢ Bring all data in the New WOUDC format: WOUDC can do that (they got the converters)
  ➢ Storage of Non-homogenized and Homogenized Data in new WOUDC data format

Download:
Data server to provide old and new data to data-investigators for validation

Wiki-Page WCCOS-JOSIE: Documentation and Info-Exchange platform

Access: Password Protected by O3S-DQA Data Protocoll)

→ Infra Structure Exist
→ Data Protocoll exist