SCIAMACHY Ozone Profile Validation

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Acknowledgment: Data from AVDC at NILU were used
Available SCIAMACHY limb ozone profiles

SCIAMACHY Offline limb ozone profiles (version 2.1)
- UV wavelengths (to be extended to UV-VIS)
- 4 ozone profiles per swath, lined up in across-track direction
- No altitude correction implemented (pointing inaccurate in 2002)
- Data in altitude or pressure vs. partial columns or mixing ratios

SCIAMACHY IFE-Bremen limb ozone profiles (version 1.6)
- Generated from Level 1 data.
- Chappuis band (VIS)
- No altitude correction implemented
- Data in altitude vs. number density
Other SCIAMACHY ozone profiles

- Nadir profiles (Van der A, KNMI; L1 calibration insufficient)
- Differential SCD profiles (Wagner, Univ. Heidelberg; experimental)
- Mesospheric ozone profiles (IFE - Univ. Bremen)
- Solar (50-70°N) & lunar (30-90 °S) occultation (IFE - Univ. Bremen)
  * SCIA on order of 10% (solar) too high compared with SAGE II in 15-35 km region (Amekudze et al., EGU poster)
Limb ozone profile introduction

- Horizontal scans at -5 to +80 km with ~2.5 km intervals
- Scan order reversed for consecutive scans
- Geolocations stored are for individual pixels, in chronological order
- Optimal estimation / Tikhonov algorithms (both include a priori)
- Retrievals yield partial column density profiles

Offline product:

- Mixing ratios profiles given derived using AFGL standard atmospheres
  (these are P,T profiles reported)
Comparisons performed with

Satellite data:
* HALOE v19, SAGE II, SAGE III, SBUV/2
* no altitude offset correction
* ppmv units as basis

Groundbased data:
* lidar, microwave, FTIR, balloon sondes (~15 sites)
* altitude offset varied, optimized per location
* number density units (from ppmv and/or partial columns), often also ppmv
SCIAMACHY OFFLINE v2.1 DATA
**HALOE (v19)**

in number densities:
- at 21 – 43 km: 
  
  [-8, 20%] (+/- 20%)

in VMR:
- at 22 – 43 km:
  
  [-6, +20]% (+/- 20%)

**SAGE II (6.2)**

in number densities:
- at 21 – 41 km:
  
  [3, +17%] (20–25%)

in VMR:
- at 22 – 41 km:
  
  [0, +15%] (20–25%)
Results: SAGE III (Taha et al.)

<table>
<thead>
<tr>
<th>Lat band</th>
<th>mean diff [%]</th>
<th>number</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH</td>
<td>[-30,25]</td>
<td>201</td>
</tr>
<tr>
<td>SH</td>
<td>[-40,25]</td>
<td>453</td>
</tr>
</tbody>
</table>

Numbers for 15-45 km range, alt. not corrected

Note: Altitude shift apparent below 23 km (NH) or throughout profile (SH)
### SBUV/2 (Hilsenrath et al.)

<table>
<thead>
<tr>
<th>Lat band</th>
<th>%diff*</th>
<th>number</th>
</tr>
</thead>
<tbody>
<tr>
<td>-80 to -60</td>
<td>[-45, 17]</td>
<td>61</td>
</tr>
<tr>
<td>-60 to -40</td>
<td>[-45, 20]</td>
<td>21</td>
</tr>
<tr>
<td>-40 to -20</td>
<td>[-40, 17]</td>
<td>12</td>
</tr>
<tr>
<td>-20 to 00</td>
<td>[-40, 15]</td>
<td>5</td>
</tr>
<tr>
<td>00 to 20</td>
<td>[-40, 40]</td>
<td>11</td>
</tr>
<tr>
<td>20 to 40</td>
<td>[-45, 30]</td>
<td>12</td>
</tr>
<tr>
<td>40 to 60</td>
<td>[-45, 18]</td>
<td>100</td>
</tr>
<tr>
<td>60 to 80</td>
<td>[-45, 30]</td>
<td>383</td>
</tr>
</tbody>
</table>

* (SCIA-SBUV)*100%/SBUV @ .5 – 50 hPa

**Altitude shift?**

Typically: SCIA O3 too high in lower stratosphere (under ~50 hPa level), too low in higher stratosphere.

**SH average:** [-45,18]%

**NH average:** [-45,28]%
Examples (Payern):
Sondes collocated with
4 SCIA profiles per state
(here – almost identical)

Averages of 30 sondes,
collocated with 4 x 30 SCIA
profiles at Payern
### SCIA Offline V2.1 compared with lidar & sondes

<table>
<thead>
<tr>
<th>Location</th>
<th>instrument</th>
<th>% diff*</th>
<th>number</th>
<th>alt offset [km]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uccle</td>
<td>sondes</td>
<td>[-12, +15]</td>
<td>31</td>
<td>-1.5</td>
</tr>
<tr>
<td>De Bilt</td>
<td>sondes</td>
<td>[-8, +7]</td>
<td>14</td>
<td>-1.5</td>
</tr>
<tr>
<td>Hohenpeissenberg</td>
<td>lidar &amp; sondes</td>
<td>[-8, +12]</td>
<td>24/21</td>
<td>-1.5 NH</td>
</tr>
<tr>
<td>Payern</td>
<td>sondes</td>
<td>[-1, +6]</td>
<td>30</td>
<td>-1.0</td>
</tr>
<tr>
<td>Table Mountain</td>
<td>lidar</td>
<td>[-7, +10]</td>
<td>5</td>
<td>0</td>
</tr>
<tr>
<td>Mauna Loa</td>
<td>lidar</td>
<td>[-7, +12]</td>
<td>3</td>
<td>-1.5 tropics</td>
</tr>
<tr>
<td>Lauder</td>
<td>lidar</td>
<td>[-11, +10]</td>
<td>21</td>
<td>-1.0</td>
</tr>
<tr>
<td>,,</td>
<td>sondes</td>
<td>[-12, +20]</td>
<td>11</td>
<td>-1.0 SH</td>
</tr>
</tbody>
</table>

* (SCIA-x)*100%/SCIA @ 20-40 km (lidar) or 15 km - burst (~35 km, sondes)

**Collocation criterion:** within 18 hours and 1000 km (from limb state corners)
SCIAMACHY OL v2.1 with FTIR (Blumenstock et al.)

O$_3$, Kiruna

16 coincidences outside polar vortex

UV-sensitivity below 20 km expected to be very low!

Note: sign reversed!
Multiple Instrument Comparison (Boyd et al.)

Same-SCIA-profile collocations with:
- microwave, lidar, sondes at Lauder, New Zealand (45°S)
- microwave and lidar at Mauna Loa, Hawaii (20°N)

Composite atmospheric profiles (up-to-date analyses) used for unit conversions (mixing ratio to number density profiles)

*Mid layer correction* implemented (profiles reported are shifted upward by 0.5 \( \Delta z \), or equivalent in pressure, alt/pres scale interpreted as *lower and upper boundaries*).

Difference plots (%) are relative to average of all instruments
Mean of 3 Profile Comparisons at Lauder NZ (45.0S, 169.7E), 20020820 - 20020827

Difference Calculation: 

\[ \frac{\text{Instrument-Mean}}{\text{Mean}} \times 100 \]

Error Bars eq 2*Std.DfV./sqrt(n)

Selection Criteria: +/-24hr

Satellite lat range: +/- 2.5 lon range:

SCIAMACHY O3 err max (%): 25%

INSTRUMENTS:
SCIAMACHY v2.1
Lidar
\( uWave \_ Dy \)
O3Sonde

SCIAMACHY v2.1 -rL
MID-LAYER CORRECTION MADE
LDR COMPOSITE ATMOSPHERE

Plot 44bf
Conclusions Lauder & Mauna Loa (number density profiles)

**Lauder (45°S)**
- Offline v2.1 [11 pairs]
  - lidar & mwave: -4% (4%) 17-25 km
  - +5% (4%) 25-45 km
- IFE v1.6 [12 pairs]
  - lidar & mwave: -4% (3%) 15-40 km
  - +5% (4%) 25-45 km

**Conclusions:** Offline V2.1 SCIA biased low <25 km, high 25-45 km,
IFE V1.6 SCIA biased low 15-40 km, high 40-70 km.
Offset -1.5 km applied to both data sets.

**Mauna Loa (20 °N)**
- Offline v2.1 [4 pairs]
  - lidar & mwave: 0% (1%) 18-25 km
  - 2% (4%) 25-45 km
- IFE v1.6 [21 pairs]
  - lidar & mwave: -3% (2%) 20-30 km
  - +3% (2%) 30-40 km
SCIAMACHY IFE-Bremen V1.6 DATA
IFE v 1.6 versus HALOE (A. Bracher et al.)

Mean $O_3$-profiles: -90.0° - 90.0° (61)

Comparison of $O_3$-P [1e18 m$^{-3}$] at -90.0° - 90.0° (61)
### IFE v1.6 compared with lidar & sondes

<table>
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<tr>
<th>Location</th>
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<th>% diff*</th>
<th>alt offset [km]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alomar, Ny Alesund</td>
<td>lidar</td>
<td>[-20, +15]</td>
<td>-3.0</td>
</tr>
<tr>
<td>Uccle</td>
<td>sondes</td>
<td>[-10, +40]</td>
<td>-1.5</td>
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<td>[-15, +20]</td>
<td>-1.5</td>
</tr>
<tr>
<td>Payern</td>
<td>sondes</td>
<td>[-20, +40]</td>
<td>-1.0</td>
</tr>
<tr>
<td>Table Mountain</td>
<td>lidar</td>
<td>[-7, +10]</td>
<td>0</td>
</tr>
<tr>
<td>Mauna Loa</td>
<td>lidar</td>
<td>[-7, +12]</td>
<td>-1.5</td>
</tr>
<tr>
<td>Paramaribo</td>
<td>lidar</td>
<td>[-20, +60]</td>
<td>-1.5</td>
</tr>
<tr>
<td>Lauder</td>
<td>lidar</td>
<td>[-25, +0]</td>
<td>-1.0</td>
</tr>
<tr>
<td></td>
<td>sondes</td>
<td>[-20, +30]</td>
<td>-1.0</td>
</tr>
</tbody>
</table>

* (SCIA-x)*100%/SCIA @ 10-35 km range

Collocation criterion: within 18 hours and 1000 km
IFE v1.6 compared with sondes (A.-M. Schmoltner et al.)

13 August 2003, Sondes folded w/3km FWHM

Lauder, 080313

- Limb profile V1.6
- Sonde, raw data
- Sonde, folded
### Summary offline ozone profile results

<table>
<thead>
<tr>
<th></th>
<th>HALOE</th>
<th>SAGE II</th>
</tr>
</thead>
<tbody>
<tr>
<td>21-43 km num. density</td>
<td>[-8, 20]</td>
<td>[-3, 17]</td>
</tr>
<tr>
<td>22-43 km mixing ratio</td>
<td>[-6, 20]</td>
<td>[0, 15]</td>
</tr>
<tr>
<td>SBUV/2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NH</td>
<td>[-45, 28]</td>
<td>[-30, 25]</td>
</tr>
<tr>
<td>SH</td>
<td>[-45, 18]</td>
<td>[-40, 25]</td>
</tr>
</tbody>
</table>

From sat-SCIA validation: SCIA biased high in low strat, biased low in high strat

<table>
<thead>
<tr>
<th></th>
<th>lidar or sonde</th>
<th>simultaneous lidar &amp; mwave</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(17-25 km)</td>
<td>(25-45 km)</td>
</tr>
<tr>
<td>NH (5 loc)</td>
<td>[-7, 10]</td>
<td></td>
</tr>
<tr>
<td>Mauna Loa (4 collocations)</td>
<td>[-7, 12]</td>
<td>[-1, 1]</td>
</tr>
<tr>
<td>SH (Lauder)</td>
<td>[-11, 15]</td>
<td>[-8, 0]</td>
</tr>
</tbody>
</table>

From groundbased-SCIA validation: Less consistent picture

All numbers: range of average (SCIA – X) in percent
Summary IFE-Bremen v1.6 ozone profile results

Sat-sat comparisons                  HALOE
   21-43 km num. density: [-7, 15]

IFE - HALOE: comparable result with SCIA OL - HALOE

SCIA-groundbased/sondes              lidar or sonde
   NH (7 locations)                  [-14,21]
   (sub)tropics (2 locations)        [-13,36]
   Lauder                            [-22,15]

IFE - groundbased: range about 2x larger than SCIA OL - groundbased

All numbers: range of average (SCIA - X) in percent
**Ozone: spectral windows**

Indicates fit window should shift (currently only UV)

From: A. Rozanov et al., Verification of O3 and NO2 vertical profiles from L2 offline product
To do list

- Decide on altitude shift (Envisat pointing problem) corrections in 2002 validation results
- Take into account a-priori / averaging kernels
- Separate cloud-free/clouded scenes
- Other dependencies (total ozone, viewing angle, etc.)
- Check errors introduced in unit conversions (e.g., P,T profiles used)
- Validate again after OL processor update (including VIS wavelengths)
- Use more ground-based data (and longer SCIA dataset when available)

Will lead to more uniform validation results and firmer conclusions
Notes on conclusions O3 profiles

- Different subsetting (e.g., Lauder and Mauna Loa) influences results, partially because of low-number statistics (3-30 collocations).

- Offline as well as IFE - consistent conclusions per site usually difficult (i.e. standard deviation in bias is high)

- All conclusions are very preliminary, validation is ongoing:
  1) More consistent approach between validation efforts needed
  2) Altitude corrections needed (location and time dependent). These also influence mixing ratio results, since P-profiles are used in unit conversions).
More notes on conclusions O3 profiles

- IFE data: larger set than SCIAMACHY OL profiles, will be better for investigating altitude offset and other dependencies.

- IFE algorithm has proven useful for OL algorithm updates (e.g., planned extension of fit window wavelength range)
Backup Material
Recommendations to algorithm developers (open for discussion)

- Change altitude and pressure grids by “half a bin” so users can plot profiles as they are (also provide average number densities rather than partial column densities)

- Use/provide accurate P,T profiles (now: standard atmosphere)

- Implement correction for pointing inaccuracy

- ...