VALIASI - Validation of IASI trace gas retrievals by GB - FTIR measurements

Sven Kühl
Presentation for EUMETSAT Fellowship day, 17th March 2014

Acknowledgments

AEMET, Centro de Investigación Atmosférica de Izaña
Angel Gómez-Peláez, Alberto Redondas,
Pedro Romero Campos, Omaira Garcia, Eliezer Sepúlveda

Karlsruhe Institute of Technology
Matthias Schneider, Andreas Wiegele, Susanne Dohe,
Sabine Barthlott, Frank Hase, Thomas Blumenstock

EUMETSAT
Thomas August
Comprehensive, longterm validation
Main reference: GB-FTIR
Project start: Sep. 2013, Izana, TC from IASI-A
Later: IASI-B, Karlsruhe, Kiruna, T-profiles

VALIASI
= Validation of IASI level 2 products

O$_3$  CO$_2$  H$_2$O  N$_2$O  CH$_4$  CO  T
Since 1916 (since 1984: BAPMoN, 1989: GAW)
Brewer, in situ GC, LIDAR, GPS, Sondes (since 1992)
GAW / NDACC / TCCON / AERONET / BSRN
FTIR since 1999, in cooperation with KIT-IMK
Izana Atmospheric Observatory (IZO)
Inversion layer

Rodriguez et al., 2009

A) T° C

B) RH, %

FT, Sc, MBL

TIL, top, bottom

Month
Outline

1. VALIASI
2. IZO, GB-FTIR, further Measurements at IZO
3. IASI, comparison to FTIR
4. Molecules, natural variability
5. Collocation
6. First Validation results
7. Annual cycle
8. Summary
Measurements, main building, Measurement-Tower, vicinity

Garcia et al., 2012
IZAÑA Observatory (and vicinity): measurements relevant for VALIASI

- **GPS**: H$_2$O total column
  (ERGNSS network: IARC, and four additional sites (three Tenerife and one La Palma)
- **ECC sondes**: O$_3$-, Hr-, T-, p-profile, u,v
  1/ week (Wednesday)
  2010: simultaneous launches south and north of the Izaña Observatory → spatial inhomogeneity
- **Radio sondes**: p-, T-, Hr-profile, windspeed and direction
  2/day, 11:00 and 23:00
- **Brewer**: O$_3$ total column, calibration center for Europe
- **GAW In Situ** CO, CH$_4$, N$_2$O Gas chromatography, CO$_2$ IR
  (July 2011: IZO + Teide Observatory and the Roque de los Muchachos Observatory, La Palma,
  Summer 2012: Flight campaigns → vertical profile)

+ **FTIR**: H$_2$O, O$_3$, CO$_2$, CH$_4$, N$_2$O, CO, T
vmr profiles of: \( \text{O}_3, \text{CO}, \text{CH}_4, \text{N}_2\text{O}, \text{H}_2\text{O}, \text{CO}_2, \text{T} \)
Approx. 120 days of observation per year, measurements only for cloud-free conditions
Since 1999: Bruker IFS 120 M
Since 2005: 120/125 HR
Validated by Brewer, \( \text{O}_3 \) Sondes, GAW
Comprehensive error analysis
High precision
<table>
<thead>
<tr>
<th></th>
<th>Projects</th>
<th>References</th>
<th>Microwindows</th>
<th>typ. # DOF</th>
<th>Precision exper. (theor.)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CO₂</strong></td>
<td>TCCON</td>
<td>Dohe et al., 2012</td>
<td>~ 5900, 6000 cm⁻¹</td>
<td>-</td>
<td>Correlation of 94% to in-situ</td>
</tr>
<tr>
<td><strong>CO</strong></td>
<td>NDACC</td>
<td>Velazco et al. (2007)</td>
<td>~ 2050, 2150 cm⁻¹</td>
<td>2</td>
<td>(&lt;5%)</td>
</tr>
<tr>
<td><strong>O₃</strong></td>
<td>NDACC</td>
<td>Schneider et al., 2008, Garcia et al., 2012, 2013</td>
<td>~ 1000 cm⁻¹</td>
<td>4</td>
<td>0.4-0.7%; / (~1DU, 0.6%)</td>
</tr>
<tr>
<td><strong>CH₄</strong></td>
<td>NDACC</td>
<td>Sepulveda et al., 2012, 2013</td>
<td>~ 2600, 2800, 2900 cm⁻¹</td>
<td>2.5</td>
<td>0.97% / (0.9 %)</td>
</tr>
<tr>
<td><strong>H₂O</strong></td>
<td>NDACC</td>
<td>Schneider et al., 2010, 2012</td>
<td>~ 2600 - 3000 cm⁻¹</td>
<td>3-4</td>
<td>Total column: 1% profiles: ~15% (&lt;1%)</td>
</tr>
<tr>
<td></td>
<td>MUSICA</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>N₂O</strong></td>
<td>NDACC</td>
<td></td>
<td>~ 2500 cm⁻¹</td>
<td>2.5</td>
<td>(~1%)</td>
</tr>
</tbody>
</table>
in situ GAW

Data from: Angel Gomez Pelaez

GPS H₂O prec.

Data from: Pedro Miguel Campos

Brewer O₃ total column

Data from: Alberto Redondas
FTIR – in situ GAW

$\text{CO}_2$

FTIR
XCO2

in situ

$\text{CO}$

FTIR

in situ
Abs. difference within uncertainty of spectroscopic data (UV/IR)
Precision for Brewer and FTIR: ~1 DU
Datasets for IASI validation

- FTIR
  - Columns Profiles, T

Windspeed, -direc. profiles

- IASI
  - Columns Profiles T, H₂O, O₃

GAW in situ
  - CO₂, CH₄, N₂O, CO

Brewer
  - O₃ TC

GPS
  - H₂O TC

Sondes
  - O₃, H₂O, T prf

colloc. criteria
• Infrared Atmospheric Sounding Interferometer
• Fourier transform spectrometer with high resolution between 645 and 2760 cm\(^{-1}\) (3.6 µm to 15.5 µm)
• associated Integrated Imaging Subsystem (IIS): broad band radiometer with a high spatial resolution. only used for co-registration with the Advanced Very High Resolution Radiometer (AVHRR)
• main goal of the IASI mission: provide atmospheric emission spectra to derive temperature and humidity profiles with high vertical resolution and accuracy. Additionally: determination of trace gases such as ozone, nitrous oxide, carbon dioxide and methane, as well as land- and sea surface temperature and emissivity and cloud properties.
one IASI orbit
2011-03-15

flag landsea

flag IASI clr

flag qual

N2O

0 The IASI IFOV is clear
1 The IASI IFOV is partly cloudy
2 The IASI IFOV is completely cloudy
3 The IASI IFOV is completely covered by water
4 The IASI IFOV is completely covered by land, the variability of the surface topography is low
5 The IASI IFOV is completely covered by land, the variability of the surface topography is high
6 The IASI IFOV covers land and water, the variability of the surface topography is low
7 The IASI IFOV covers land and water, the variability of the surface topography is high

0 No successful retrieval
1 Complete retrieval, errors within EURD objective
2 Incomplete retrieval, errors within EURD objective
3 Complete retrieval, errors within EURD threshold
4 Incomplete retrieval, errors within EURD threshold
5 Complete retrieval, errors outside EURD threshold
6 Incomplete retrieval, errors outside EURD threshold

3 obs. in 1x1 deg box also days with no obs. v6 : increase by factor 2
## Comparison: GB-FTIR to IASI

<table>
<thead>
<tr>
<th>GB FTIR</th>
<th>IASI</th>
</tr>
</thead>
<tbody>
<tr>
<td>FTS</td>
<td>FTS</td>
</tr>
<tr>
<td>700 to 9000 cm(^{-1})</td>
<td>645 to 2760 cm(^{-1}) (3.6 to 15.5 (\mu)m)</td>
</tr>
<tr>
<td>0.005 cm(^{-1}), S/N ~ 2000</td>
<td>0.5 cm(^{-1})</td>
</tr>
<tr>
<td>direct solar absorption</td>
<td>thermal emission</td>
</tr>
<tr>
<td>day</td>
<td>day + night</td>
</tr>
<tr>
<td>continuous (when clear sky)</td>
<td>10:00 + 22:00 (at Izana latitude)</td>
</tr>
<tr>
<td>2370 m to TOA</td>
<td>Surface to TOA (sensitivity)</td>
</tr>
<tr>
<td>28.3 N / 16.5 W</td>
<td>± 1 (0.5) deg (12 km)</td>
</tr>
<tr>
<td>land</td>
<td>sea (land)</td>
</tr>
<tr>
<td>8 min sampling (4 min CO(_2))</td>
<td>8 sec (30x4 pixel)</td>
</tr>
</tbody>
</table>
Column below 2370 m

- Use independent measurements (SCIA, TES, …)
- In situ for 2370 km and below?
- MUSICA/AMISOC flight campaign summer 2013
- O$_3$, H$_2$O sondes (but ...)
- study IASI sensitivity for boundary layer (thermal contrast, land sea, day night)
- use IASI profile (a priori) and AK information → add to FTIR profile (for v6)
- Use model data: WACCM
### WACCM data on column below IZO
(partial column for 0 to 2370 m)

<table>
<thead>
<tr>
<th></th>
<th>H₂O</th>
<th>O₃</th>
<th>CO</th>
<th>CH₄</th>
<th>N₂O</th>
<th>CO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-</td>
<td></td>
<td>(11 DU)</td>
<td>4.1e17</td>
<td>9.2e18</td>
<td>1.65e18</td>
<td>2.0e21</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(sondes: 8-10 DU)</td>
<td>Very strong annual cycle</td>
<td>± 0.2e18</td>
<td>± 0.05e18</td>
<td>± 0.05e21</td>
</tr>
</tbody>
</table>

**REMARKS:**
Correlation not affected!
Absolute values/differences not considered now
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### Molecules

(from Goody and Yung, 1989)

![Graph showing the distribution of various molecules across different altitudes and mixing ratios.](image)

<table>
<thead>
<tr>
<th></th>
<th>H$_2$O</th>
<th>CO</th>
<th>O$_3$</th>
<th>CO$_2$</th>
<th>CH$_4$</th>
<th>N$_2$O</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Daily variability</strong></td>
<td>very strong</td>
<td>mod. to strong</td>
<td>low to mod.</td>
<td>low</td>
<td>low</td>
<td>very low</td>
</tr>
<tr>
<td><strong>Annual Cycle</strong></td>
<td>very strong</td>
<td>very strong</td>
<td>moderate</td>
<td>moderate</td>
<td>moderate</td>
<td>small</td>
</tr>
<tr>
<td><strong>year to year (trend)</strong></td>
<td>(+)</td>
<td>-</td>
<td>±</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td><strong>spatial</strong></td>
<td>&lt; 10 km</td>
<td>&lt; 50 km</td>
<td>&gt; 50 km</td>
<td>~50 km</td>
<td>~50 km</td>
<td>&gt; 50 km</td>
</tr>
</tbody>
</table>
FTIR profiles variability

- N$_2$O
- O$_3$
- H$_2$O
- CH$_4$
- CO

March
June
September
December
Seasonal cycles - Meteorology

Figure 3. Seasonal cycle of single and multiple thermal tropopause occurrence frequency and wind speed over Tenerife derived from radiosondes data for the 1992–2011 period. Results are shown for single (solid stars with solid line), double (solid circles with dashed line), and triple (solid squares with dash-dotted line) tropopause events. Open circles with solid line denotes the sum of occurrence frequency for double and triple thermal tropopauses.

Rodriguez and Cuevas, JGR, 2013
Temporal and spatial collocation

Temporal criterium: depends on natural variability of target gas and FTIR uncertainty

A) Intra-day variability < FTIR uncertainty: **DAILY MEANS**
B) Intra-day variability > FTIR uncertainty: **±1h IASI overpass**

GAW, Brewer, GPS

Spatial criterium:

1) Determine region for air masses probed by FTIR
2) consider variability observed by IASI
different seasonal cycles
land, sea, day night
Windspeed, direction
Temporal collocation

Example for $O_3$

Intraday variability larger than FTIR uncertainty $\rightarrow$

FTIR measurements throughout the day can differ significantly to those at IASI overpass time (10-12h)

Brewer observations
$\sim$ 20 to 100 per day

one observation = mean value for approx. 3.5 min.
consists of exactly 20 single meas.

$O_3$

FTIR uncertainty
0.7%
For optimal collocation: only consider FTIR observations within 1 hour of IASI measurements.
CO₂ CH₄ N₂O:

almost no diurnal variation

→ FTIR uncertainty larger than Intruday variability observed by GAW in situ measurements

→ Daily means of FTIR

No loss of information
No effect on validation results
Spatial collocation

air masses probed by FTIR measurements determined by:
Vertical Column, Observation geometry (SZA, SAA)
effective vertical column length → distance

FTIR

VC2

VC1

SZA

LOS

d1

d2
Effective Column:
FTIR profiles of number density

- N$_2$O
- CH$_4$
- CO
- O$_3$
- H$_2$O
Distance for top of effective column along LOS from FTIR, at surface

H₂O: 5-10 km
N₂O, CH₄, CO, CO₂: 20 km
O₃: 40 km
**Summary: collocation**

<table>
<thead>
<tr>
<th>Region FTIR</th>
<th>H₂O</th>
<th>O₃</th>
<th>CO</th>
<th>CH₄</th>
<th>N₂O</th>
<th>CO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>spatial</td>
<td>0.25 deg</td>
<td>1 deg</td>
<td>0.5 deg</td>
<td>0.5 deg</td>
<td>0.5 deg</td>
<td>0.5 deg</td>
</tr>
<tr>
<td>temporal</td>
<td>± 1h</td>
<td>± 1h</td>
<td>± 1h</td>
<td>Daily mean</td>
<td>Daily mean</td>
<td>Daily mean</td>
</tr>
</tbody>
</table>

Validation performed for

- different sets of collocation criteria
- results compared to optimal criteria
FTIR dataset

- For comparison:
- Jun 2008 to Dec 2013 (= v4-v5 of IASI lv2), cloud free days!
- 7561 profiles for CH$_4$, N$_2$O, H$_2$O, (CO$_2$)
- 1349 profiles for CO, 1594 for O$_3$
- 50% of profiles in 2012+2013

IASI dataset

- v4 : Jun 2008 to Sep 2010
- v5 : Sep 2010 to now
- Daily means for 1deg (0.5 deg) boxes around IZO
- Cloud free, sea-land pixel, day-night separate

v5: approx. 1200 days → IZO: 400 cloud free
→ IASI: 300 colloc. days (180 for 0.5 deg)
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IASI - FTIR

* 1 deg box, sea pixel, daytime, v4-v5
* collocation criteria: 1degS, 0.5 deg, ± 1h
day-night / land-sea
* Correlation coefficient (Pearson)
* Total columns: O₃, CO, CH₄, N₂O, CO₂
* Profiles H₂O, partial columns: O₃
$O_3$

**v4**

$allV4 : day\_sea\_Q5 : 1deg$

- $r = 0.62$
- $MD = -13.8$

**v5**

$allV5 : day\_sea\_Q5 : 1deg$

- $r = 0.92$
- $MD = -7.9$
**CO**

**v4**

```
allV4 : day_sea_Q5 : 1deg
```

- **r = 0.67**
- **RMD = 43.8 %**

**v5**

```
allV5 : day_sea_Q5 : 1deg
```

- **r = 0.78**
- **RMD = 23.7 %**
CH$_4$

**v4**

- $r = -0.35$
- RMD = -3.8 %

**v5**

- $r = 0.39$
- RMD = 0.3 %
N$_2$O

$\text{CO}_2$

v4

\[ r = -0.27 \]

\[ \text{RMD} = 2.4\% \]

v5

\[ r = 0.31 \]

\[ \text{RMD} = -5.4\% \]
Summary on v4 / v5

<table>
<thead>
<tr>
<th></th>
<th>O₃</th>
<th>CO</th>
<th>CH₄</th>
<th>N₂O</th>
<th>CO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>v4</td>
<td>0.62</td>
<td>0.67</td>
<td>-0.35</td>
<td>-0.27</td>
<td>0.13</td>
</tr>
<tr>
<td>v5</td>
<td>0.92</td>
<td>0.78</td>
<td>0.39</td>
<td>0.31</td>
<td>0.05</td>
</tr>
</tbody>
</table>

1 deg box around IZO (center)
temp colloc. : daily mean

Following studies for v5 data:
different spatial colloc. (1 deg south, 0.5 deg)
temp colloc. : ± 1h IASI overpass
Daily mean ± 1 h

\[ \text{O}_3 \]

1deg

1deg S

\[ r = 0.92 \quad \text{MD} = -7.9 \]

\[ r = 0.93 \quad \text{MD} = -7.2 \]

\[ r = 0.87 \quad \text{MD} = -9.1 \]

\[ r = 0.9 \quad \text{MD} = -8.8 \]
Daily mean

\[ \text{CH}_4 \]

\[ 0.5\text{deg} \]

\[ 0.5\text{deg S} \]

\[ \pm 1\text{ h} \]
## Summary on collocation

<table>
<thead>
<tr>
<th></th>
<th>O₃</th>
<th>CO</th>
<th>CH₄</th>
<th>N₂O</th>
<th>CO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>1deg</td>
<td>0.92</td>
<td>0.78</td>
<td>0.39</td>
<td>0.31</td>
<td>0.05</td>
</tr>
<tr>
<td>1deg, t</td>
<td>0.93</td>
<td>0.82</td>
<td>0.44</td>
<td>0.34</td>
<td>0.15</td>
</tr>
<tr>
<td>1degS</td>
<td>0.87</td>
<td>0.74</td>
<td>0.39</td>
<td>0.32</td>
<td>0.07</td>
</tr>
<tr>
<td>1degS, t</td>
<td>0.9</td>
<td>0.8</td>
<td>0.44</td>
<td>0.39</td>
<td>0.21</td>
</tr>
<tr>
<td>0.5deg</td>
<td>0.93</td>
<td>0.8</td>
<td>0.37</td>
<td>0.25</td>
<td>0.12</td>
</tr>
<tr>
<td>0.5deg, t</td>
<td>0.94</td>
<td>0.82</td>
<td>0.49</td>
<td>0.34</td>
<td>0.23</td>
</tr>
<tr>
<td>0.5degS</td>
<td>0.92</td>
<td>0.78</td>
<td>0.41</td>
<td>0.38</td>
<td>0.08</td>
</tr>
<tr>
<td>0.5degS, t</td>
<td>0.93</td>
<td>0.8</td>
<td>0.52</td>
<td>0.46</td>
<td>0.16</td>
</tr>
</tbody>
</table>
Summary on day night

<table>
<thead>
<tr>
<th></th>
<th>(O_3)</th>
<th>CO</th>
<th>(CH_4)</th>
<th>(N_2O)</th>
<th>(CO_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>day</td>
<td>0.92</td>
<td>0.78</td>
<td>0.39</td>
<td>0.30</td>
<td>0.05</td>
</tr>
<tr>
<td>night</td>
<td>0.86</td>
<td>0.76</td>
<td>0.42</td>
<td>0.36</td>
<td>0.15</td>
</tr>
</tbody>
</table>
### Land - sea

<table>
<thead>
<tr>
<th></th>
<th>O$_3$</th>
<th>CO</th>
<th>CH$_4$</th>
<th>N$_2$O</th>
<th>CO$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>sea</td>
<td>0.92</td>
<td>0.78</td>
<td>0.39</td>
<td>0.30</td>
<td>0.05</td>
</tr>
<tr>
<td>land</td>
<td>0.84</td>
<td>0.71</td>
<td>0.06</td>
<td>0.07</td>
<td>0.46</td>
</tr>
</tbody>
</table>

- **0**: The IASI IFOV is completely covered by water
- **1**: The IASI IFOV is completely covered by land, the variability of the surface topography is low
- **2**: The IASI IFOV is completely covered by land, the variability of the surface topography is high
- **3**: The IASI IFOV covers land and water, the variability of the surface topography is low
- **4**: The IASI IFOV covers land and water, the variability of the surface topography is high
H₂O profiles

Schneider and Hase, ACP, 2011

IASI H₂O [ppm] vs ground-based FTS H₂O [ppm]

@3 km
ρ: 0.88

@5 km
ρ: 0.89

@9 km
ρ: 0.89

IASI PROFFIT-nadir H₂O [ppm] vs IASI EUMETSAT H₂O [ppm]

@0.5 km
ρ: 0.766

@3 km
ρ: 0.982

@6.5 km
ρ: 0.991

@10 km
ρ: 0.996
Annual cycles
$O_3$, only v5
Detrended

PC1: ~6-12km
PC2: ~6-16km
Summary
Summary

• Natural variability
• collocation criteria
• Temporal: FTIR unc.
• Spatial: FTIR probed airmasses and var. IASI observations
Summary

• Natural variability
• collocation criteria
• Temporal: FTIR unc.
• Spatial: FTIR probed airmasses and var. IASI observations

• Partial column below IZO: WACCM
• correlation coef. FTIR-IASI
• Improvement from v4 to v5
• Large: O$_3$, CO, mod.: CH$_4$
• Low for N$_2$O and CO$_2$
Summary

• Natural variability
• collocation criteria
• Temporal: FTIR unc.
• Spatial: FTIR probed airmasses and var. IASI observations

• Partial column below IZO: WACCM
• correlation coef. FTIR-IASI
• Improvement from v4 to v5
• Large: O$_3$, CO, mod.: CH$_4$
• Low for N$_2$O and CO$_2$

• Different collocation criteria (temp/spat)
• Best corr. for optimal coll. for O$_3$ and CO
• For CH$_4$ and N$_2$O best corr. for ±1h IASI overpass
Summary

- Natural variability
- collocation criteria
- Temporal: FTIR unc.
- Spatial: FTIR probed airmasses and var. IASI observations
- Partial column below IZO: WACCM
- correlation coef. FTIR-IASI
- Improvement from v4 to v5
- Large: O$_3$, CO, mod.: CH$_4$
- Low for N$_2$O and CO$_2$

- Different collocation criteria (temp/spat)
- Best corr. for optimal coll. for O$_3$ and CO
- For CH$_4$ and N$_2$O best corr. for ±1h IASI overpass
- day night: slight diff.
- land pixel: surf. alt. too var.
- Annual cycle: good agreement for O$_3$ and CO
- Agreement but also discr. for CH$_4$, N$_2$O and CO$_2$
Outlook

- Version 6 data: profiles for $O_3$ and CO, + AK, interpretation of discrepancies
  → part.col. below IZO
- More data: retrieval for 2x pixels
- Land data: high resolution info on topography
- Transport: windspeed, direction, Trajectories
- IASI-B, collocation criteria, outliers for IASI
- Include FTIR - stations at Karlsruhe and Kiruna
- T profiles
Wind direction

Footprint of source region for airmasses above IARC (shown are probabilities in %). Courtesy of Dr. Dietrich Feist, MPI for Biogeochemistry, Jena, Germany.