SCIAMACHY Validation with Solar FTIR Spectrometry at the NDSC Primary Station Zugspitze

DLR Contract: 50 EE 0007

Principle Investigator:
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Acknowledgment:
Michael Buchwitz (Uni Bremen)
Rüdiger de Beek (Uni Bremen)
Andreas Richter (Uni Bremen)
Zugspitze Solar FTIR: NDSC Primary-Status Instrument

0.00186 cm\(^{-1}\) resolution
(OPD = 486 cm) Bruker IFS120HR FT-spectrometer

- SFIT1.09e/2.38
- FASCATM 2.03 raytracing
Species: CO, CH₄, N₂O, O₃, NO₂

Contract-Commitment:

Commissioning Phase: Intense measurement phase between L+3 and L+6; measurement intensity: two weeks per month; columns be made available within 45 days.

Main validation phase: Intense measurement phase between L + 6 and L + 18 months; measurement intensity: one week per month; columns will be made available within 90 days.

Long-term validation phase: L+18 – project end: Routine operation (once a week).

We did much more: permanent 4 weeks per month operation on all clear sky days

„5.5 months Commissioning Phase“: including weekends

15 July - 31 Dec 2002: 60 Measurement days at Zugspitze within first 5.5 months.

Main validation phase:
15 July 2002 – 1 July 2003: 127 measurement days within first 11.5 months.

All retrievals have been submitted to Cal/Val database

Long-term validation phase:
15 July 2002 – 15 Oct 2004: 278 measurement days within 27 months = 2.3 measurement days / week.
Zugspitze FTIR: Relative Activity during Commissioning (15 Jul – 1 Dec 2002)

- Measurement Days 15 Jul – 1 Dec 02
- Data submitted to the Cal/Val data base 15 Jul – 1 Dec 02

Proc. ESA-ACVE1 Meeting, Dec 2002
Permanent Ground Truthing Facility Zugspitze/Garmisch according to the WMO requirements. Validation of and Synergistic use with Satellite Measurements.

MAPS, MOPITT, SAGE, ENVISAT

Selected by EUMETSAT as European Site for operational AIRS/IASI Validation

Example: 2002 AIRSVAL Campaign
3-months-7-days-a-week operation data delivery twice a day within 12 h
Zugspitze FTIR: Quality control/intercomparison

(taken from “Zugspitze FTIR NDSC Report Form 2003”):
Name, date, and location of last intercomparison and/or validation:
• 1996 intercomparison with Jungfraujoch: coincident measurements and independent analyses of HF, HCl. Agreement within 2 per cent

• In 2001 evaluation of the Zugspitze time series since 1995 of HCl and ClONO2, and comparison to the Jungfraujoch series; showed very good overall agreement!

• In spring 2003 comparison of the Zugspitze time series (1996-2002) of CO to the Jungfraujoch series; showed very good overall agreement!

• Intense 3 months water vapor validation campaign at Zugspitze (mid Aug – mid Nov 2002) with permanent FTIR water vapor measurements compared to 4 radio sondes launched on site daily and permanent GPS water column measurements on site. Very good agreement of FTIR to sonde columns within a few per cent! Detailed FTIR validation study also relative to GPS measurements under way._
Zugspitze FTIR: Quality control/intercomparison

Example CO

Monthly CO total columns or mixing ratios related to normal values, averaged over all the years, except 1998

Alpine stations

Yurganov, et al., J. Geophys. Res. 109, 2004
Zugspitze FTIR: Quality control/intercomparison

Example $N_2O$

+ also done for all other species!
Ozone Operational NRT Product - July 2003: FTIR versus SCIA DOAS0 (UV)

FTIR: Individual measurements (15-min integr.)
SCIA: Daily average of all pixels within 500-km radius

Total Column (cm^-2)

Time of year 2002/03

IMK-IFU Garmisch-Partenkirchen, Ralf Sussmann  Zugspitze FTIR NDSC
Karlsruhe Research Center  DLR Contr. 50 EE 0007
Ozone Operational Product - April 2004: FTIR versus SCIA Master Set

![Graph showing ozone column density comparison between FTIR and SCIA Master Set DOAS_0 measurements within 500 km.]

- **Zugspitze FTIR:** individual measurements
- **SCIA Master Set DOAS_0:** individual pixels within 500 km

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**Zugspitze FTIR NDSC**

**Karlsruhe Research Center**  
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Ozone Operational – Dec 2004: FTIR versus SCIA Master Set and Reprocessing

- SCIA Master Set; averages of pixels within 500 km
- Zugspitze FTIR daily averages
- SCIA Reprocessing; averages of pixels within 500 km

<table>
<thead>
<tr>
<th>Date</th>
<th>Total Column (cm⁻²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jul-02</td>
<td>5.0E+18</td>
</tr>
<tr>
<td>Oct-02</td>
<td>6.0E+18</td>
</tr>
<tr>
<td>Feb-03</td>
<td>7.0E+18</td>
</tr>
<tr>
<td>Jun-03</td>
<td>8.0E+18</td>
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<tr>
<td>Oct-03</td>
<td>9.0E+18</td>
</tr>
<tr>
<td>Feb-04</td>
<td>1.0E+19</td>
</tr>
<tr>
<td>Jun-04</td>
<td>1.1E+19</td>
</tr>
<tr>
<td>Oct-04</td>
<td>1.2E+19</td>
</tr>
</tbody>
</table>

IMK-IFU Garmisch-Partenkirchen, Ralf Sussmann

Zugspitze FTIR NDSC

Karlsruhe Research Center

DLR Contr. 50 EE 0007
O$_3$ Column Scaling Factor: \[ \text{FTIR} = (\text{SCIA Master Set, Reprocessing}) \times 0.95(\pm0.01) \]

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</tr>
<tr>
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</tr>
</tbody>
</table>

- Red: SCIA Master Set; averages of pixels within 500 km
- Blue: Zugspitze FTIR daily averages
- Pink: SCIA Reprocessing; averages of pixels within 500 km

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Zugspitze FTIR NDSC
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NO$_2$ Operational NRT Product – July 2003: FTIR versus SCIA DOAS1 (vis)

FTIR: Individual measurements (15-min integr.)

SCIA: Daily average of all pixels within 500-km radius

Total Column (cm$^{-2}$)

FTIR Zugspitze Column

Version 3.51
Version 3.52
Version 3.53
Version 4.00
Version 4.01

Time of year 2002/03

Jul 02 Aug 02 Okt 02 Nov 02 Jan 03 Mrz 03 Apr 03 Jun 03

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NO$_2$ Scientific Product UB 1.0 – July 2003: FTIR versus UB 1.0

- Zugspitze FTIR individ. measurements (15-min integration)
- SCIA Scientific UB1.0; individ. pixels within 200 km

Date

Jul-02 Aug-02 Oct-02 Dec-02 Feb-03 Apr-03 Jun-03

Total Column (cm$^{-2}$)
NO$_2$ Scientific Prod. UB1.0: *Pollution episodes removed from satellite data*

- Zugspitze FTIR individ. measurements (15-min integration)
- SCIA Scientif. UB1.0; individ. pixels within 200 km

**Date**

- Jul-02
- Aug-02
- Oct-02
- Dec-02
- Feb-03
- Apr-03
- Jun-03

**Total Column (cm$^{-2}$)**

- 1.0E+16
- 8.0E+15
- 6.0E+15
- 4.0E+15
- 2.0E+15
- 0.0E+00
**NO$_2$ Column Scaling Factor:** $\text{FTIR} = \text{SCIA UB 1.0} \times 1.30 (\pm 0.02)$

![Graph showing the NO$_2$ column scaling factor comparison between FTIR and SCIA UB 1.0 measurements.](image)

- **Zugspitze FTIR individ. measurements (15-min integration)**
- **SCIA Scientif. UB1.0; individ. pixels within 200 km**

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**Karlsruhe Research Center**  
**Zugspitze FTIR NDSC**  
**DLR Contr. 50 EE 0007**
NO$_2$ Scientific – 2004: FTIR versus UB 1.5 (1E+15 slant col. added) and UB 1.0

Date

0.0E+00 2.0E+15 4.0E+15 6.0E+15 8.0E+15 1.0E+16 1.2E+16

Total Column (cm$^{-2}$)

2nd NO2 Column Scaling Factor: FTIR = SCIA UB 1.5 * 1.20(±0.02)
NO$_2$ Operational Product - 2004: Master Set, Reprocessing versus UB 1.5, FTIR

![Graph showing total column (cm$^{-2}$) vs. date]

**IMK-IFU Garmisch-Partenkirchen**, Ralf Sussmann  
Zugspitze FTIR NDSC  
Karlsruhe Research Center, DLR Contr. 50 EE 0007
NO₂ Operational Product - Wrong Annual Cycle: Role of Solar Zenith Angle

Date
Jun-02 Jul-02 Aug-02 Sep-02 Sep-02 Oct-02 Nov-02 Dec-02

SZA("TOA") (deg)
20 30 40 50 60 70 80

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CO Operational NRT Product Versions July-2003: FTIR versus SCIA BIAS2 (NIR)

FTIR: Individual measurements (15-min integr.)

SCIA: Daily average of all pixels within 500-km radius

FTIR Zugspitze Column
version 3.51
version 3.52 data out of this scale
version 3.53
version 4.00
version 4.01

Time of year 2002/03
CO Scientif. WFMD v0.4 Prod.: FTIR versus WFMD Averaging Kernels

Pressure (hPa)

SCIA SZA=60°
SCIA SZA=70°
FTIR SZA=60°
FTIR SZA=70°
Uniform Sampling

CO Total Column Averaging Kernel
CO WFMD v0.4: FTIR indiv. measurements versus WFMD indiv. pixels <500 km

WFMD data for 33 days Jan–Oct 2003

Zugspitze FTIR: Anomaly of pressure corrected CO columns, individ. measurements, 20 min integr.

SCIA_WFMD_v0.4: CO/O2 columns anomaly, individ. pixels within 500 km; includ. cloud contaminated pixels (69%)

SCIA_WFMD_v0.4: CO/O2 columns anomaly, individ. pixels within 500 km; cloud flagged pixels removed

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Zugspitze FTIR NDSC
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CO WFMD v0.4: FTIR daily averages versus WFMD pixel averages <2000 km

- Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns
- SCIA_WFMD_v0.4 CO/O2 column anomaly: average of pixels within 2000 km; cloud contaminated pixels removed
CO WFMD v0.4: FTIR daily averages versus WFMD pixel averages <2000 km

- Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns
- SCIA_WFMD_v0.4 CO/O2 column anomaly: average of pixels within 2000 km; cloud contaminated pixels removed

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CO WFMD v0.4: FTIR daily averages versus WFMD pixel averages <2000 km

- **Zugspitze FTIR CO column anomaly**: daily means of pressure corrected columns
- **SCIA_WFMD_v0.4 CO/O2 column anomaly**: average of pixels within 2000 km; cloud contaminated pixels removed

**Graph Details**
- X-axis: Date
- Y-axis: Column anomaly
- Data points from Dec-02 to Feb-04

**Sources**
- IMK-IFU Garmisch-Partenkirchen, Ralf Sussmann
- Zugspitze FTIR NDSC
- Karlsruhe Research Center
- DLR Contr. 50 EE 0007
## CO WFMD v0.4: Linear Response to Annual Cycle?

<table>
<thead>
<tr>
<th>Data Source</th>
<th>Slope</th>
<th>Slope error</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zugspitze FTIR</td>
<td>-9.5E-4</td>
<td>9.8E-5</td>
<td>-0.70</td>
</tr>
<tr>
<td>SCIA 2000 km</td>
<td>-1.2E-3</td>
<td>4.9E-4</td>
<td>-0.43</td>
</tr>
<tr>
<td>SCIA 1000 km</td>
<td>-6.4E-4</td>
<td>5.9E-4</td>
<td>-0.21</td>
</tr>
<tr>
<td>SCIA 1000 km incl. clds</td>
<td>-4.4E-4</td>
<td>4.3E-4</td>
<td>-0.18</td>
</tr>
</tbody>
</table>
CO WFMD Sep-04 „Add-Release“: Data Set increased from 33 Days to 153 Days

- Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns
- SCIA_WFMD_v0.4 CO, release Sep05; ground altitude corr. with barometr. eq.; column anomaly: average of pixels within 1000 km; cloud contaminated pixels removed; retrieval error < 60 %
CO Day-to-Day Scatter: \( \text{STDV FTIR} = 7.3\% \) \( \text{STDV SCIA WFMD v0.4} = 25.4\% \)

Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns

SCIA_WFMD_v0.4 CO, release Sep05; ground altitude corr. with barometr. eq.; column anomaly: average of pixels within 1000 km; cloud contaminated pixels removed; retrieval error < 60%
CO Column Scaling Factor: \textit{Zugspitze FTIR = SCIA WFMD v0.4 * 0.78(± 0.06)}
N₂O Operational NRT Product July-2003: FTIR versus SCIA BIAS1 (NIR)

FTIR: Individual measurements (15-min integr.)

SCIA: Individual pixels within 500-km radius

Total Column (cm⁻²)

Time of year 2002/03

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N$_2$O Scientific WFMD v0.4: FTIR versus WFMD < ±2000 km latitudinal band

- Zugspitze FTIR N2O column anomaly: daily means of pressure corrected columns
- SCIA_WFMD_v0.4 N2O/O2 column anomaly: average of pixels within a latitudinal band ± 2000 km; cloud contaminated pixels removed; retrieval error <100 %
CH$_4$ Operational NRT Prod. Versions – July-2003: FTIR versus SCIA BIAS2 (NIR)

FTIR: Individual measurements (15-min integr.)

SCIA: Daily average of all pixels within 500-km radius

Total Column (cm$^{-2}$)

Time of year 2002/03

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Zugspitze FTIR NDSC

Karlsruhe Research Center

DLR Contr. 50 EE 0007
XCH$_4$ WFMD Product: FTIR versus WFMD v0.4 and WFMD v0.41

- Zugspitze FTIR
- SCIAMACHY v.0.4
- SCIAMACHY v.0.41

Pixel averages within 2000 km; retrieval error < 10 %

Date
Dec-02  Mar-03  May-03  Aug-03  Nov-03
SCIAMACHY Validation by Zugspitze FTIR: CONCLUSIONS AS TO 7-DEC-2004

1. Operational total ozone (Master Set plus Reprocessing) shows good pixel-to-pixel reproducibility and a realistic day-to-day scatter (pixel average within 500 km) – comparable to the ground FTIR. Column scaling factor: Zugspitze FTIR = SCIA * 0.95(±0.01).

2. Operational total NO$_2$ (Master Set plus Reprocessing) shows serious difficulties in monitoring the annual cycle (fall-winter decrease) above Zugspitze.

3. Scientific total NO$_2$ (UB 1.0, 1.5) perfectly monitors the annual cycle. It shows a realistic day-to-day scatter (200-km selection radius) after exclusion of pollution episodes. The column scaling factor (UB 1.5) is: Zugspitze FTIR = SCIA * 1.20(±0.02).

4. Scientific WFMD CO v0.4 shows a day-to-day scatter that is too high by a factor of 3.5 compared to the ground FTIR for a 1000-km selection radius. Higher selection radii are required to reflect the CO annual cycle in terms of a linear response. In the „September-2003 Release“ an unrealistic enhancement around Jul-2003 shows up. Column scaling factor is: FTIR = SCIA * 0.78(±0.06).

5. WFMD N$_2$O v0.4 day-to-day scatter is too high by a factor 10 even for averaging all pixels within a ±2000-km latitudinal band.

6. WFMD XCH$_4$ has shown a quality break-through from v0.4 to v.0.41 (time dependent correction, ice issue). However, systematic ice features still dominate over the day-to-day scatter for a 2000-km selection radius, thus masking the CH4 annual cycle.