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Chapter 1 | Introduction

1.1 Aim and scope of this document

Odin/SMR performs passive limb measurements of the atmosphere, mainly at wavelengths and frequencies around 0.6 mm and 500 GHz, respectively. From these measurements, profiles of O$_3$, ClO, N$_2$O, HNO$_3$, H$_2$O, CO, and isotopologues of H$_2$O, and O$_3$, that are species of interest for studying stratospheric and mesospheric chemistry and dynamics, can be derived. Odin/SMR has been in operation for approximately 20 years, and thus, the Level2 dataset can potentially be applied for scientifically interesting trend analysis.

The project aims at producing a new Odin/SMR Level2 product dataset with improved long term consistency and precision. This dataset will be based on updated/revised processing algorithms and input data. A verification dataset (VDS) has been created. The VDS is a representative subset of the Odin/SMR Level1B dataset and collocated correlative measurements from similar instruments, i.e. data from Odin/OSIRIS, Aura/MLS, ENVISAT/MIPAS, ISS/JEM/SMILES, and Meteor3M/SAGEIII. See Rydberg et al. (2016b) for descriptions of data and instruments included in the VDS.

From the VDS a diagnostic dataset (DDS) has been created, containing Level2 products produced with the updated processing system. The aim of this document is to describe the DDS and the main results of comparing it with the correlative measurements from other instruments, as well as with the Level2 data from the older 2.0/2.1 versions of the Odin/SMR processing chain.

1.2 Document structure

This document is organized as follows: Chapter 2 describes the Odin/SMR Level2 data products. Chapter 3 contains comparisons for several of the Odin/SMR frequency modes and their Level2 data products with collocated measurements from various instruments. Chapter 4 contains conclusions, and the appendix contains additional information on the various observation modes of Odin/SMR.
Chapter 2 | Odin/SMR Level2 data products

2.1 The Odin mission

The Odin satellite was launched on the 20th of February 2001, into a sun-synchronous 18:00 hour ascending node orbit, carrying two co-aligned limb sounding instruments: OSIRIS (Optical spectrograph and infrared imaging system) and SMR (Sub-millimetre radiometer) Murtagh et al. (2002). Originally, Odin was used for both atmospheric and astronomical observations, but since 2007 only its aeronomy mission is active. Odin is a Swedish-led project, in cooperation with Canada, France and Finland. Both of Odin’s instruments are still functional, and the present operation of the satellite is partly performed as an ESA third party mission.

2.2 The SMR instrument

The Odin/SMR package is highly flexible Frisk et al. (2003). In short, the four main receiver chains can be tuned to cover frequencies in the ranges 486–504 GHz and 541–581 GHz, but the maximum total instantaneous bandwidth is only 1.6 GHz. This bandwidth is determined by the two auto-correlation spectrometers (ACs) used for atmospheric observations. The two ACs can be coupled to any of the four front-ends, but only two or three front-ends are used simultaneously. The ACs cover 400 or 800 MHz per front-end, depending on configuration. In the configuration applied for atmospheric sounding, the channels of the ACs have a spacing of 1 MHz, while the frequency resolution is only 2 MHz. To cover all molecular transitions of interest (see Table 2.1 and Table 2.2 for an overview), a number of “observation modes” have been defined. Each observation mode makes use of two or three frequency bands. Single sideband operation is obtained by tunable Martin–Pupplet interferometers. The nominal sideband suppression is better than 19 dB across the image band.

Odin/SMR also has a receiver chain around the 118 GHz oxygen transition that was heavily used during Odin’s astronomy mission. For the atmospheric mission, this front-end was planned to be used for retrieving temperature profiles, but a technical problem (drifting LO frequency) and the fact that the analysis requires treatment of Zeeman splitting have given these data low priority.

The main reflector of Odin/SMR has a diameter of 1.1 m, giving a vertical resolution at the tangent point of about 2 km. The vertical scanning of the two instruments’ line-of-sight is achieved by a rotation of the satellite platform, with a rate matching a vertical speed of the tangent altitude of 750 m/s. Measurements are performed during both upward and downward scanning. The lower end of the scan is typically at about 7 km, the upper end
Table 2.1: Characteristics of Odin/SMR Level2 main data products for version 2 of the processing chain.

<table>
<thead>
<tr>
<th>Product</th>
<th>Frequency [GHz]</th>
<th>Vertical coverage</th>
<th>Vertical resolution</th>
<th>Precision</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₃</td>
<td>501.5 (FM 01)</td>
<td>~19–50 km</td>
<td>~2 km</td>
<td>0.5–2 ppmv</td>
<td>Urban et al. (2005)</td>
</tr>
<tr>
<td>ClO</td>
<td>501.3 (FM 01)</td>
<td>~19–67 km</td>
<td>1.5–2 km</td>
<td>0.15–0.2 ppbv</td>
<td>Urban et al. (2005)</td>
</tr>
<tr>
<td>N₂O</td>
<td>502.3 (FM 01)</td>
<td>~15–70 km</td>
<td>~1.5 km</td>
<td>15–35 ppbv</td>
<td>Urban et al. (2005)</td>
</tr>
<tr>
<td>O₃</td>
<td>544.9 (FM 02)</td>
<td>~18–70 km</td>
<td>~1.5 km</td>
<td>0.2–0.4 ppmv</td>
<td>Urban et al. (2005)</td>
</tr>
<tr>
<td>HNO₃</td>
<td>544.4 (FM 02)</td>
<td>~21–67 km</td>
<td>1.5–2 km</td>
<td>1 ppbv</td>
<td>Urban et al. (2005)</td>
</tr>
</tbody>
</table>

Table 2.2: Characteristics of Odin/SMR Level2 science data products for version 2 of the processing chain.

<table>
<thead>
<tr>
<th>Product</th>
<th>Frequency [GHz]</th>
<th>Vertical coverage</th>
<th>Vertical resolution</th>
<th>Precision</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>578.6 (FM 22)</td>
<td>~17–110 km</td>
<td>3–4 km</td>
<td>25 ppbv–2 ppmv</td>
<td>Dupuy et al. (2004)</td>
</tr>
<tr>
<td>H₂¹⁶O</td>
<td>556.9 (FM 19)</td>
<td>~40–100 km</td>
<td>~3 km</td>
<td>0.5–1 ppmv</td>
<td>Urban et al. (2007)</td>
</tr>
<tr>
<td>H₂¹⁸O</td>
<td>488.5 (FM 17)</td>
<td>~20–70 km</td>
<td>~3 km</td>
<td>0.5–1 ppmv</td>
<td>Urban et al. (2007)</td>
</tr>
<tr>
<td>HD₂</td>
<td>490.6 (FM 17)</td>
<td>~20–70 km</td>
<td>3–4 km</td>
<td>0.5 ppbv</td>
<td>Urban et al. (2007)</td>
</tr>
<tr>
<td>H₂¹⁸O</td>
<td>489.1 (FM 08)</td>
<td>~20–65 km</td>
<td>3–4 km</td>
<td>20–30 ppbv</td>
<td>Urban et al. (2007)</td>
</tr>
<tr>
<td>H₂¹⁷O</td>
<td>552.0 (FM 21)</td>
<td>~20–70 km</td>
<td>~3 km</td>
<td>0.4 ppbv</td>
<td>Urban et al. (2007)</td>
</tr>
<tr>
<td>NO</td>
<td>551.7 (FM 21)</td>
<td>~40–100 km</td>
<td>~7 km</td>
<td>40%</td>
<td>Sheese et al. (2013)</td>
</tr>
<tr>
<td>^1⁸O²¹⁶O¹⁸O</td>
<td>490.4 (FM 17)</td>
<td>~27–41 km</td>
<td>4–6 km</td>
<td>25%</td>
<td>Urban et al. (2013)</td>
</tr>
<tr>
<td>^1⁶O²¹⁶O¹⁸O</td>
<td>490.0 (FM 17)</td>
<td>~25–45 km</td>
<td>3–4 km</td>
<td>25%</td>
<td>Urban et al. (2013)</td>
</tr>
<tr>
<td>^1⁶O²¹⁷O¹⁷O</td>
<td>490.6 (FM 17)</td>
<td>~31–39 km</td>
<td>5–6 km</td>
<td>25%</td>
<td>Urban et al. (2013)</td>
</tr>
</tbody>
</table>

varies between 70 and 110 km, depending on observation mode. In correspondence, the horizontal sampling ranges from 1 scan per 600 km to 1 scan per 1000 km. Measurements are in general performed along the orbit plane, providing a latitude coverage between 82.5°S and 82.5°N. Since the end of 2004 Odin is also pointing off-track during certain periods, e.g. during the austral summer season, allowing the latitudinal coverage to be extended towards the poles.

2.3 Odin/SMR Level2 data products

Odin/SMR data are categorized into main and science Level2 products, and Table 2.1 and Table 2.2 describe the characteristics of these products, respectively. The main products are retrieved from the so called “stratospheric” observation mode of Odin/SMR, and this mode cover approximately 50% of the Odin/SMR observation time. In this mode spectra in frequency bands around 501 and 544 GHz are collected. The science data products are derived from less frequently applied observation modes (typically applied a few days per month).

2.3.1 Main data products

Ozone, ClO, N₂O, and HNO₃ profiles are the main Odin/SMR Level2 products. ClO and N₂O profiles are retrieved from spectra covering transitions around 501 GHz, and
HNO$_3$ from spectra around 544 GHz. Ozone can be retrieved from both the 501 and the 544 GHz band. Table 2.1 describes characteristics of these Level2 products that have been derived from earlier Odin/SMR Level2 data studies. The characteristics can not be expected to be changed/improved dramatically for a new Level2 data product, because these characteristics depend on the physics of the measurement and the sensor.

Possibly more important than the characteristics described in Table 2.1 are the accuracy and stability of the profiles, since the latter enable trend studies. The overall aim of the new Level2 data processing also reflects this aspect, and the objective is therefore that the accuracy and stability outperforms that from earlier Odin/SMR Level2 data products.

### 2.3.2 Science data products

Profiles of H$_2$O, CO, NO and isotopologues of H$_2$O, and O$_3$ are considered as science data products for Odin/SMR, and characteristics of these products are described in Table 2.2. Observations covering the science data products are performed on a less frequent basis than the main data products. The aim of the Level2 processing of the science data products is in principle identical to that for the main data products, although the main data products will be given a higher priority.
Chapter 3  |  Comparisons with other instruments

This chapter contains comparisons between the Level2 data products of Odin/SMR and collocated measurements from various instruments as accumulated in the Validation Data Set (VDS) (Rydberg et al. (2016b)). The initial VDS covered the period 2003–2015 but this has been extended to 2019. This implies that the DDS has also been extended to the same period. The comparisons are organised primarily on frequency mode, secondarily on data product. For each product, average deviations from the various instruments at different altitudes are investigated, followed by an investigation of the overall correlation between the measurements and both Odin/SMR v2 and v3. The Odin/SMR measurement response and averaging kernels are also investigated for each data product Eriksson (2017). This has been carried out for the main data products i.e. those from FM 01, FM 02, FM 08, FM 13 and FM 19. The other science mode products require separate treatment since they must be compared to special products from the other instruments. They have therefore been excluded from the project and this report. However many of the “lessons learnt” in the project will be useful. From the correlation some key performance indicators are obtained and presented in a table. Of these the most important are the Pearson correlation and slope, both of which should be as close as possible to unity for a good match, and the intercept, which should ideally be zero.
CHAPTER 3. COMPARISONS WITH OTHER INSTRUMENTS
3.1 Frequency mode 01

3.1.1 Overview

Frequency mode 01 monitors two bands, 501.180–501.580 GHz and 501.980–502.380 GHz. Its main use is retrievals of O₃, ClO and N₂O. This ozone product has previously been used as the main Odin/SMR ozone product despite the weak line and thereby noisy profiles. Spectra from this observation mode are shown in Figure 3.1. We hope that this reprocessing will make the FM 02 ozone the main product.

![Figure 3.1: Annual median spectra for FM 01 for altitude interval 35–45 km at equatorial latitudes during the arctic winter.](image)

3.1.2 Comparison of retrieved profiles

3.1.2.1 O₃

The retrievals for O₃ have been compared with data from the MIPAS, MLS, OSIRIS and SAGE III instruments. Annual average differences to these instruments are shown in Figure 3.2. In Figure 3.3 individual retrievals for the instruments for 2003–2019 (depending on the instrument) are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a considerable improvement with the updated version of the processing, with much better overall correlation and coherency, and most of the systematic under estimation having been removed compared to all instruments except for SAGE III. Compared to SAGE III, the results were bad for Odin/SMR v2.X, but are even worse for Odin/SMR v3. This may be attributed to the fact that the collocated measurements for SAGE III are all from altitude range 40–50 km, which is the upper range of altitudes for this frequency mode, and the lower range for the SAGE III instrument, as seen in Figure 3.2d.

A clear drift in the results is seen after 2009 and data from 2010–2017 should be treated with extreme care. The reason for the drift has now been identified as an instrument
problem where an unstable oscillator has widened the instrument line-profile. This may be possible to correct for in a later version of the data but will require an in depth study of the problem and possible corrections strategies. Data from 2018 and onward seems to be free of this problem thanks to a retuning of some parameters on-board the satellite. The useful range for the product and the vertical resolution is shown in Figure 3.4. Based on an analysis of the averaging kernels and comparisons with the other instruments the product is useful for the range 19–50 km with a resolution of around 5 km. The resolution is slightly degraded compared to the version 2.x product due to increased vertical correlation used to stabilise the retrievals.

Figure 3.2: Average difference in percent between retrievals of O$_3$ from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 01.
3.1. Frequency mode 01

(a) correlation of collcated instruments with Odin/SMR v2.X
(b) correlation of collcated instruments with Odin/SMR v3

Figure 3.3: Correlation between retrievals of O₃ using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments for frequency mode 01. The period is restricted to 2003-2008 in order to avoid the errors caused by the LO from 2009-2018.

(a) median measurement response with 1σ and 2σ percentiles
(b) median averaging kernels

Figure 3.4: Measurement response and averaging kernels for O₃ retrievals for Odin/SMR v3 at different altitudes for frequency mode 01.
3.1.2.2 N$_2$O

The retrievals for N$_2$O have been compared with data from the MIPAS and MLS instruments. Annual average differences to these instruments are shown in Figure 3.5. In Figure 3.6 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. Only a minor improvement is seen with the updated version of the processing. Figure 3.7 suggests that the product is useful over the range 15–50 km with a vertical resolution of around 5 km.

(a) average difference to MIPAS

(b) average difference to MLS

Figure 3.5: Average difference in percent between retrievals of N$_2$O from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 01. (Retrievals yielding concentrations $\leq$ 0.03 ppm have been filtered out.)

(a) correlation of collocated instruments with Odin/SMR v2.X

(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.6: Correlation between retrievals of N$_2$O using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments for frequency mode 01.
3.1. Frequency mode 01

Figure 3.7: Measurement response and averaging kernels for N$_2$O retrievals for Odin/SMR v3 at different altitudes for frequency mode 01.

3.1.2.3 ClO

The retrievals for ClO have been compared with data from the MLS instrument. Annual average differences to MLS are shown in Figure 3.8. In Figure 3.9 individual retrievals from MLS for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. No sizeable improvement is seen for the new version of the Odin/SMR processing chain compared to MLS, and the correlation and coherency between the two remains poor, however, Figure 3.9 suggests that this is due to noisy nature of the MLS retrievals, which show a very large spread – sometimes even large negative concentrations – for the retrievals where both Odin/SMR versions yield low ClO concentrations. A further explanation is that, since ClO concentrations have a diurnal cycle, collocation in time is very important for comparisons, and due to the orbits of the two instruments, this is only really satisfied near the poles. In this comparison we have not attempted to separate periods of chlorine activation from period with a normal vertical distribution. From previous experience we know that the diurnal effect can be very large in such comparisons. Figure 3.10 suggests that the product is useful in the range 18–55 km with a vertical resolution of around 5 km.
CHAPTER 3. COMPARISONS WITH OTHER INSTRUMENTS

Figure 3.8: Average difference in percent between retrievals of ClO from Odin/SMR v3 and collocated measurements from MLS at different altitudes for frequency mode 01. (Retrievals yielding concentrations ≤ 0.3 ppb have been filtered out.)

Figure 3.9: Correlation between retrievals of ClO using Odin/SMR versions 2.X and 3 and collocated measurements MLS for frequency mode 01.
3.1. Frequency mode 01

Figure 3.10: Measurement response and averaging kernels for ClO retrievals for Odin/SMR v3 at different altitudes for frequency mode 01.

3.1.3 Discussion

The Pearson correlation between the Odin/SMR retrievals and the other instruments was calculated for the overlap periods for both versions of the processing chain. The results are summarised in Table 3.1, and show that the new algorithm is an improvement compared to all the instruments (with the exception of SAGE) for all species used in this investigation. The improvement is considerable for the O₃, but only slight for N₂O and ClO, with the latter still showing very poor correlation with the collocated MLS data. Correlations and fits were also calculated for the individual years in the period (see Figure 3.11), but no trends of note were seen until 2012, when an instrument problem occurred or possibly increased which renders retrievals from frequency mode 01 unreliable outside the arctic summer months. The problem caused asymmetric broadening of the lines resulting in bad fits and reduced species concentrations. It may be possible to compensate for the effect in a later reprocessing and rescue the data but this is not yet clear. The problem was fixed late in 2017 through retuning of driving circuits by the instrument scientist. Averaging of some weeks of spectra show that the distortions of the lines has been removed.

3.1.4 Conclusions

Based on the discussion above, retrievals based on frequency mode 01 can be used with confidence for the species O₃ and N₂O for the period 2003–2008. Retrievals of ClO based on this frequency mode should be used with some caution taking account of the local time of the observations.

For the period 2012–2017 all retrievals from frequency mode 01 should be used with caution, if at all, due to the problem discussed in Sec. 3.1.3. The only exceptions are retrievals from the middle of the arctic summer, which are not affected by this problem as a result of the satellite being colder during this period Eriksson and Urban (2006). The problem was fixed in late 2017, wherefore data from 2018 and onwards should have the same quality as that of 2003–2008. This is confirmed by the comparisons.
Table 3.1: Pearson correlation and fit parameters of the old and new Odin/SMR retrievals for frequency mode 01, compared with collocated data from other instruments for the period 2003–2019. \( \langle \text{res.} \rangle \) is the mean residual.

<table>
<thead>
<tr>
<th>Species</th>
<th>Instrument</th>
<th>SMR</th>
<th>corr.</th>
<th>slope</th>
<th>intercept</th>
<th>( \langle \text{res.} \rangle )</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₃</td>
<td>MIPAS (KIT) v3</td>
<td>0.900</td>
<td>0.979</td>
<td>0.044ppm</td>
<td>1.056ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.789</td>
<td>0.908</td>
<td>0.007ppm</td>
<td>1.497ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MIPAS (ESA) v3</td>
<td>0.887</td>
<td>0.959</td>
<td>0.108ppm</td>
<td>1.128ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.778</td>
<td>0.885</td>
<td>0.098ppm</td>
<td>1.548ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MLS v3</td>
<td>0.898</td>
<td>0.999</td>
<td>0.129ppm</td>
<td>1.030ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.778</td>
<td>0.923</td>
<td>0.095ppm</td>
<td>1.436ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OSIRIS v3</td>
<td>0.918</td>
<td>1.005</td>
<td>0.053ppm</td>
<td>0.890ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.783</td>
<td>0.951</td>
<td>-0.101ppm</td>
<td>1.426ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SAGE III v3</td>
<td>0.439</td>
<td>1.023</td>
<td>0.371ppm</td>
<td>0.943ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.275</td>
<td>0.840</td>
<td>0.654ppm</td>
<td>1.193ppm</td>
<td></td>
</tr>
<tr>
<td>N₂O</td>
<td>MIPAS (KIT) v3</td>
<td>0.983</td>
<td>0.985</td>
<td>2.844ppb</td>
<td>16.750ppb</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.975</td>
<td>0.979</td>
<td>2.786ppb</td>
<td>20.055ppb</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MIPAS (ESA) v3</td>
<td>0.017</td>
<td>0.000</td>
<td>67.659ppb</td>
<td>19.677ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.086</td>
<td>0.007</td>
<td>67.000ppb</td>
<td>1.148ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MLS v3</td>
<td>0.976</td>
<td>0.960</td>
<td>2.062ppb</td>
<td>19.809ppb</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.968</td>
<td>0.940</td>
<td>2.632ppb</td>
<td>22.881ppb</td>
<td></td>
</tr>
<tr>
<td>ClO</td>
<td>MLS v3</td>
<td>0.259</td>
<td>0.098</td>
<td>0.177ppb</td>
<td>0.436ppb</td>
<td></td>
</tr>
<tr>
<td></td>
<td>v2.x</td>
<td>0.238</td>
<td>0.109</td>
<td>0.160ppb</td>
<td>0.441ppb</td>
<td></td>
</tr>
</tbody>
</table>

Figure 3.11: Pearson correlation (\( \rho \)) of Odin/SMR v3 (---) and v2.X (---) retrievals of O₃ with collocated measurements. Note the decline in \( \rho \) after 2012.
3.2 Frequency mode 02

3.2.1 Overview

Frequency mode 02 monitors the band 544.102–544.902 GHz. Its main use is retrievals of O$_3$ and HNO$_3$. This mode was intended to be the main measurement of ozone in the stratosphere but in previous versions of the data products suffered with large systematic biases. We believe that this was caused by an incorrect line broadening constant. This also resulted in an unrealistic pointing offset being derived for this band. In this version of the product the coefficient was adjusted to remove the pointing offset and at the same time greatly improved the ozone values. Spectra from this observation mode are shown in Figure 3.12.

![Figure 3.12: Annual median spectra for FM 02 for altitude interval 35–45 km at equatorial latitudes during the arctic winter.](image)

3.2.2 Comparison of retrieved profiles

3.2.2.1 O$_3$

The retrievals for O$_3$ have been compared with data from the MIPAS, MLS, OSIRIS and SAGE III instruments. Annual average differences to these instruments are shown in Figure 3.13. In Figure 3.14 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a considerable improvement with the updated version of the processing, with much better over-all correlation and coherency, and most of the systematic under estimation having been removed compared to all the considered instruments. The largest improvement is compared to SAGE III, though, as seen in Figure 3.13d, there are still large systematic differences depending on the altitude. This could be a result of the difference in local time at the measurement location. At these altitudes ozone starts to exhibit a diurnal variation. This speculation could be supported by the good agreement with SAGE since it is an occultation instrument and therefore measures closest to Odin’s local time. Figure 3.15 suggests that the product is useful over the range 17–77 km with
a vertical resolution of around 3.5 km.

Figure 3.13: Average difference in percent between retrievals of O$_3$ from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 02. (Retrievals yielding concentrations ≤ 0.1 ppm have been filtered out.)
3.2. Frequency mode 02

Figure 3.14: Correlation between retrievals of O$_3$ using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments for frequency mode 02.

Figure 3.15: Measurement response and averaging kernels for O$_3$ retrievals for Odin/SMR v3 at different altitudes for frequency mode 02.
3.2.2.2 HNO$_3$

The retrievals for HNO$_3$ have been compared with data from the MIPAS and MLS instruments. Annual average differences to these instruments are shown in Figure 3.16. In Figure 3.17 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a considerable improvement with the updated version of the processing compared to both considered instruments with respect to the over-all correlation and coherency is much better, however a large altitude dependent difference seems to have been introduced, resulting in Odin/SMR over estimating the concentrations. The reason for this has not been identified despite considerable effort. At the current time we are without ideas as to how to proceed to improve the discrepancy. Figure 3.18 suggests that the product is useful over the range 20–60 km with a vertical resolution of around 6 km.

Figure 3.16: Average difference in percent between retrievals of HNO$_3$ from Odin/SMR v3 and collocated measurements from various instruments at different altitudes. (Retrievals yielding concentrations $\leq 0.5$ ppb have been filtered out.)

Figure 3.17: Comparison of individual retrievals for the MIPAS and MLS instruments with the new and old versions of the Odin/SMR processing chain.
3.2. Frequency mode 02

(a) correlation of collocated instruments with Odin/SMR v2.X
(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.17: Correlation between retrievals of HNO$_3$ using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments.

(a) median measurement response with 1σ and 2σ percentiles
(b) median averaging kernels

Figure 3.18: Measurement response and averaging kernels for HNO$_3$ retrievals for Odin/SMR v3 at different altitudes for frequency mode 02.
3.2.2.3 Temperature

The retrievals for temperature have been compared with data from the MLS instrument. Annual average differences to this instrument are shown in Figure 3.19. In Figure 3.20 individual retrievals from MLS for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a considerable improvement with the updated version of the processing, with much better over-all correlation and coherency, though a small systematic under estimation of the temperature remains, in particular at high altitudes. Figure 3.21 suggests that the product is useful over the range 20–60 km with a vertical resolution of around 7.5 km.

Figure 3.19: Average difference in K between retrievals of temperature from Odin/SMR v3 and collocated measurements from MLS at different altitudes.
3.2. Frequency mode 02

(a) correlation of collocated instruments with Odin/SMR v2.X  
Odin/SMR v3

(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.20: Correlation between retrievals of temperature using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments.

(a) median measurement response with 1σ and 2σ percentiles  
(b) median averaging kernels

Figure 3.21: Measurement response and averaging kernels for temperature retrievals for Odin/SMR v3 at different altitudes for frequency mode 02.
### 3.2.3 Discussion

The Pearson correlation between the Odin/SMR retrievals and the other instruments was calculated for the entire period for both versions of the processing chain. The results are summarised in Table 3.2, and show that the new algorithm is an improvement compared to all the instruments for all species used in this investigation. The improvement is considerable for both $O_3$ and HNO$_3$.

Table 3.2: Pearson correlation and fit parameters of the old and new Odin/SMR retrievals for frequency mode 02, compared with collocated data from other instruments for the period 2003–2019.

| Species | Instrument | SMR | corr. | slope | intercept | |⟨res.⟩|
|---------|------------|-----|-------|-------|-----------|-------|
| $O_3$   | MIPAS (KIT) v3 | 0.970 | 0.931 | -0.067 ppm | 0.724 ppm |
|         | v2.x       | 0.922 | 0.794 | -0.234 ppm | 1.429 ppm |
|         | MIPAS (ESA) v3 | 0.973 | 0.931 | -0.025 ppm | 0.716 ppm |
|         | v2.x       | 0.921 | 0.789 | -0.212 ppm | 1.439 ppm |
|         | MLS v3     | 0.974 | 0.968 | -0.011 ppm | 0.603 ppm |
|         | v2.x       | 0.905 | 0.824 | -0.195 ppm | 1.337 ppm |
|         | OSIRIS v3  | 0.976 | 0.952 | 0.027 ppm  | 0.523 ppm |
|         | v2.x       | 0.913 | 0.793 | -0.092 ppm | 1.378 ppm |
|         | SAGE III v3 | 0.926 | 1.071 | -0.102 ppm | 0.400 ppm |
|         | v2.x       | 0.736 | 0.782 | -0.124 ppm | 0.780 ppm |
| HNO$_3$ | MIPAS (KIT) v3 | 0.958 | 0.978 | 0.101 ppb  | 0.873 ppb |
|         | v2.x       | 0.814 | 0.996 | -0.096 ppb | 2.077 ppb |
|         | MIPAS (ESA) v3 | 0.958 | 1.003 | 0.158 ppb  | 0.869 ppb |
|         | v2.x       | 0.810 | 1.028 | -0.021 ppb | 2.133 ppb |
|         | MLS v3     | 0.739 | 0.643 | 0.717 ppb  | 2.366 ppb |
|         | v2.x       | 0.643 | 0.723 | -0.502 ppb | 2.963 ppb |
| Temp.   | MLS v3     | 0.959 | 0.925 | 15.274 K   | 6.012 K |
|         | v2.x       | 0.768 | 0.688 | 68.847 K   | 14.417 K |

### 3.2.4 Conclusions

Based on the discussion above, retrievals based on frequency mode 02 can be used with confidence for the species $O_3$ and for temperature. For HNO$_3$, some caution is warranted.
3.3 Frequency mode 08

3.3.1 Overview

Frequency mode 08 monitors two bands, 488.950–489.350 GHz and 488.350–488.750 GHz. Its main use is retrievals of water vapour in the lower stratosphere. O₃ is also retrieved. This mode showed considerable sideband leakage and served as the model for a new sideband correction that has been applied to all bands. This model includes a mathematical description of the Martin–Pulpett interferometer including a term to allow for thermal expansion of the optical bench (Eriksson and Urban (2006)). The thermal expansion coefficients have been updated using a more extensive dataset. Spectra from this observation mode are shown in Figure 3.22. For some unknown reason two different command macros were utilised for this mode resulting in slight different frequency coverage and different settings for the sideband filter. Examples of the effects and the differences can be found in Eriksson and Urban (2006).

![Figure 3.22: Annual median spectra for FM 08 for altitude interval 40–50 km at equatorial latitudes for the 97 µm sideband path during the arctic winter.](image)

3.3.2 Comparison of retrieved profiles

3.3.2.1 O₃

The retrievals for O₃ have been compared with data from the MIPAS, MLS, OSIRIS and SAGE III instruments. Annual average differences to these instruments are shown in Figure 3.23. In Figure 3.24 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a considerable improvement with the updated version of the processing compared to all considered instruments as can be seen in the correlation plots and the value of the slope parameters. The other parameters are affected by the difference in the biases between the old and new processing chains and must be treated.
with care. There are however some indications of a change in the last three years that requires further investigation. The over-all correlation and coherency is much better, though a systematic under estimation remains. Figure 3.25 suggests that the product is useful over the range 16–70 km with a vertical resolution of around 5 km.

(a) average difference to MIPAS  
(b) average difference to MLS

(c) average difference to OSIRIS  
(d) average difference to SAGE III

Figure 3.23: Average difference in percent between retrievals of O₃ from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 08.
3.3. Frequency mode 08

Figure 3.24: Correlation between retrievals of O₃ using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments for frequency mode 08.

(a) correlation of collocated instruments with Odin/SMR v2.X  
(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.25: Measurement response and averaging kernels for O₃ retrievals for Odin/SMR v3 at different altitudes for frequency mode 08.

(a) median measurement response with 1σ and 2σ percentiles  
(b) median averaging kernels
3.3.2.2 H$_2$O

The retrievals for H$_2$O have been compared with data from the MIPAS, MLS and SAGE III instruments. Annual average differences to these instruments are shown in Figure 3.26. In Figure 3.27 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. Though the results show a considerably improved coherency with the updated version of the processing compared to all considered instruments, the correlation is still poor, and the water content is still systematically underestimated, in particular for higher concentrations. Again there appears to have been a change in performance in the last few years. Figure 3.28 suggests that the product is useful over the range 19–78 km with a vertical resolution of around 4.5 km.

Figure 3.26: Average difference in percent between retrievals of H$_2$O from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 08.

(a) average difference to MIPAS

(b) average difference to MIPAS - ESA

(c) average difference to MLS

(d) average difference to SAGE III
3.3. Frequency mode 08

(a) correlation of collocated instruments with Odin/SMR v2.X

(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.27: Correlation between retrievals of H$_2$O using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments for frequency mode 08.

(a) median measurement response with 1σ and 2σ percentiles

(b) median averaging kernels

Figure 3.28: Measurement response and averaging kernels for H$_2$O retrievals for Odin/SMR v3 at different altitudes for frequency mode 08.
3.3.3 Discussion

The Pearson correlation between the Odin/SMR retrievals and the other instruments was calculated for the entire period for both versions of the processing chain. The results are summarised in Table 3.3, and show that the new algorithm is an improvement compared to all the instruments for all species used in this investigation. The improvement is considerable for both O₃ and H₂O. However there still seems to be a systematic underestimation of both products. It is unclear if this is due to spectroscopic problems or some sort of underestimation of the intensity. Spectroscopic data are taken from the HITRAN 12 database updated with the latest laboratory results; see Eriksson (2017).

Table 3.3: Pearson correlation and fit parameters of the old and new Odin/SMR retrievals for frequency mode 08, compared with collocated data from other instruments for the period 2003–2019.

| Species | Instrument     | SMR | corr. | slope     | intercept   | ⟨|res.|⟩ |
|---------|----------------|-----|-------|-----------|-------------|-----|
| O₃      | MIPAS (KIT)    | v3  | 0.851 | 1.004    | -0.207 ppm  | 1.582 ppm |
|         |                | v2.x| 0.911 | 0.872    | -0.059 ppm  | 1.179 ppm |
|         | MIPAS (ESA)    | v3  | 0.843 | 0.956    | -0.052 ppm  | 1.639 ppm |
|         |                | v2.x| 0.906 | 0.831    | 0.085 ppm   | 1.260 ppm |
|         | MLS            | v3  | 0.879 | 1.001    | -1.130 ppm  | 1.378 ppm |
|         |                | v2.x| 0.878 | 0.884    | 0.031 ppm   | 1.238 ppm |
|         | OSIRIS         | v3  | 0.853 | 0.983    | 0.132 ppm   | 1.408 ppm |
|         |                | v2.x| 0.909 | 0.913    | -0.091 ppm  | 1.089 ppm |
|         | SAGE III       | v3  | 0.837 | 1.078    | -0.144 ppm  | 0.566 ppm |
|         |                | v2.x| 0.737 | 0.975    | -0.324 ppm  | 0.650 ppm |
| H₂O     | MIPAS (KIT)    | v3  | 0.426 | 0.596    | 1.851 ppm   | 2.026 ppm |
|         |                | v2.x| 0.432 | 0.377    | 2.816 ppm   | 1.662 ppm |
|         | MIPAS (ESA)    | v3  | 0.428 | 0.437    | 2.892 ppm   | 2.250 ppm |
|         |                | v2.x| 0.455 | 0.320    | 3.146 ppm   | 1.854 ppm |
|         | MLS            | v3  | 0.490 | 0.702    | 0.870 ppm   | 2.094 ppm |
|         |                | v2.x| 0.411 | 0.486    | 2.022 ppm   | 1.907 ppm |
|         | SAGE III       | v3  | 0.608 | 0.496    | 2.106 ppm   | 1.502 ppm |
|         |                | v2.x| 0.285 | 0.161    | 4.460 ppm   | 1.567 ppm |

3.3.4 Conclusions

Based on the discussion above, retrievals based on frequency mode 08 can be used with confidence for the species O₃ while noting that the values may be underestimated by 5–10 %. The data should be used with some caution for H₂O but this requires more investigation.
3.4 Frequency mode 13

3.4.1 Overview

Frequency mode 13 monitors the band 556.598–557.398 GHz. Its main use is retrievals of H$_2$O and O$_3$. This is the strongest water vapour line available in the sub-mm wave spectrum and is used to reach the highest possible altitude particularly to study water vapour around the mesopause region. The line centre is saturated up to approximately 90 km and therefore temperatures can be derived throughout the mesosphere. This band and FM 19 remain problematic and have been subject to a dedicated study (Grieco et al. (2020b)) since the first version of this report to understand the effect of instrumental and other influences. Various instrumental uncertainties such as sideband filter values and non-linearity effects in the amplifiers and spectrometers have been investigated without any clear conclusion. However a value for the maximum suppression value different from that in the first version of the report was selected leading to some improvements in the agreement in both temperature and water vapour. Even the uncertainty in the pressure broadening coefficient has been revisited. Spectra from this observation mode are shown in Figure 3.29.

![Figure 3.29: Annual median spectra for FM 13 for altitude interval 65–75 km at equatorial latitudes during the arctic winter.](image)

3.4.2 Comparison of retrieved profiles

3.4.2.1 O$_3$

The retrievals for O$_3$ have been compared with data from the MIPAS, MLS and OSIRIS instruments. Annual average differences to these instruments are shown in Figure 3.30. In Figure 3.31 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a better overall coherency with the updated version of the processing compared to all considered instruments, but a systematic under estimation of the concentrations has been introduced. The reason for this is that a previously introduced (ver 2.1) empirical correction to the intensities has been remove since there was no physical basis for...
its inclusion. We suspect that some sort of non-linearity is causing the underestimation. Investigations of this band are continuing. Above about 65 km diurnal variability in the ozone concentration introduce problems when comparing with instruments on different platforms. We assume that this is the main reason for the differences at such altitudes. Figure 3.32 suggests that the product is useful over the range 44–80 km with a vertical resolution of around 6 km.

Figure 3.30: Average difference in percent between retrievals of $\text{O}_3$ from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 13.

(a) average difference to MIPAS  
(b) average difference to MLS  
(c) average difference to OSIRIS
3.4. Frequency mode 13

(a) correlation of collocated instruments with Odin/SMR v2.0
Odin/SMR v3

Figure 3.31: Correlation between retrievals of O₃ using Odin/SMR versions 2.0 and 2.1 with collocated measurements from various instruments for frequency mode 13.

(b) median measurement response with 1σ and 2σ percentiles

Figure 3.32: Measurement response and averaging kernels for O₃ retrievals for Odin/SMR v3 at different altitudes for frequency mode 13.
3.4.2.2 H$_2$O

The retrievals for H$_2$O have been compared with data from the MIPAS and MLS instruments. SAGE does not provide reliable water vapour profiles above 33km (Rydberg et al. (2016b)). Annual average differences to these instruments are shown in Figure 3.33. In Figure 3.34 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a slightly improved overall coherency with the updated version of the processing compared to both considered instruments, but a systematic under estimation of the concentrations has been introduced, and the correlation, in particular with MIPAS, remains poor. This would suggest that the MIPAS values are unreliable for this data product. After consultation with KIT we have compared with MIPAS middle atmosphere and upper atmosphere modes and found much better agreement (Grieco et al. (2020b)). Figure 3.35 suggests that the product is useful over the range 44–110 km with a vertical resolution of around 4.5 km.

(a) average difference to MIPAS
(b) average difference to MLS

Figure 3.33: Average difference in percent between retrievals of H$_2$O from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 13.
3.4. Frequency mode 13

(a) correlation of collocated instruments with Odin/SMR v2.X
(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.34: Correlation between retrievals of H$_2$O using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments for frequency mode 13.

(a) median measurement response with 1σ and 2σ percentiles
(b) median averaging kernels

Figure 3.35: Measurement response and averaging kernels for H$_2$O retrievals for Odin/SMR v3 at different altitudes for frequency mode 13.
3.4.2.3 Temperature

The retrievals for temperature have been compared with data from the MLS instrument. Annual average differences to this instrument are shown in Figure 3.36. In Figure 3.37 individual retrievals from MLS for 2003-2019 are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show little or no improvement with the updated version of the processing. Whereas with the previous version of the system, the temperature was systematically over estimated, a small under estimation of the temperature is now seen. This is a result of the removal of the arbitrary scaling factor. Figure 3.38 suggests that the product is useful over the range 44–95 km with a vertical resolution of around 5.5 km.

![Temperature comparison with MLS](image)

Figure 3.36: Average difference in K between retrievals of temperature from Odin/SMR v3 and collocated measurements from MLS at different altitudes.
3.4. Frequency mode 13

(a) correlation of collocated instruments with Odin/SMR v2.X

(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.37: Correlation between retrievals of temperature using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments.

(a) median measurement response with 1σ and 2σ percentiles

(b) median averaging kernels

Figure 3.38: Measurement response and averaging kernels for temperature retrievals for Odin/SMR v3 at different altitudes for frequency mode 13.


3.4.3 Discussion

The Pearson correlation between the Odin/SMR retrievals and the other instruments was calculated for the entire period for both versions of the processing chain. The results are summarised in Table 3.4, and show that the new algorithm shows little or no improvement compared to all the instruments for the species used in this investigation.

Table 3.4: Pearson correlation and fit parameters of the old and new Odin/SMR retrievals for frequency mode 13, compared with collocated data from other instruments for the period 2003–2019.

| Species | Instrument       | SMR | corr. | slope     | intercept | |⟨res.⟩| |
|---------|------------------|-----|-------|-----------|-----------|-----------------|-----------------|
| O3      | MIPAS (KIT) v3   | 0.643| 0.470 | 0.503 ppm | 0.801 ppm | 0.470 ppm       | 0.503 ppm       |
|         | v2.x             | 0.750| 0.886 | 0.128 ppm | 0.489 ppm | 0.886 ppm       | 0.128 ppm       |
|         | MIPAS (ESA) v3   | 0.750| 0.696 | 0.282 ppm | 0.560 ppm | 0.696 ppm       | 0.282 ppm       |
|         | v2.x             | 0.788| 0.905 | 0.201 ppm | 0.451 ppm | 0.905 ppm       | 0.201 ppm       |
|         | MLS v3           | 0.436| 0.262 | 0.658 ppm | 1.183 ppm | 0.262 ppm       | 0.658 ppm       |
|         | v2.x             | 0.829| 0.979 | -0.083 ppm| 0.500 ppm | 0.979 ppm       | -0.083 ppm      |
|         | OSIRIS v3        | 0.845| 0.845 | 0.176 ppm | 0.332 ppm | 0.845 ppm       | 0.176 ppm       |
|         | v2.x             | 0.765| 0.884 | 0.207 ppm | 0.372 ppm | 0.884 ppm       | 0.207 ppm       |
| O3      | MIPAS (KIT) v3   | 0.432| 0.706 | -0.376 ppm| 3.254 ppm | 0.706 ppm       | -0.376 ppm      |
|         | v2.x             | 0.445| 0.823 | -0.187 ppm| 3.086 ppm | 0.823 ppm       | -0.187 ppm      |
| H2O     | MIPAS (ESA) v3   | 0.824| 0.803 | 1.061 ppm | 1.821 ppm | 0.803 ppm       | 1.061 ppm       |
|         | v2.x             | 0.787| 0.842 | 1.508 ppm | 2.275 ppm | 0.842 ppm       | 1.508 ppm       |
|         | MLS v3           | 0.923| 0.935 | -0.362 ppm| 1.345 ppm | 0.935 ppm       | -0.362 ppm      |
|         | v2.x             | 0.897| 0.964 | -0.448 ppm| 1.534 ppm | 0.964 ppm       | -0.448 ppm      |
| Temp.   | MLS v3           | 0.968| 1.029 | -2.859 K  | 8.773 K   | 1.029 ppm       | -2.859 K        |
|         | v2.x             | 0.965| 1.043 | -3.836 K  | 11.260 K  | 1.043 ppm       | -3.836 K        |

3.4.4 Conclusions

Based on the discussion above, retrievals based on frequency mode 13 should be used with caution for both O3 and H2O. The temperature retrievals, on the other hand, appear reliable albeit with a cold bias of 3–5 K. For water vapour he comparisons with MLS seem to suggest a consistent -20 % bias.
3.5 Frequency mode 19

3.5.1 Overview

Frequency mode 19 monitors the band 556.598–557.398 GHz. Its main use is retrievals of H$_2$O and O$_3$. FM 19 is an alternative mode for measuring water vapour in the mesosphere. This band and FM 13 remain problematic and have been subject to a dedicated study (Grieco et al. (2020b)) since the first version of this report to understand the effect of instrumental and other influences. Various instrumental uncertainties such as sideband filter values and non-linearity effects in the amplifiers and spectrometers have been investigated without any clear conclusion. However, a value for the maximum suppression value different from that in the first version of the report was selected leading to some improvements in the agreement in both temperature and water vapour. Even the uncertainty in the pressure broadening coefficient has been revisited. Spectra from this observation mode are shown in Figure 3.39.

![Figure 3.39: Annual median spectra for FM 19 for altitude interval 42–48 km at equatorial latitudes during the arctic winter.](image)

3.5.2 Comparison of retrieved profiles

3.5.2.1 O$_3$

The retrievals for O$_3$ have been compared with data from the MIPAS, MLS, OSIRIS and SAGE III instruments. Annual average differences to these instruments are shown in Figure 3.40. In Figure 3.41 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a better over-all coherency with the updated version of the processing compared to SAGE III and OSIRIS, but worse correlation with MIPAS and MLS, and a systematic under estimation of the concentrations remains compared to all considered instruments. Above about 65 km diurnal variability in the ozone concentration introduces problems when comparing with instruments on different platforms. We assume that this is the main reason for the differences at such altitudes. Figure 3.42 suggests that the product is useful over the range 44–80 km with a vertical resolution of around 6 km.
CHAPTER 3. COMPARISONS WITH OTHER INSTRUMENTS

Figure 3.40: Average difference in percent between retrievals of O$_3$ from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 19.

(a) average difference to MIPAS
(b) average difference to MLS
(c) average difference to OSIRIS
(d) average difference to SAGE III
3.5. Frequency mode 19

(a) Correlation of collocated instruments with Odin/SMR v2.0/2.1
(b) Correlation of collocated instruments with Odin/SMR v3

Figure 3.41: Correlation between retrievals of $O_3$ using Odin/SMR versions 2.0/2.1 and 3 and collocated measurements from various instruments for frequency mode 19.

(a) Median measurement response with $1\sigma$ and $2\sigma$ percentiles
(b) Median averaging kernels

Figure 3.42: Measurement response and averaging kernels for $O_3$ retrievals for Odin/SMR v3 at different altitudes for frequency mode 19.
3.5.2.2 $\text{H}_2\text{O}$

The retrievals for $\text{H}_2\text{O}$ have been compared with data from the MIPAS and MLS instruments. Annual average differences to these instruments are shown in Figure 3.43. In Figure 3.44 individual retrievals for the instruments for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a slightly improved over-all coherency with the updated version of the processing compared to both considered instruments, but a systematic under estimation of the concentrations has been introduced. Comparisons with MLS suggest a -20% bias as with FM13 but with a increasing bias with altitude. The MIPAS product used seems to be unreliable at these altitudes.

The SAGE III instrument also measures $\text{H}_2\text{O}$, but the there are too few collocated measurements with frequency mode 19 for a relevant analysis. Figure 3.45 suggests that the product is useful over the range 44–110 km with a vertical resolution of around 4 km.

![Figure 3.43: Average difference in percent between retrievals of $\text{H}_2\text{O}$ from Odin/SMR v3 and collocated measurements from various instruments at different altitudes for frequency mode 19.](image)

(a) average difference to MIPAS  
(b) average difference to MLS
3.5. Frequency mode 19

(a) correlation of collocated instruments with Odin/SMR v2.X
(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.44: Correlation between retrievals of H₂O using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments for frequency mode 19.

(a) median measurement response with 1σ and 2σ percentiles
(b) median averaging kernels

Figure 3.45: Measurement response and averaging kernels for H₂O retrievals for Odin/SMR v3 at different altitudes for frequency mode 19.
CHAPTER 3. COMPARISONS WITH OTHER INSTRUMENTS

3.5.2.3 Temperature

The retrievals for temperature have been compared with data from the MLS instrument. Annual average differences to this instruments are shown in Figure 3.46. In Figure 3.37 individual retrievals from MLS for the entire period are plotted against the retrievals from the new and old versions of the Odin/SMR processing chain. The results show a little or no improvement with the updated version of the processing. Whereas with the previous version of the system, the temperature was under estimated for lower temperatures and over estimated for higher, and a small systematic under estimation of the temperature is still seen. Figure 3.48 suggests that the product is useful over the range 44–95 km with a vertical resolution of around 5 km.

![Frequency mode 19: Temperature comparison with MLS](image)

Figure 3.46: Average difference in K between retrievals of temperature from Odin/SMR v3 and collocated measurements from MLS at different altitudes.
3.5. Frequency mode 19

(a) correlation of collocated instruments with Odin/SMR v2.X
(b) correlation of collocated instruments with Odin/SMR v3

Figure 3.47: Correlation between retrievals of temperature using Odin/SMR versions 2.X and 3 and collocated measurements from various instruments.

(a) median measurement response with 1σ and 2σ percentiles
(b) median averaging kernels

Figure 3.48: Measurement response and averaging kernels for temperature retrievals for Odin/SMR v3 at different altitudes for frequency mode 19.
3.5.3 Discussion

The Pearson correlation between the Odin/SMR retrievals and the other instruments was calculated for the entire period for both versions of the processing chain. The results are summarised in Table 3.5, and show that the new algorithm is a general improvement compared to all the instruments for all species used in this investigation. Specifically the improvement is largest for water vapour and temperature while the secondary ozone product shows some variability. The agreement is best with OSIRIS over a limited height region. This is to be expected since they are on the same platform. For MLS and MIPAS diurnal variability biases the results. The improvement is considerable for both \( \text{O}_3 \) and \( \text{H}_2\text{O} \).

Table 3.5: Pearson correlation and fit parameters of the old and new Odin/SMR retrievals for frequency mode 19, compared with collocated data from other instruments for the period 2003–2019.

| Species | Instrument       | SMR | corr. | slope   | intercept | \(|\langle \text{res.} \rangle|\) |
|---------|------------------|-----|-------|---------|-----------|----------------|
| \( \text{O}_3 \) | MIPAS (KIT) v3 | 0.678 | 0.492 | 0.505 ppm | 0.780 ppm |
|         | v2.x            | 0.800 | 0.810 | -0.099 ppm | 0.591 ppm |
|         | MIPAS (ESA) v3  | 0.787 | 0.739 | 0.275 ppm | 0.523 ppm |
|         | v2.x            | 0.845 | 0.861 | -0.070 ppm | 0.479 ppm |
|         | MLS v3          | 0.476 | 0.292 | 0.655 ppm | 1.150 ppm |
|         | v2.x            | 0.810 | 0.767 | 0.089 ppm | 0.533 ppm |
|         | OSIRIS v3       | 0.883 | 0.894 | 0.161 ppm | 0.257 ppm |
|         | v2.x            | 0.847 | 0.878 | -0.042 ppm | 0.422 ppm |
|         | SAGE III v3     | 0.895 | 0.918 | 0.092 ppm | 0.363 ppm |
|         | v2.x            | 0.885 | 0.819 | 0.068 ppm | 0.395 ppm |
| \( \text{H}_2\text{O} \) | MIPAS (KIT) v3 | 0.444 | 0.720 | -1.153 ppm | 3.699 ppm |
|         | v2.x            | 0.411 | 0.635 | -0.556 ppm | 3.590 ppm |
|         | MIPAS (ESA) v3  | 0.867 | 0.937 | 0.525 ppm | 1.536 ppm |
|         | v2.x            | 0.819 | 0.839 | 0.785 ppm | 1.762 ppm |
|         | MLS v3          | 0.926 | 0.911 | -0.569 ppm | 1.442 ppm |
|         | v2.x            | 0.920 | 0.884 | -0.416 ppm | 1.451 ppm |
|         | Temp. MLS v3    | 0.976 | 1.085 | -18.131 K | 7.551 K  |
|         | v2.x            | 0.965 | 1.084 | -21.231 K | 8.798 K  |

3.5.4 Conclusions

Based on the discussion above, retrievals based on frequency mode 19 should be used with caution for both \( \text{O}_3 \) and \( \text{H}_2\text{O} \), but can be used with confidence for temperature retrievals.
3.6 Frequency mode 22 and 24

3.6.1 Overview

Frequency modes 22 and 24 monitor the band around the CO line at 576.268 GHz. Its main use is retrievals of CO and when possible O₃. The receiver used for these modes suffered a failure shortly after launch resulting in an inability to stabilise the frequency. However it recovered between October 2003 until October 2004 for reasons that can only be guessed at. In order to recover the CO product a special algorithm had to be developed to first detect if the CO line was at all present in the spectra of a given scan. This involved distinguishing the CO and O₃ lines and then if the CO line was present re-tuning the frequency scale. It was also necessary to account for rapid changes in the frequency during a vertical scan and within the integration time. The details are given in Grieco et al. (2020a).

Spectra from this observation mode are shown in Figure 3.49.

![Figure 3.49: Spectra for the CO mode showing one example where the line is present and one without.](image)

3.6.2 Comparison of retrieved profiles

3.6.2.1 CO

The retrievals for CO have been compared with data from the MIPAS and MLS instruments. The comparison does not follow the same methodology as for the other modes, rather a special approach has had to be employed. The MIPAS instrument was operated in several modes and the most useful ones covering the extended altitude range of the Odin measurements are the Middle Atmosphere and the Upper atmosphere modes. A detailed analysis in presented in Grieco et al. (2020a) with only the conclusions presented here.

3.6.3 Discussion

Comparisons with MIPAS, ACE-FTS and OSO show a positive bias of SMR of up to +20 % at low altitudes (50-60 km) and a negative bias of up to -20 % at high altitudes (80-115 km). Something different is found with regards to MLS – i.e. negative difference at all altitudes, ranging from -40 % to -10 % – which is in accordance with the stated MLS bias (Errera et al. (2019)).
3.6.4 Conclusions

Based on the discussion above, the (CO) data set has been recovered for a large fraction of the mission and can be used in the altitude range 50–115 km.
Chapter 4 | Conclusions

4.1 General comments

Table 4.1 shows an overview of the characteristics of the main data products from the updated Odin/SMR processing chain for the frequency modes investigated in Chapter 3. The vertical coverage has been defined as the altitude interval where the measurement response for the retrievals is > 0.8. The vertical resolution and precision are calculated from the ±2σ percentiles of the full widths at half maximum of the averaging kernels and the comparison with the other datasets respectively.

The results presented in Table 4.1 should be compared with the results for the old processing chain, presented in Tables 2.1 and 2.2.

Table 4.1: Characteristics of Odin/SMR Level2 main Version 3.0 data products.

<table>
<thead>
<tr>
<th>Product</th>
<th>Frequency [GHz]</th>
<th>Vertical coverage</th>
<th>Vertical resolution</th>
<th>Precision</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₃</td>
<td>501.5 (FM 01)</td>
<td>19–53 km</td>
<td>5.3–5.5 km</td>
<td>0.70–0.85 ppmv</td>
</tr>
<tr>
<td>ClO</td>
<td>501.3 (FM 01)</td>
<td>18–58 km</td>
<td>5.3–5.6 km</td>
<td>0.07–0.08 ppbv</td>
</tr>
<tr>
<td>N₂O</td>
<td>502.3 (FM 01)</td>
<td>15–62 km</td>
<td>4.4–5.6 km</td>
<td>5.00–6.10 ppbv</td>
</tr>
<tr>
<td>O₃</td>
<td>544.9 (FM 02)</td>
<td>17–77 km</td>
<td>2.9–4.9 km</td>
<td>0.18–0.26 ppmv</td>
</tr>
<tr>
<td>HNO₃</td>
<td>544.4 (FM 02)</td>
<td>20–61 km</td>
<td>5.0–7.2 km</td>
<td>0.24–0.28 ppbv</td>
</tr>
<tr>
<td>Temperature</td>
<td>544.9 (FM 02)</td>
<td>21–64 km</td>
<td>7.5–7.9 km</td>
<td>1.13–2.18 K</td>
</tr>
<tr>
<td>O₃</td>
<td>489.2 (FM 08)</td>
<td>16–71 km</td>
<td>4.1–6.0 km</td>
<td>0.29–0.39 ppmv</td>
</tr>
<tr>
<td>H₂O</td>
<td>489.5 (FM 08)</td>
<td>19–78 km</td>
<td>4.0–4.7 km</td>
<td>0.32–0.55 ppmv</td>
</tr>
<tr>
<td>O₃</td>
<td>556.9 (FM 13)</td>
<td>44–80 km</td>
<td>6.1–6.7 km</td>
<td>0.19–0.24 ppmv</td>
</tr>
<tr>
<td>H₂O</td>
<td>556.7 (FM 13)</td>
<td>44–110 km</td>
<td>4.3–4.8 km</td>
<td>0.06–0.33 ppbv</td>
</tr>
<tr>
<td>Temperature</td>
<td>556.9 (FM 13)</td>
<td>44–95 km</td>
<td>5.3–5.6 km</td>
<td>1.85–2.73 K</td>
</tr>
<tr>
<td>O₃</td>
<td>556.9 (FM 19)</td>
<td>43–81 km</td>
<td>5.8–6.6 km</td>
<td>0.19–0.24 ppmv</td>
</tr>
<tr>
<td>H₂O</td>
<td>556.7 (FM 19)</td>
<td>43–109 km</td>
<td>4.1–4.4 km</td>
<td>0.13–0.26 ppbv</td>
</tr>
<tr>
<td>Temperature</td>
<td>556.9 (FM 19)</td>
<td>43–93 km</td>
<td>5.2–5.5 km</td>
<td>1.72–2.65 K</td>
</tr>
</tbody>
</table>

4.2 Recommendations

4.2.1 Ozone

The best ozone product for general use is that from FM 02. The new product is in much better agreement with other instruments and does not seem to show any temporal drifts although a thorough analysis of drifts has not yet been attempted. The other ozone
products show some biases but could be used in conjunction with simultaneously measured products if account is taken of this.

4.2.2 Chlorine Monoxide

The ClO product should be reliable until 2009 and after January 2018. Unfortunately a gradually deteriorating instrument malfunction has disturbed the intervening period. It may be possible to correct for this effect by simulating the effects of the deterioration on the spectra but this has not been attempted in version 3.0 of the data.

4.2.3 Water vapour

Water vapour continues to be a difficult product. the FM 08 product has improved and is stable over time although shows a 15 % low bias compared to MLS. For the upper stratosphere and mesosphere FM 13 appears to be the best product, but also shows a small bias of around 15 % and some variability above 70 km that needs further investigation. A much more detailed analysis of the new mesospheric water vapour product is available in Grieco et al. (2020b).

4.2.4 Temperature

FM 02 provides stratospheric temperatures with a possible increasing bias with altitude. There does not appear to be any systematic drift with time. For higher altitudes FM 13 can be used with knowledge of a possible cold bias of 3–5 K

4.3 Remaining work

While a substantial effort has been made in this project there are always things that show up and are worthy of attention in a future reprocessing. This is an attempt to summarise these.

1. The unfortunate degradation in the FM 01 performance over a long period is well worth an attempt to correct the data and retrieve the ClO measurements between 2009 and 2018.

2. Although great efforts have been made to understand the altitude dependent bias in the nitric acid profiles in FM 02, it would be useful to resolve the problem in the future.

3. Remaining biases in many of the ozone products are often of the same magnitude and direction indicating an underlying cause that has yet to be identified.

4. The current validation study has not permitted the investigation of long term drifts. Indications from the Level1 data indicate that some such drifts may exist and the effect of these on the Level2 products and any mitigation strategies should be investigated.
Bibliography


Appendix A | API description

This section describes the API calls used to get data from the DDS. The data is accessed through a hierarchical REST API where deeper URIs return more specific data. All call URIs have a common root `rest_api/v5`, which has been omitted below for clarity. All GET calls return JSON objects unless otherwise noted. Key/value pairs are listed as name of the key along with the type of the corresponding value within parentheses, followed by a brief description of the contents. See the sections on the different data sources for specifications on the structure of their respective JSON objects. This description is only for the Odin/SMR version 3 Level2 data. For details on how to access the collocated measurements from the VDS, see Rydberg et al. (2016b), for more details on the Level2 data format see Rydberg et al. (2016a); Pérot et al. (2017), and for a more general description of the Odin/SMR API, see http://odin.rss.chalmers.se/apidocs/index.html.

A.1 API calls

A.1.1 level2/DDS/

Method: GET

Get project information.

A.1.1.0.1 Parameters: None.

A.1.1.0.2 Data structure: Returns JSON object with the following structure:

```json
{
    'Data': [
    {
        'FreqMode': <int>,
        'URLS': {
            'URL-comment': <string: URL for comments for scans>,
            'URL-failed': <string: URL for failed scans>,
            'URL-scans': <string: URL for scans>
        }
    },
    ...]
    'Count': <int: number of FreqModes in project>,
    'Type': 'level2_project_freqmode'
}
```

A.1.2 level2/DDS/area

Method: GET

Get data in provided area.
APPENDIX A. API DESCRIPTION

A.1.2.0.1 Parameters:

- `product (array of strings)`: Return data only for these products
- `min_lat (float)`: Minimum latitude (-90 to 90)
- `max_lat (float)`: Maximum latitude (-90 to 90)
- `min_lon (float)`: Minimum longitude (0 to 360)
- `max_lon (float)`: Maximum longitude (0 to 360)
- `min_pressure (float)`: Minimum pressure (Pa)
- `max_pressure (float)`: Maximum pressure (Pa)
- `min_altitude (float)`: Minimum altitude (m)
- `max_altitude (float)`: Maximum altitude (m)
- `start_time (date)`: Return data after this date (inclusive)
- `end_time (date)`: Return data before this date (exclusive)

Provide latitude and/or longitude limits to get data for a certain area of the earth. If no latitude or longitude limits are provided, data for the whole earth is returned. Choose between min/max altitude and min/max pressure.

A.1.2.0.2 Data structure: Returns JSON object with the following structure:

```json
{
    'Data': <array of Level2 Data Structures as described below>,
    'Count': <int: number of matching data>,
    'Type': 'L2'
}
```

A.1.3 level2/DDS/locations

Method: `GET`

Get data close to provided location.

A.1.3.0.1 Parameters:

- `product (array of strings)`: Return data only for these products
- `location (array of strings; required)`: Return data close to these locations (‘lat,lon’).
- `radius (float; required)`: Return data within this radius from the provided locations (km).
- `min_pressure (float)`: Minimum pressure (Pa)
- `max_pressure (float)`: Maximum pressure (Pa)
- `min_altitude (float)`: Minimum altitude (m)
- `max_altitude (float)`: Maximum altitude (m)
• start_time *(date)*: Return data after this date (inclusive)
• end_time *(date)*: Return data before this date (exclusive)

Provide one or more locations and a radius to get data within the resulting circles on the earth surface. Choose between min/max altitude and min/max pressure.

**A.1.3.0.2 Data structure:** Returns JSON object with the same structure as endpoint A.1.2.

**A.1.4 level2/DDS/products/**
Method: *GET*
Get available products.

**A.1.4.0.1 Parameters:** None.

**A.1.4.0.2 Data structure:** Returns JSON object with the following structure:

```json
{
  'Data': ['array of strings: product names'],
  'Count': 'int: number of available products',
  'Type': 'level2_product_name'
}
```

**A.1.5 level2/DDS/<string:date>/**
Method: *GET*
Get data for the provided date.

**A.1.5.0.1 Parameters:**
• product *(array of strings)*: Return data only for these products
• min_pressure *(float)*: Minimum pressure (Pa)
• max_pressure *(float)*: Maximum pressure (Pa)
• min_altitude *(float)*: Minimum altitude (m)
• max_altitude *(float)*: Maximum altitude (m)
• start_time *(date)*: Return data after this date (inclusive)
• end_time *(date)*: Return data before this date (exclusive)

Choose between min/max altitude and min/max pressure.

**A.1.5.0.2 Data structure:** Returns JSON object with the same structure as endpoint A.1.2.

**A.1.6 level2/DDS/<int:frequencymode>/comments/**
Method: *GET*
Get list of comments for a frequency mode.
A.1.6.0.1 Parameters:
- offset (int): Skip scans before returning
- limit (int; default: 1000): Number of scans to return

A.1.6.0.2 Data structure: Returns JSON object with the following structure:

```json
{  
  'Data': [  
    {  
      'Comment': 'string: comment from processing',  
      'URLS': {  
        'URL_failed': 'string: URL for failed scans with comment',  
        'URL_scans': 'string: URL for successful scans with comment'  
      }  
    },  
    ...  
  ],  
  'Count': 'int: number of unique comments',  
  'Type': 'level2_scan_comment'  
}
```

A.1.7 level2/DDS/<int:frequencymode>/failed/

Method: GET
Get list of matching scans that failed the level2 processing.

A.1.7.0.1 Parameters:
- start_time (date): Return data after this date (inclusive)
- end_time (date): Return data before this date (exclusive)
- comment (string): Return scans with this comment
- offset (int): Skip scans before returning
- limit (int; default: 1000): Number of scans to return

A.1.7.0.2 Data structure: Returns JSON object with the following structure:

```json
{  
  'Data': [  
    {  
      'Date': 'string: date',  
      'Error': 'string: error message',  
      'ScanID': 'int: scan number',  
      'URLS': {  
        'URL_ancillary': 'string: URL for Level2 ancillary data',  
        'URL_level2': 'string: URL for Level2 data',  
        'URL_log': 'string: URL for Level1 log data',  
        'URL_spectra': 'string: URL for Level1 spectra'  
      }  
    },  
    ...  
  ],  
  'Count': 'int: number of matching scans',  
  'Type': 'level2_failed_scan_info'  
}
```
A.1.8  level2/DDS/<int:frequencymode>/products/

Method:  *GET*

Get available products for a given project and frequency mode.

**A.1.8.0.1 Parameters:** None.

**A.1.8.0.2 Data structure:** Returns JSON object with the same structure as endpoint A.1.4.

A.1.9  level2/DDS/<int:frequencymode>/scans/

Method:  *GET*

Get list of matching scans.

**A.1.9.0.1 Parameters:**
- *start_time (date):* Return data after this date (inclusive)
- *end_time (date):* Return data before this date (exclusive)
- *comment (string):* Return scans with this comment
- *offset (int):* Skip scans before returning
- *limit (int; default: 1000):* Number of scans to return

**A.1.9.0.2 Data structure:** Returns JSON object with the following structure:

```
{
    "Data": [
        {
            "Date": <string: date>,
            "ScanID": <int: scan number>,
            "URLS": {
                "URL_ancillary": <string: URL for Level2 ancillary data>,
                "URL_level2": <string: URL for Level2 data>,
                "URL-log": <string: URL for Level1 log data>,
                "URL-spectra": <string: URL for Level1 spectra>
            }
        },
        ...
    ],
    "Count": <int: number of matching scans>,
    "Type": "level2_scan_info"
}
```

A.1.10  level2/DDS/<int:frequencymode>/<int:scannumber>/

Method:  *GET*

Get level2 data, info, comments, and ancillary data for one scan and frequency mode.

**A.1.10.0.1 Parameters:** None.
APPENDIX A. API DESCRIPTION

A.1.10.0.2 Data structure: Returns JSON object with the following structure:

```json
{ 'Data': { 'L2': '<Level2 Data Structure as described below>', 'L2anc': '<Level2 Ancillary Data Structure as described below>', 'L2c': '<Level2 Comments Data Structure as described below>', 'L2i': '<Level2 Info Data Structure as described below>', 'Count': null, 'Type': 'mixed' }
}
```

A.1.11 level2/DDS/<frequencymode>/<scannumber>/L2/
Method: GET
Get level2 data for one scan and frequency mode.

A.1.11.0.1 Parameters :
- product (array of strings): Return data only for these products

A.1.11.0.2 Data structure: Returns JSON object with the following structure:

```json
```

A.1.12 level2/DDS/<int:frequencymode>/<int:scannumber>/L2anc/
Method: GET
Get ancillary data for one scan and frequency mode.

A.1.12.0.1 Parameters: None.
A.1.12.0.2 Data structure: Returns JSON object with the following structure:

```
{ 'Data': [ 
  
  'FreqMode': <int: frequency mode>,
  'InvMode': <string: inversion mode used in retrieval>,
  'LST': <float: local solar time>,
  'Lat1D': <float: approximate latitude of retrieval>,
  'Latitude': <array of floats: latitudes for retrieval at altitudes>,
  'Lon1D': <float: approximate latitude of retrieval>,
  'Longitude': <array of floats: longitude for retrieval at altitudes>,
  'MJD': <float: Modified Julian Date for retrieval>,
  'Orbit': <int: orbit number>,
  'Pressure': <array of floats: pressure at altitudes [Pa]>,
  'SZA': <array of floats: solar zenith angle for retrieval at altitudes>,
  'SZA1D': <float: approximate solar zenith angle for retrieval>,
  'ScanID': <int: scan number>,
  'Theta': <array of floats: potential temperature>
},
  
  'Count': 1,
  'Type': 'string'
]
```

A.1.13 level2/DDS/<int:frequencymode>/<int:scannumber>/L2i/

Method: GET

Get level2 auxiliary data for one scan and frequency mode.

A.1.13.0.1 Parameters: None.

A.1.13.0.2 Data structure: Returns JSON object with the following structure:

```
{ 'Data': { 
  'BlineOffset': <array of arrays of floats: baseline offsets for spectra>,
  'ChannelsID': <array of floats: channel identifier>,
  'FitSpectrum': <array of arrays of floats: fitted spectra [K]>,
  'FreqMode': <int: frequency mode>,
  'FreqOffset': <float: retrieved LO frequency offset [Hz]>,
  'InvMode': <string: inversion mode used in retrieval>,
  'LOFreq': <array of floats: LO frequency for each spectrum in scan [Hz]>,
  'MinLmFactor': <float: minimum Levenberg–Marquard factor of OEM>,
  'PointOffset': <float: retrieved pointing offset [degree]>,
  'Residual': <float: residual of retrieved and measured spectra>,
  'SBpath': <float: sideband path used for retrieving spectra [m]>,
  'STW': <array of floats: satellite time words for spectra>,
  'ScanID': <int: scan number>,
  'Tsat': <float: satellite onboard temperature [K]>,
  'URLS': { 
    'URL-ancillary': <string: URL for Level2 ancillary data>,
    'URL-level2': <string: URL for Level2 data>,
    'URL-log': <string: URL for Level1 log data>,
    'URL-spectra': <string: URL for Level1 spectra>
  }
},
  'Count': null,
  'Type': 'L2i'
}
```
A.1.14  level2/DDS/<int:frequencymode>/<int:scannumber>/L2c/

Method: GET

Get level2 comments for one scan and frequency mode.

A.1.14.0.1  Parameters: None.

A.1.14.0.2  Data structure: Returns JSON object with the following structure:

```json
{
    'Data': <array of strings: comments>,
    'Count': <int: number of comments for scan>,
    'Type': L2c
}
```

A.2 Example usage

This is a brief example of how to use the Odin/SMR API to access the DDS in Python. The basic procedure for navigating the call hierarchy is the same in all major programming languages and browsers.

```python
# Setup the namespace:
import requests

# Start by making a request to the root URI of the DDS API:
r0 = requests.get('http://odin.rss.chalmers.se/rest_api/v5/level2/DDS/')

# The request contains the returned JSON object, which in Python is a dictionary, which can be printed or inspected to find out its keys and contents. Let's assume that we have done that, or that we have read the API documentation, so that we know that 'FreqMode' is a key.
# Use this to single out the frequency mode of interest, in this case 2:
FM2 = [x for x in r0.json()['Data'] if x['FreqMode'] == 2][0]

# Make a new request using the URI provided in the JSON object:
r1 = requests.get(FM2['URLs']['URL−scans'])

# Filter out data from 2012−03−11 and fetch the level2 data for the first scan in the list:
day = [x for x in r1.json()['Data'] if x['Date'] == '2012−03−11']
r2 = requests.get(day[0]['URLs']['URL−level2'])

# The Level2 data available to us, along with the ancillary and auxiliary data:
L2 = r2.json()['Data']['L2']
L2anc = r2.json()['Data']['L2anc']
L2aux = r2.json()['Data']['L2i']

# Now we have the data at hand and can proceed with crunching it!
```
# Appendix B | Observation modes

Table B.1: Odin/SMR operational modes in aeronomy for AC1 and AC2 and the sub-mm frontends (FM = frequency mode)

<table>
<thead>
<tr>
<th>Backend</th>
<th>Frontend</th>
<th>LO freq [GHz]</th>
<th>Source mode</th>
<th>FM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC1</td>
<td>495 A2</td>
<td>492.750</td>
<td>Transport</td>
<td>23</td>
</tr>
<tr>
<td></td>
<td></td>
<td>499.698</td>
<td>Transport</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td>549 A1</td>
<td>548.502</td>
<td>Stratospheric</td>
<td>02</td>
</tr>
<tr>
<td></td>
<td></td>
<td>553.050</td>
<td>Water isotope</td>
<td>19</td>
</tr>
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<td>547.752</td>
<td>Water isotope</td>
<td>21</td>
</tr>
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<td></td>
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<td>553.302</td>
<td>Transport</td>
<td>23</td>
</tr>
<tr>
<td>555 B2</td>
<td>553.298</td>
<td></td>
<td>Summer mesosphere</td>
<td>13</td>
</tr>
<tr>
<td>572 B1</td>
<td>572.762</td>
<td></td>
<td>Transport</td>
<td>24</td>
</tr>
<tr>
<td>AC2</td>
<td>495 A2</td>
<td>497.880</td>
<td>Stratospheric</td>
<td>01</td>
</tr>
<tr>
<td></td>
<td></td>
<td>492.750</td>
<td>Water isotope</td>
<td>08</td>
</tr>
<tr>
<td></td>
<td></td>
<td>494.750</td>
<td>Water isotope</td>
<td>17</td>
</tr>
<tr>
<td></td>
<td></td>
<td>499.698</td>
<td>Transport</td>
<td>25</td>
</tr>
<tr>
<td>572 B1</td>
<td>572.762</td>
<td></td>
<td>Summer mesosphere</td>
<td>14</td>
</tr>
<tr>
<td></td>
<td>572.964</td>
<td></td>
<td>Transport</td>
<td>22</td>
</tr>
</tbody>
</table>

Table B.2: Odin/SMR frontend and backend frequency specification for modes that are measured during part of the summer (when only backend AC2 is used, which is the case for 2013 and onwards). These modes are normally measured by backend AC1 (e.g. FM 102 and FM 2, FM 119 and FM 19, FM 121 and FM 21, and FM 113 and 13, are all identical except the Backend used).

<table>
<thead>
<tr>
<th>Backend</th>
<th>Frontend</th>
<th>LO freq [GHz]</th>
<th>Source mode</th>
<th>FM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC2</td>
<td>549 A1</td>
<td>548.502</td>
<td>Stratospheric</td>
<td>102</td>
</tr>
<tr>
<td></td>
<td></td>
<td>553.050</td>
<td>Water isotope</td>
<td>119</td>
</tr>
<tr>
<td></td>
<td></td>
<td>547.752</td>
<td>Water isotope</td>
<td>121</td>
</tr>
<tr>
<td>555 B2</td>
<td>553.298</td>
<td></td>
<td>Summer mesosphere</td>
<td>113</td>
</tr>
</tbody>
</table>
Table B.3: Odin/SMR frontend and backend frequency specification

<table>
<thead>
<tr>
<th>FM</th>
<th>SMR mode</th>
<th>LO Freq. [GHz]</th>
<th>Freq. Range [GHz]</th>
<th>Species</th>
<th>Name / ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>s1a or sc1a</td>
<td>497.880</td>
<td>501.180–501.580</td>
<td>ClO, O3, N2O</td>
<td>SM-AC2a / 01</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>501.980–502.380</td>
<td></td>
<td>SM-AC2b / 02</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>SM-AC2ab / 29</td>
</tr>
<tr>
<td>02</td>
<td>s1a</td>
<td>548.502</td>
<td>544.102–544.902</td>
<td>HNO3, O3</td>
<td>SM-AC1e / 03</td>
</tr>
<tr>
<td>08</td>
<td>w3a or w5a</td>
<td>492.750</td>
<td>488.950–489.350</td>
<td>H18O, O3, H16O</td>
<td>IM-AC2a / 13</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>488.350–488.750</td>
<td></td>
<td>IM-AC2b / 14</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>IM-AC2ab / 30</td>
</tr>
<tr>
<td>17</td>
<td>w4a or w5b</td>
<td>494.250</td>
<td>489.950–490.750</td>
<td>HDO, 18O3</td>
<td>IM-AC2c / 21</td>
</tr>
<tr>
<td>19</td>
<td>w3a or w4a</td>
<td>553.050</td>
<td>556.550–557.350</td>
<td>H2O, O3</td>
<td>IM-AC1c / 22</td>
</tr>
<tr>
<td>21</td>
<td>w5a or w5b</td>
<td>547.752</td>
<td>551.152–551.552</td>
<td>NO, O3, H17O</td>
<td>IM-AC1de / 31</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>551.752–552.152</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>sm1a</td>
<td>553.298</td>
<td>556.598–557.398</td>
<td>H16O2, O3</td>
<td>HM-AC1c / 19</td>
</tr>
<tr>
<td>14</td>
<td>sm1a</td>
<td>572.762</td>
<td>576.062–576.862</td>
<td>CO, O3</td>
<td>HM-AC2c / 20</td>
</tr>
<tr>
<td>22</td>
<td>co1a</td>
<td>572.964</td>
<td>576.254–576.654</td>
<td>CO, O3, HO2, 18O3</td>
<td>HM-AC2ab / 32</td>
</tr>
<tr>
<td></td>
<td></td>
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<td>577.069–577.469</td>
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<td></td>
</tr>
<tr>
<td>23</td>
<td>co1a</td>
<td>492.750</td>
<td>488.350–488.750</td>
<td>H16O2, O3</td>
<td>HM-AC1d / 33</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>553.302–557.102</td>
<td></td>
<td>HM-AC1c / 34</td>
</tr>
<tr>
<td>24</td>
<td>sc1a</td>
<td>572.762</td>
<td>576.062–576.862</td>
<td>CO, O3</td>
<td>HM-AC1e / 35</td>
</tr>
<tr>
<td>25</td>
<td>ut1a</td>
<td>499.698</td>
<td>502.998–504.198</td>
<td>H16O2, O3</td>
<td>TM-ACs1 / 36</td>
</tr>
</tbody>
</table>

Table B.4: Order of sub-bands from lowest frequency range to highest for some of the most common frequency modes. Sub-bands that are in bad condition have been emphasised, broken bands are in bold.

<table>
<thead>
<tr>
<th>FM</th>
<th>Freq. Range [GHz]</th>
<th>Sub-band order</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>501.180–501.585</td>
<td>2 1 5 6</td>
</tr>
<tr>
<td></td>
<td>501.980–502.380</td>
<td>4 3 7 8</td>
</tr>
<tr>
<td>02</td>
<td>544.102–544.902</td>
<td>1 2 6 5 8 7 3 4</td>
</tr>
<tr>
<td>08</td>
<td>488.950–489.350</td>
<td>8 7 3 4 6 5 1 2</td>
</tr>
<tr>
<td>17</td>
<td>489.950–490.750</td>
<td>8 7 3 4 6 5 1 2</td>
</tr>
<tr>
<td>19</td>
<td>556.550–557.350</td>
<td>4 3 7 8 2 1 5 6</td>
</tr>
<tr>
<td>21</td>
<td>551.152–551.552</td>
<td>4 3 7 8</td>
</tr>
<tr>
<td></td>
<td>551.752–552.152</td>
<td>2 1 5 6</td>
</tr>
</tbody>
</table>