Odin/SMR

Requirement Baseline Document

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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_2O, HNO_3, H_2O, CO, and isotopologues of H_2O, 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 14 years, and thus, the Level2 dataset can potentially be applied for scientifically interesting trend analysis. The current Level2 data version is Version 2-0 (for the 544 GHz band) and 2-1 (for all other data). Following various validation exercises a number of issues have been identified. In particular various artefacts were noted in the level 1 data used, including strange baselines, glitches and jumps in the power level. It has become clear that many of these are caused by the implementation of the calibration scheme, in particular in how the load spectra were selected. The main aim of the project is to reprocess all Odin/SMR data in order to create a fully consistent and homogeneous dataset of stratospheric species profiles. This should be done using the latest versions of the calibration scheme and settings for the inversion algorithm, and revised ancillary and auxiliary data.

The aim of this document is to define Odin/SMR Level2 products to be generated, and then establish a structured set of individual high-level requirements for

- the products to be generated,
- the algorithms to be implemented either in the form of refinements to existing algorithms or as newly developed alternative algorithms,
- all input data required to generate the data products,
- methods and sources to be used to validate the products.

1.2 Document structure

This document is organized as follows: Chapter 2 describes the Odin/SMR Level2 data products. Chapter 3 describes the requirements for the Odin/SMRLevel2 algorithms and input data. Chapter 4 describes requirements for validation of Odin/SMRdata products.

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 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

In this section an overview of Odin/SMR Level2 data products and requirements are given. Table 2.1 and Table 2.2 describe characteristics of the main and science Level2 products. The main products are retrieved from the so called "stratospheric" observation mode of Odin/SMR. In this mode spectra in frequency bands around 501 and 544 GHz are collected, and this mode is the most commonly applied mode. 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, N_2O, and HNO_3 profiles are the main Odin/SMR Level2 products. ClO and N_2O 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 has 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.

A requirement is therefore that an inventory/review is performed of the Level1B algorithm and data, and all other input data, applied in the Level2 processing (see Chapter 3). A further requirement is that the new Level2 dataset is validated by comparison to correlative datasets, both during the development phase and and in its final stage (see further Chapter 4).

2.3.2 Science data products

Profiles of H_2O, CO, NO and isotopologues of H_2O, 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.

Table 2.1: Characteristics of Odin/SMR Level2 main data products.

Product	**Frequency mode**	**Frequency [GHz]**	**Vertical coverage**	**Vertical resolution**	**Precision**	**Reference**
O_3	1	501.5	∼19–50 km	∼2 km	0.5–2 ppmv	(Urban et al., 2005)
ClO	1	501.3	∼19–67 km	1.5–2 km	0.15–0.2 ppbv	(Urban et al., 2005)
N_2O	1	502.3	∼15–70 km	∼1.5 km	15–35 ppbv	(Urban et al., 2005)
O_3	2	544.9	∼18–70 km	∼1.5 km	0.2–0.4 ppmv	(Urban et al., 2005)
HNO_3	2	544.4	∼21–67 km	1.5–2 km	1 ppbv	(Urban et al., 2005)

Table 2.2: Characteristics of Odin/SMR Level2 science data products.

Product	**Frequency mode**	**Frequency [GHz]**	**Vertical coverage**	**Vertical resolution**	**Precision**	**Reference**
CO	14	578.6	∼17–110 km	3–4 km	25 ppbv–2 ppmv	(Dupuy et al., 2004)
$H_2{}^{16}O$	13,19	556.9	∼40–100 km	∼3 km	0.5–1 ppmv	(Urban et al., 2007)
$H_2{}^{16}O$	8	488.5	∼20–70 km	∼3 km	0.5–1 ppmv	(Urban et al., 2007)
HDO	17	490.6	∼20–70 km	3–4 km	0.5 ppbv	(Urban et al., 2007)
$H_2{}^{18}O$	8	489.1	∼20–65 km	3–4 km	20-30 ppbv	(Urban et al., 2007)
$H_2{}^{17}O$	21	552.0	∼20–70 km	∼3 km	0.4 ppbv	(Urban et al., 2007)
NO	21	551.7	∼40–100 km	∼7 km	40 %	(Sheese et al., 2013)
${}^{16}O\,{}^{18}O\,{}^{16}O$	17	490.4	∼27–41 km	4–6 km	25 %	(Urban et al., 2013)
${}^{16}O\,{}^{16}O\,{}^{18}O$	17	490.0	∼25–45 km	3–4 km	25 %	(Urban et al., 2013)
${}^{16}O\,{}^{16}O\,{}^{17}O$	17	490.6	∼31–39 km	5–6 km	25 %	(Urban et al., 2013)

Chapter 3 | Odin/SMR Level2 algorithms and input data

3.1 Overview

The basic target of the Level2 algorithms is to convert observed and calibrated Level1B spectra to atmospheric species profiles. The retrieval problem is in general non-unique and non-linear for Odin/SMR and the Odin/SMR level2 data products will be derived by an Optimal estimation method (OEM) implementation, as described in the Odin/SMR ATBD for level2 processing (Eriksson, 2016). The OEM implementation combines measurement information with Ancillary–Auxiliary data and applies a forward model (Figure 3.1). High level requirements for each component is described in the following sections.

3.2 Forward model requirements

Forward model requirements are described in Sect. 2.2 and 2.4.2 in the ATBD for level2 processing. In short, these requirements are:

- limb sounding requires that refraction and the spherical shape of the Earth is considered when determining the propagation path, which excludes all plane-parallel models,
- the forward model must be able to deliver Jacobians,
- the forward model must be able to incorporate effects of sensor characteristics (e.g. antenna angular response, sideband filtering, frequency response of each spectrometer channel).

ARTS, the Atmospheric radiative transfer simulator, is a publicly available Free open-source software project. ARTS is in compliance with the requirements for Odin/SMR Level2 data processing. Thus, no further refinements of ARTS are necessary to perform.

3.2.1 Spectroscopic data

Spectroscopic data can be seen as basic input to the forward model, and it is of high importance that this data is as correct as possible. The positions and strengths of molecular transitions are known with a relatively high accuracy. In contrast, effects of pressure broadening and non-resonant absorption are less well known. Spectroscopic parameters can for instance be found in the High-resolution transmission molecular absorption (HITRAN) database. However, a requirement is that a literature review is performed, in order to identify the best possible spectroscopic data to apply (covered within WP 2.2.2 - Consolidation of AUX/ANC Data Files).

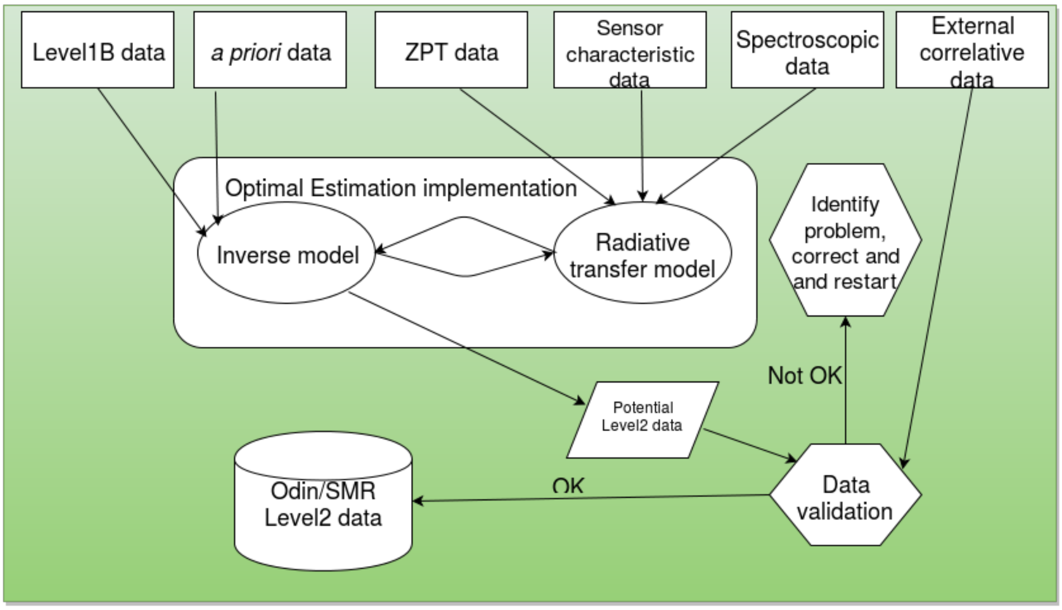

Figure 3.1: Schematic of the Level2 processing and input data.

3.3 OEM implementation requirements

The basis of the required OEM (Optimal estimation method) implementation for Odin/SMR is described in Chapter 4 of the ATBD for level2 processing. In short, the basic considerations/requirements of the OEM implementation are:

- the OEM implementation must contain an interface to the applied forward model,
- the retrieval problem is in general non-unique, hence a constraint to the solution must be applied,
- measurement information must be combined with *a priori* information, and the OEM implementation must contain functions to create parametric covariance matrices,
- the retrieval problem is non-linear, hence an iterative procedure is required to find the solution,
- the iteration scheme needs a convergence test and stop criteria.

A matlab implementation, that is part of the Atmlab package, of OEM will be applied. This package is available through the ARTS site, at `www.radiativetransfer.org/tools`. It provides an interface to ARTS and other necessary functionality, and has been used by several groups for retrieval processing. However, the exact setup of the retrieval processing has to be seen specific for Odin/SMR and tests must be performed to identify best setup. Level2 data validation is covered in Chapter 4.

3.4 Level1B data requirements

The accuracy of the Level1B dataset is important for the quality of the Level2 dataset for obvious reasons. Following various validation exercises a number of issues of Odin/SMR Level1 data have been identified, including strange baselines, glitches and jumps in the power level. A requirement is therefore that a review of the calibration scheme and the processing algorithms is performed, and that any errors that are found are corrected if possible. A further requirement is that Level1 data is quality classified, and that corrupt data is weeded out. The accuracy of Level1 data should be verified by comparison to simulated measurements (see Chapter 4). In short, the best available Odin/SMR Level1B data should be applied, and the Level1B data must not contain any errors that are known.

3.5 Ancillary–Auxiliary data requirements

3.5.1 Climatology *a priori* data

A priori data, or a climatology database covering all species of interest is required, as the OEM implementation needs a starting estimate for each profile to be retrieved. The climatology must also cover the relevant vertical range for each species, and latitudinal and seasonal variations. A requirement is that a literature review is performed, in order to identify the best possible climatology data (covered within WP 2.2.2 - Consolidation of AUX/ANC Data Files).

3.5.2 ZPT data

External ZPT data (altitude, pressure, temperature) is given as input to the Level2 processing. Data from the selected source must be available for the complete Odin mission. Furthermore, the data should be as accurate as possible and contain no known artificial trends.

A commonly used data source for this type of application, is European centre for medium-range weather forecasts (ECMWF). In principle, there are two possible ECMWF products to choose between, i.e. data from the operational model or from ERA-Interim. ERA-Interim is a global atmospheric reanalysis from 1979, and is based on the same version of assimilation system, whereas the operational product has changed assimilation version during the Odin mission.

Thus, a requirement is that a temperature trend analysis is performed for candidate data sources, in order to verify that the data contains no spurious trend, that can propagate to an artificial trend in Odin/SMR Level2 data.

3.5.3 Sensor characteristic data

The forward model simulation must take into account sensor characteristic data, such as the antenna angular response, sideband filtering, and frequency response of each spectrometer channel. A requirement is that the best possible data is applied.

Chapter 4 | Data validation

4.1 Validation objective and method

The basic idea of validation is to check that a product meets its specification. An ideal validation exercise would be to compare Odin/SMR Level2 data profiles to the truth, and to evaluate if the differences between Odin/SMR and the truth is within the specified errors. Furthermore, validation can be seen as an iterative process: validation results are used to trace systematic errors in the instrument and the applied processing algorithms, and thus to improve Level1 and Level2 products.

The problem is that the true trace gas species concentration, within the Odin/SMR field of view in the upper atmosphere, is seldom known. Thus, a true validation is complicated. The best one can do is therefore to compare Odin/SMR Level2 data to best possible correlative datasets, and to derive a mean bias against various reference datasets.

The "validation" must be performed in at least two phases. The first phase is validation for a diagnostic/verification dataset, i.e. a sub-part of the Odin/SMR dataset. This dataset will be used to judge the performance of the updated processing chain, and to allow continuous improvements to the processing chain during development. The dataset should be representative in the sense that it contains all types of data (both "good" and "problematic") while not being overly large (less than 10% of the complete dataset). The second phase is to perform validation for the finally selected processing setup and for the complete dataset.

4.2 Level1B verification

The quality of the Level1B dataset should be verified. A minimum requirement is that calibrated spectra should be compared with radiative transfer model simulations where the observed signal can be accurately predicted. In practice, this means observations with low tangent point at high latitudes and with low tropospheric temperature gradient. Furthermore, simulations should be based on the best possible input data. Time-series of measurements and simulations should be evaluated in order to identify/verify the calibration accuracy and any drifts.

4.3 Level2 validation

All main Level2 data species must be compared to correlative datasets from other satellite instruments, such as Microwave limb sounder (MLS) on the Aura satellite, and the Michelson interferometer for passive atmospheric sounding (MIPAS), a mid-infrared emission spectrometer mounted on the European environmantal satellite (ENVISAT). Furthermore, Odin/SMRozone profiles can be compared to high quality balloon-borne measurements, and such comparisons are presented in (Jégou et al., 2008). However, ozone profiles derived from balloon-borne measurements do not cover the upper atmosphere (typically maximum altitude is below 35 km).

A minimum requirement for the Odin/SMR Level2 products is that mean bias profiles against reference datasets are established. The following reference datasets must be considered:

- the previous Odin/SMR Level2 dataset for O_3, ClO, N_2O, HNO_3,
- best possible correlative dataset derived from satellite-borne measurements for O_3, ClO, N_2O, and HNO_3,
- ballon-borne measurements (between 20–35 km) for O_3.

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