

***Validation Report - GRAS Level 1b Bending
Angle FCDR Release 1***

Doc.No. : EUM/OPS/DOC/18/1008023
Issue : v3 e-signed
Date : 15 April 2019
WBS/DBS :

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Document Change Record

Version	Version Date (as on profile)	DCR* No. if applicable	Description of Changes
1C	15 January 2019		Final version ready for DRR
1D	22 February 2019		Implemented DRR RIDs (EUM/OPS/FRM/18/1041007), e.g. various text bits, Fig. 4 added, Fig. 6, 8, 10 updated to include hemisphere, Fig. 11 included a zoom on 2013/2014 period.
2	7 March 2019		Version with RIDs from DRR members addressed and marked in the text
3	15 April 2019		Final version with RIDs 26, 51, 57, 59 from DRR members addressed after confirmation at the collocation meeting

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1 INTRODUCTION

1.1 Purpose and scope

This document details the validation results for Release-1 of the Fundamental Climate Data Record (FCDR) of reprocessed Level 1b bending angles from the Global Navigation Satellite System (GNSS) Receiver for Atmospheric Sounding (GRAS) instrument on Metop-A using the wave-optics-based retrieval implemented in the Yaros version 1.4 software [RD 4], hereinafter referred to as Release 1 - GRAS Level 1b Bending Angle FCDR. The generation of the data record was triggered by the EU ERA-CLIM2 project [RD 6], which asked for Level 1b Radio Occultation (RO) bending angle data from the GRAS instrument for assimilation in European Centre for Medium-Range Weather Forecasts (ECMWF) Numerical Weather Prediction (NWP) model-based re-analysis.

The Release 1 - GRAS Level 1b Bending Angle FCDR comprises GRAS data from Metop-A for the period 2006–2016, and provides a consistent record of bending angle data from which, for example, stratospheric temperature, pressure and tropospheric temperature, pressure and humidity profiles can be derived, which in turn can be used for climate monitoring and data assimilation. The data record can be regarded a FCDR, i.e., a long-term data record of calibrated and quality-controlled sensor data designed to allow the generation of homogeneous products that are accurate and stable enough for climate monitoring and data assimilation for re-analysis of the recent climate. Note here that the radio occultation technique is based on time measurements and thus requires no calibration.

The “reference” data used to evaluate Release 1 - GRAS Level 1b Bending Angle FCDR comprise reanalysis data from ECMWF re-analysis ERA-Interim¹, Level 1b bending angles from Metop-B (processed with the same s/w version as Metop-A data), Level 1b bending angles from Metop-A derived by the University Corporation for Atmospheric Research (UCAR), and Level 1b bending angles from the CHAMP and COSMIC instruments derived by UCAR. ROM SAF products are not used for data evaluation here since their processing up to higher levels (refractivity, temperature, pressure, humidity) is partly based on the here presented Release 1 - GRAS Level 1b Bending Angle FCDR products and they do an extensive validation within this reprocessing, thus please refer to [RD 17].

The Release 1 - GRAS Level 1b Bending Angle FCDR has been validated by evaluating trends in the time-series (direct evaluation), comparing against ERA-Interim reanalysis on a global scale (global analysis) as well as for different latitude bands, comparing against bending angle retrievals from other satellites or providers (match-up evaluation), and analysing the observations departures using ERA-Interim reanalysis as background.

A Product User Guide to Release 1 [RD 1] accompanies this validation report, where more general information on product format, features, access and support is given. Information on the actual data format can be found in the Product Format Specifications document [RD 2].

1.2 Structure of this document

This document is organised as follows:

Section 1 Introduction

¹ Note that even though a re-analysis is using the same assimilation software version for the complete data set, it suffers from model errors and can also in addition suffer time varying errors since the observation data characteristics change, see e.g. [RD 18] for the impact of RO data availability. It is thus not an independent reference, but serves here as a commonly used “reference” (in quotes).

Section 2	Background
Section 3	Validation strategy
Section 4	Validation results
Section 5	Product evaluation
Section 6	Summary and Conclusions
Section 7	References

1.3 Acronyms

<i>Acronym</i>	<i>Meaning</i>
BUFR	Binary Universal Form for the Representation of meteorological data
CDR	Climate Data Record
CHAMP	Challenging Mini-satellite Payload
ECMWF	European Centre for Medium-Range Weather Forecasts
FCDR	Fundamental Climate Data Record
GNSS	Global Navigation Satellite System
GO	Geometrics Optics
GPS	Global Positioning System
GRAS	GNSS Receiver for Atmospheric Sounding
NH	Northern Hemisphere
NRT	Near-Real-Time
NWP	Numerical Weather Prediction
POD	Precise Orbit Determination
QBO	Quasi-Biennial Oscillation
RO	Radio Occultation
ROPP	Radio Occultation Processing Package
SH	Southern Hemisphere
SLTA	Straight Line Tangent Altitude
SNR	Signal to Noise Ratio
UCAR	University Corporation for Atmospheric Research
WO	Wave Optics

1.4 Definitions

The following definitions are used throughout the document.

Data levels:

- Level 0 - Reconstructed raw sounding data at full time resolution with all available supplemental instrument information to be used in subsequent processing included.
- Level 1a – individual occultations full information such as phases and amplitudes, Signal to Noise Ratios (SNRs), as well as all other information e.g. from the Precise Orbit Determination (POD), needed to process it further to Level 1b.
- Level 1b - Level 1a sounding data that have been processed to bending-angles and impact parameters, tangent point location, and quality information.

Products types:

- Near-Real-Time (NRT)- refers to data delivered for Numerical Weather Prediction (NWP) applications and is generally provided within less than 2h 15min (for EUMETSAT GRAS products). Data presented here is re-processed and thus has a higher quality compared to the NRT products.
- Fundamental Climate Data Record - is a well-characterised, long-term data record, usually involving a series of instruments, with potentially changing measurement approaches, but with overlaps and calibrations sufficient to allow the generation of products that are accurate and stable, in both space and time, to support climate applications. FCDRs are typically calibrated radiances, backscatter of active instruments, or radio occultation bending angles. FCDRs also include the ancillary data used to calibrate them [RD 5].

Statistics:

- Observations minus background departures - refers to departures that are derived using the $(O-B)/B$ [%] quantity. O represents the observed profile, B the background profile (e.g. as taken from ECMWF ERA-Interim [RD 14]). This representation allows a better comparison for the exponentially varying bending-angle profiles. B is sometimes not taken from the ECMWF re-analysis, but from a match of another bending-angle observation; then referring to $(O_1-O_2)/O_2$ where O_1 generally denotes the EUMETSAT data and O_2 the other bending-angle observation. All profile data validation is based on “thinned” data, meaning that the high resolution profile data (which has > 1000 data points per profile) is thinned to a resolution varying with altitude (higher resolution near the surface of about 150m, to about 300m near 60km). This thinned profile data, comprising 247 data points, is also used in the NRT product delivery to NWP users. The high resolution data is though also part of the GRAS Level 1b FCDR [RD 2].
- Robust estimator for statistics based on Tukey’s bi-weight, for more details please refer to [RD 11] - it refers to an estimator that provides an effective tool to reduce weight for outliers from noisy distributions, returning bias, standard deviation² and percentage of data points falling into the $\pm 2\sigma$ interval. This would be 95% for an ideal Gauss distribution, for GRAS it is around 92% at the upper troposphere.
- Weight - provides information on the number of outliers filtered out in the robust estimator (see above); at higher altitudes, for ideal Gauss distributions, it should be about 95%. In the lower part of the atmosphere, it also shows the penetration of the occultations, meaning how many manage to reach down to a particular impact height level.
- Standard deviation - output of the robust estimator, represents the standard deviation of the data set once outliers are de-weighted.
- Bias - output of the robust estimator, represents the systematic difference of the two data set once outliers are de-weighted.
- Number of occultations - the average number of occultations per day over the plotted or analysed time range. Taking into account all valid occultations processed (percentage of invalid occultations is given in failure rate).
- Failure Rate - Percentage of all occultations that do not provide valid neutral bending angles (e.g. because one of the frequencies is not tracked) or that are very short (covering less than 20km in impact height space).
- Structural uncertainty - a residual uncertainty that still persists between processing streams, even if the processing starts from the same level 0 / original data. It is caused by

² Note that this Validation Report and the Product User Guide [RD 1] generally discuss data quality in bias and standard deviation terms, which in metrology are called systematic and random uncertainty.

assumptions/implementations made in the processing, such as e.g. how to filter noisy data, how to interpolate (linear or exponential).

Other:

- Match up - A sensor “point” measurement that is matched with another sensor’s “point” measurement sufficiently close in space and time (usually 300km/3hours is used here). For radio occultation matching, the “point” measurement is taken at the reference tangent point.
- Straight Line Tangent Altitude (SLTA): the tangent altitude of the direct LEO/GNSS satellite ray with respect to the Earth WGS84 Ellipsoid; it is generally $>0\text{km}$, but in the lower troposphere can go to values $<-200\text{km}$ due to the bending of the ray. For EUMETSAT data, the reference tangent point corresponds to $\text{SLTA} = 0\text{km}$.
- Bending angle: the actual geometry of the limb sounding radio occultation measurement technique is shown in Figure 1. The figure shows the bending angle as the angle between the actual, measured, and the straight line propagation from the GNSS satellite to the LEO satellite. The SLTA altitude is also shown.

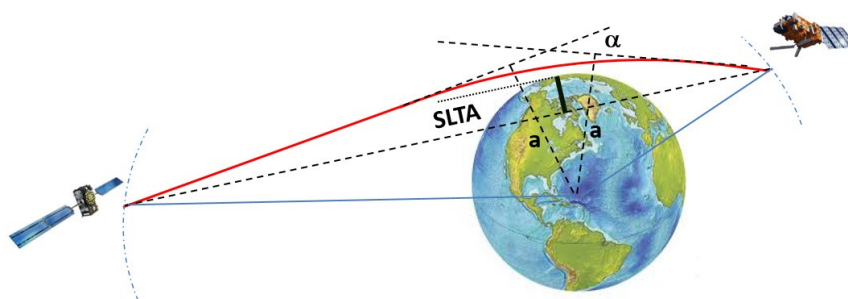


Figure 1 Radio occultation geometry, showing the bending angle α , the impact parameter a , and the straight line tangent altitude (SLTA). Note that α is generally below 1° and is measured in μrad , thus the figure is greatly exaggerated.

2 BACKGROUND

In this chapter background information is given on the GRAS radio occultation (RO) instruments, on the data that have been processed, on the algorithms that have been used for the reprocessing, as well as a summary on the reprocessing procedure. Please refer to [RD 7] for a more general introduction to RO.

2.1 GRAS instrument

The GRAS instrument is flying on the Metop satellites, Metop-A has been in orbit since 19 October 2006, Metop-B since 17 September 2012, Metop-C since 7 November 2018, all in a sun-synchronous orbit with a 09:30 Equator crossing time, orbit altitude of 820 km. At time of writing, all GRAS instrument are operating nominally.

GRAS observes GPS signals on the L1 and L2 frequencies, both on the zenith pointing antenna for Precise Orbit Determination (POD), and on the velocity and anti-velocity pointing antennas (rising and setting occultations). Occultation measurements are performed from the Earth surface to about 80km altitude. The instrument has for the occultation chain a closed-loop tracking mode on L1 and L2 frequencies and an L1 open-loop tracking mode to improve the penetration into the lower troposphere. The instrument can either do open-loop and closed-loop tracking on L1 or closed-loop only tracking on L1 and L2. Please refer to [RD 9] for more information on the GRAS instruments.

2.2 GRAS data

The provided data record includes Level 1b bending angles from the GRAS instrument on Metop-A. The data record covers the period 2006 to end 2016, and consists of approximately 2.5 million occultations for GRAS on Metop-A. Note that reprocessing activities of more recent data are ongoing; for the most recent NRT data, please refer to the EUMETSAT archive.

Table 1 provides the start and end time of the EUMETSAT reprocessed data, the number of nominal/non-nominal occultations, and the average number of occultations per day. The EUMETSAT data record was generated using Yaros version 1.4, utilizing all available GRAS data. Note that these are about 10% more occultations than the GRAS data that are made available by UCAR [RD 13]; the data set presented here also covers a longer time period.

Table 1 Data coverage of Release 1 - GRAS Level 1b Bending Angle FCDR. Degraded occultations determined from setting of Product Confidence Descriptor [RD 10]. Average number of occultations per day uses all occultations.

Mission	Start Record	End Record	Tot. Occs / Degr. Occs	Avg. Occs/Day
<i>EUMETSAT</i>				
Metop-A	2006-10-27 09:57	2016-12-31 21:54	2,464,280 / 247,104	663

2.3 Reprocessing algorithm

The reprocessing of the GRAS RO data is based on a “wave optics” retrieval algorithm, and is fully consistent³ with the operational GRAS processing as introduced in November 2016. The reprocessed GRAS data thus extends the current (at the time of writing) operationally available data backwards in

³ Although the operational processing uses a mainly C++ based implementation of the algorithms, it is validated against the reference processor used for this reprocessing, assuring that the 2 implementations lead to the same result if they process the same data.

time towards shortly after the Metop-A launch in October 2006. This data set in particular provides significant improvements over the early Metop-A NRT data, as shown in the Product User Guide to Release 1 [RD 1]. A general introduction on the principles of RO sounding can be found in, e.g., [RD 7] and [RD 8].

2.4 Reprocessing procedure

The actual data processing from Level 0 to Level 1a and Level 1b is summarized in this section. The procedure to retrieve Level 1b bending-angle data starts with GRAS Level 0 data reconstruction, followed by the POD from the zenith antenna data, after which the Level 1a processing is performed (e.g. to determine phases and amplitudes), and finally the Level 1b processing is done (e.g. to determine bending angles over impact parameters). The sequence of processing steps is very similar to the operational setup for GRAS data provision in NRT and the data is produced in daily batches for improved orbit determination setup (The NAPEOS POD s/w [RD 17] is run per complete day, centred on that day, with 3h overlaps into the previous and the next day; orbit manoeuvres are split into 2 POD runs, prior and after). A more detailed description of the reprocessing procedure as well as more information on the Release 1 - GRAS Level 1b Bending Angle FCDR data can be found in the Product User Guide to Release 1 [RD 1] and the Product Format Specifications document [RD 2].

3 VALIDATION STRATEGY

In this chapter the validation strategy and validation data sets are presented. The EUMETSAT reprocessed data record is compared to reprocessed data records provided by UCAR for quality evaluation, thus characteristics for both data records are included in the following sections. The UCAR data records that are used for comparison are the COSMIC, Metop-A, and Metop-B data records resulting from their reprocessing in 2016 [RD 13].

3.1 Overall approach

All mission data (from EUMETSAT and UCAR) are mapped onto a standard vertical grid, the same as also used in the operational BUFR⁴ generation at EUMETSAT, for the NRT data stream. This consists of 247 impact height levels spanning from 2.1 km to 59.9 km. The vertical resolution is adapted to the information content of the RO measurement, thus more levels are provided in the lower troposphere, coarser information on the atmosphere is provided at altitude of about 60km. Impact heights are calculated from the standard impact parameter by subtracting the radius of curvature. The lowest vertical level represents rays getting all the way down to the surface, it is not at 0 km since the bending of the rays is taken into account.

RO bending-angle data is generally processed on a higher resolution than these 247 levels, there can be several thousands in the actually “raw” bending-angle data. For processing and assimilation purposes this is thinned / smoothed to a lower resolution. The EUMETSAT RO data has a specific netCDF-4 entry that includes thinned data on 247 levels [RD 2]. The UCAR data is pre-processed from the available high resolution with the ROPP [RD 10] tool to be available on the same 247 levels. Note that the exact algorithm for the thinning from a higher vertical bending-angle profile resolution to a lower one impacts the statistics. For the UCAR thinning, we applied a standard ROPP implemented thinning that is based on first searching for the impact parameters in the high resolution data that are right above / below the sought after thinned level, and then the linear interpolation in log space of the bending angles at these nearest data points to the required thinned level. Advantage of this thinning method is that the original

⁴ The Binary Universal Form for the Representation of meteorological data (BUFR) data is sent to NWP centres for assimilation; it is defined to provide sufficient vertical resolution, matching the NWP model resolution

data is kept as close as possible to the UCAR provided processing. There is however also the disadvantage of higher noise terms introduced with this method - but the data set is very large and this additional noise will be averaged out.

3.2 Validation assessments

The quality of Release 1 - GRAS Level 1b Bending Angle FCDR is analysed through the following five assessments:

1. **Global analysis:** in this analysis all data sets are compared with each other globally, using the ERA-Interim re-analysis as “reference”, however the limitations outlined Section 1.1 apply.
2. **Direct evaluation:** analysis of seasonal and annual trends in the time-series of Level 1b GRAS data. This analysis requires only Level 1b GRAS data. No additional information is taken, and thus avoids, e.g., the mixture of reanalysis and actual measurement errors;
3. **Match-up evaluation:** pairs Level 1b GRAS data processed by EUMETSAT with Level 1b GRAS data processed by another centre (direct match-ups), or with Level 1b data from another mission. For direct matching, it is assured that only the same occultations are compared by (1) a main matching criteria that the reference time is within a few minutes (reference times and the geo-location are differently defined by the 2 centres, EUMETSAT e.g. uses an SLTA⁵ value of 0km for geo-location, UCAR uses the SLTA value where the excess path reaches 500m; the provided reference time can depend on how deep the occultation penetrates), and (2) the same GPS satellite is observed in occultation. For match-ups with another mission, observations pairs that are within 3h and 300km are taken. The resulting statistics are thus a mixture of the measurement errors (if not using a direct match), co-location uncertainties (if not using a direct match), and differences in processing characteristics;
4. **Reanalysis evaluation:** departure analysis in which the observations are evaluated against an ERA-Interim background. ERA-Interim provides a consistent data set “reference” over the full investigated record. The resulting statistics are a mixture of reanalysis errors and the actual measurement/processing errors. The re-analysis errors should have a consistent model error since they are run with the same assimilation software version for the complete data set, but it can suffer time varying errors since the observation data characteristics change, see e.g. [RD 18] for the impact of RO data availability.
5. **Product evaluation:** analysing annual trends in bending angles for different latitudes and altitudes, derived both from the here analysed Release 1 - GRAS Level 1b Bending Angle FCDR data, as well as the ECMWF ERA-Interim data.

Either all occultation data is shown, or the data is separated into setting and rising occultations, or into different latitude bands. These latitude bands are either considering 30° spacing, independent of whether they are on the Northern or Southern Hemisphere, or they separate that further by Hemisphere.

3.3 Validation datasets

3.3.1 ECMWF data

ECMWF re-analysis ERA-Interim data [RD 14] is primarily used to validate the bending-angle profiles of the different RO missions since it provides a consistent data set, covering the full time period. The data set includes global atmospheric fields of temperature, water vapour and surface pressure and geopotential on 60 model levels up to about 65km altitude. The data is stored at EUMETSAT with a 6h time and a 1° latitude, longitude resolution. The ECMWF data is interpolated to the occultation position (time

⁵ Straight Line Tangent Altitude (SLTA) is the tangent altitude of the direct LEO/GNSS satellite ray with respect to the Earth WGS84 Ellipsoid; it is generally >0km, but in the lower troposphere can go to values <-200km.

interpolation is not used as it has a minor impact on the statistics) and then forward propagated to bending angles using the ROPP tool at version 9.0⁶ [RD 10].

The ERA-Interim re-analysis started to assimilate CHAMP data from May 2001, with the first CHAMP data being available, COSMIC data entered in December 2006, and GRAS data in May 2008, it is thus not a fully independent data set. Note also that RO data was by configuration error not assimilated in late 2013, early 2014. The re-analysis does, however, also assimilate millions of other ground and satellite based data. The impact of GRAS assimilation is shown in Figure 2, which is determined by using the mentioned robust estimator for statistics based on Tukey's bi-weight, hereinafter referred to as robust statistics. The average weight for this data set is 92%, thus over the whole profile 3% of the data has been de-weighted/removed by the robust statistics from a nominal Gauss distribution. This averaged 3% of the reduced weight data (see right plot in Figure 2), can be slightly higher at higher altitudes where the POD and orbit/clock noise is more visible, and is generally slightly less in the core region between 10km to 35km. At lower altitudes the decreasing penetration is visible, this is however not included in the average 92% number.

As can be seen from Figure 2, the bias hardly changes between April and June 2008, only the standard deviation is slightly reduced after GRAS data were assimilated in June 2008. For comparison, the same months are also shown for the year 2007. Removing all RO data from ERA-Interim (thus primarily COSMIC, GRAS-A and GRAS-B, but also TerraSAR-X and Grace data end 2013) had a larger impact, as can be seen when comparing December 2013 with January 2014; as said above, in November/December 2013 the RO assimilation in ERA-Interim was accidentally switched off at ECMWF.

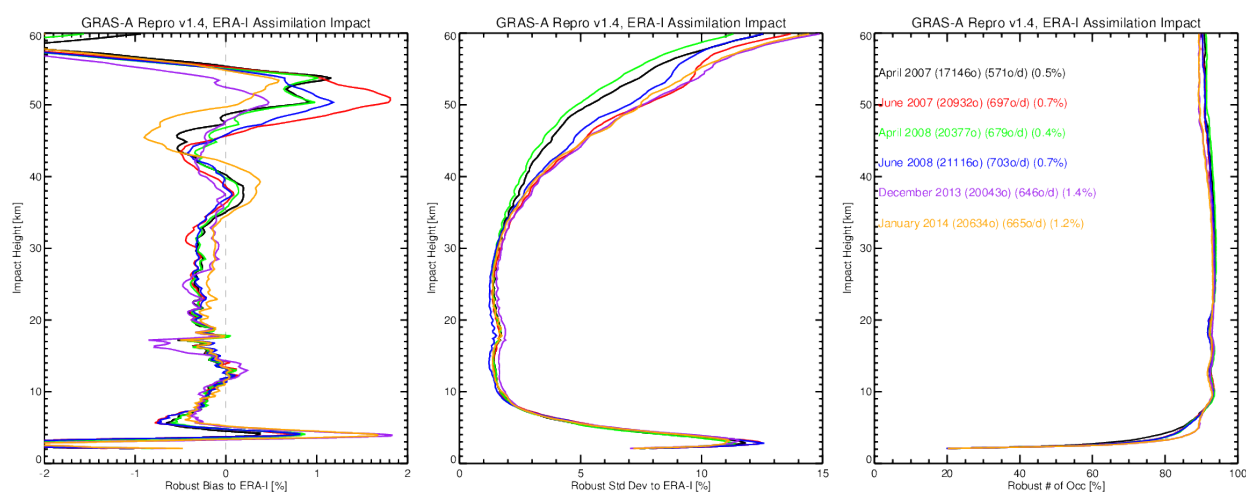


Figure 2 Release 1 - GRAS Level 1b Bending Angle FCDR bending-angle comparison to ERA-Interim forward propagated ones around the month when GRAS was assimilated into ERA-Interim, as well as one year before assimilation. In addition, the month when all RO was accidentally removed from ERA-Interim (Dec 2013), as well as when it was reactivated (Jan 2014) is included. Robust bias (left), standard deviation (middle), outlier distribution (right). The legend gives in addition the total number of occultations, average occultations per day and the failure rate.

3.3.2 Metop-A data from UCAR

⁶ The actual version used internally is ROPP v9.1, which includes a correction to deal with incorrectly named/processed UCAR data (undulation is actually included in the UCAR impact height variable).

The Metop-A Level 1b GRAS data from UCAR are used for match-up evaluations against Metop-A Level 1b GRAS data from EUMETSAT, i.e., the Release 1 - GRAS Level 1b Bending Angle FCDR data. These Metop-A results from UCAR's reprocessing in 2016 [RD 13]. Note that the UCAR Metop-A data has gaps around end 2007, beginning 2008.

3.3.3 Metop-B data from EUMETSAT

Metop-B Level 1b GRAS data has been processed by EUMETSAT in a similar fashion as the Metop-A data validated here and is primarily used for general and match-up evaluations against Metop-A Level 1b data from EUMETSAT, i.e., the Release 1 - GRAS Level 1b Bending Angle FCDR data. All occultations obtained within the investigated period up to 2016 are included.

3.3.4 COSMIC and CHAMP data from UCAR

The COSMIC and CHAMP Level 1b data from UCAR are primarily used for match-up evaluations against Metop-A Level 1b GRAS data from EUMETSAT, i.e., the Release 1 - GRAS Level 1b Bending Angle FCDR data. These COSMIC and CHAMP data results are from UCAR's reprocessing in 2013 (COSMIC, providing data up to April 2014) and 2016 (CHAMP, providing data up to October 2008) [RD 13].

4 PRODUCT VALIDATION

In this chapter the results of the product validation are presented. The Release 1 - GRAS Level 1b Bending Angle FCDR has been validated by evaluating trends in the time-series (direct evaluation), comparing against ERA-Interim reanalysis on a global scale (global analysis), comparing against bending-angle retrievals from other satellites or providers (match-up evaluation), and analysing the observations departures using ERA-Interim reanalysis as background.

4.1 Global analysis

The global analysis compares all data sets with each other on a global scale, using the ERA-Interim reanalysis as "reference"⁷. The results for the Metop-A GRAS instrument are shown in Figure 3. As an outlook to following activities for the Copernicus Climate Change Service (C3S), Figure 4 shows some results already obtained for the GRAS instrument on Metop-B. These figures look very similar since both GRAS instruments have almost identical sampling and instrument characteristics, only the total number of occultations, as given in the legend, is higher for the GRAS instrument on Metop-A than for the GRAS instrument on Metop-B since Metop-A GRAS started to collect data already from 2006 onwards. On a daily basis, both instruments are however providing very similar numbers of occultations. Note that the total number of occultations available, as well as the daily average, is different to Table 1 since here addition quality control (e.g. removing occultations that have no L2 data, removing short occultations) is applied.

Regarding the results from processing at EUMETSAT or UCAR, bias and standard deviation look very similar for both GRAS data records, at least for altitudes above about 7 km. Below this altitude, the different Wave Optics (WO) processing implementations lead to different biases, which are, as expected, similar for Metop-A and -B. The exact reason for the larger peak around 5 km in the EUMETSAT processed data is currently unknown, it is under investigation whether this is an issue in the EUMETSAT or UCAR processing. It is found at all latitude bands and is highest for mid-latitudes in the Southern Hemisphere and for low latitudes (see later Figure 11). It is also found to be significantly higher in winter 2013/2014, when GRAS data was not assimilated at ECMWF (Figure 2). The magnitude of the peak also varies when comparing to UCAR processed data (see later Figure 7 and Figure 9). The standard

⁷ Within the limitations outlined in Section 1.1.

deviations are slightly different around the tropopause and above 22 km. The different filtering/smoothing of the data is very likely the root cause here. This is also the reason for lower EUMETSAT standard deviations above about 55 km, where the EUMETSAT processing applies an adaptable filter widths, leading to slightly lower values. Regarding the data quality/robustness, both data sets are similar above about 10 km, although the EUMETSAT data set provides more occultations per day than the UCAR data set. Below 10 km, the penetration into the troposphere is higher for the EUMETSAT data record. Note that the different standard deviations are not caused by the slightly different number of occultations entering the statistics, aligning the EUMETSAT data set to include only occultations provided by UCAR, yields almost identical statistics.

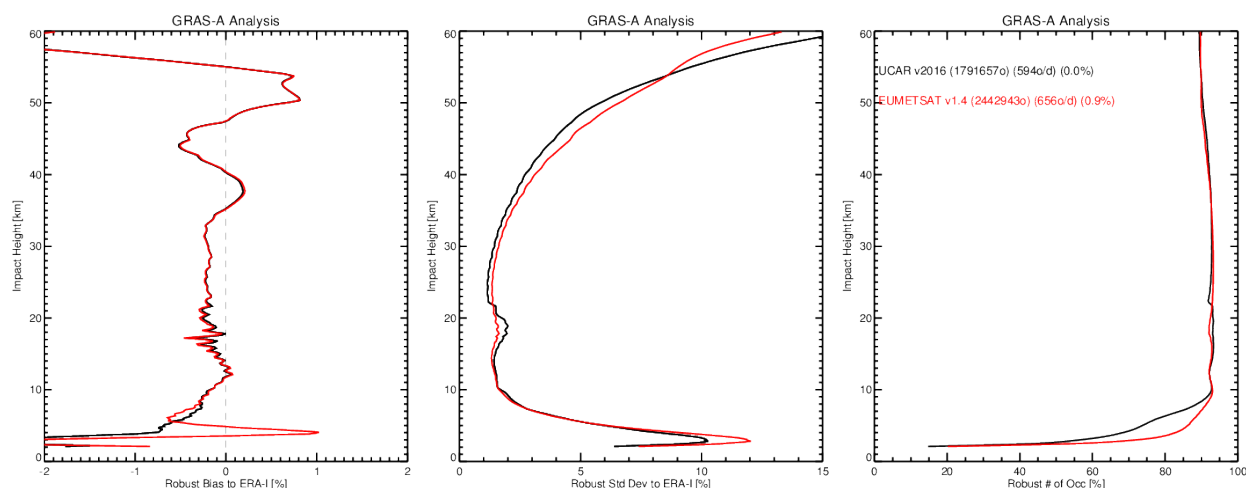


Figure 3 Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR bending-angle comparison to ERA-Interim forward propagated ones for the complete Metop-A GRAS data record, by UCAR at version 2016 (black line) and EUMETSAT at Yaros version 1.4. (red line). Robust bias (right), standard deviation (middle), outlier distribution (right), otherwise as Figure 2.

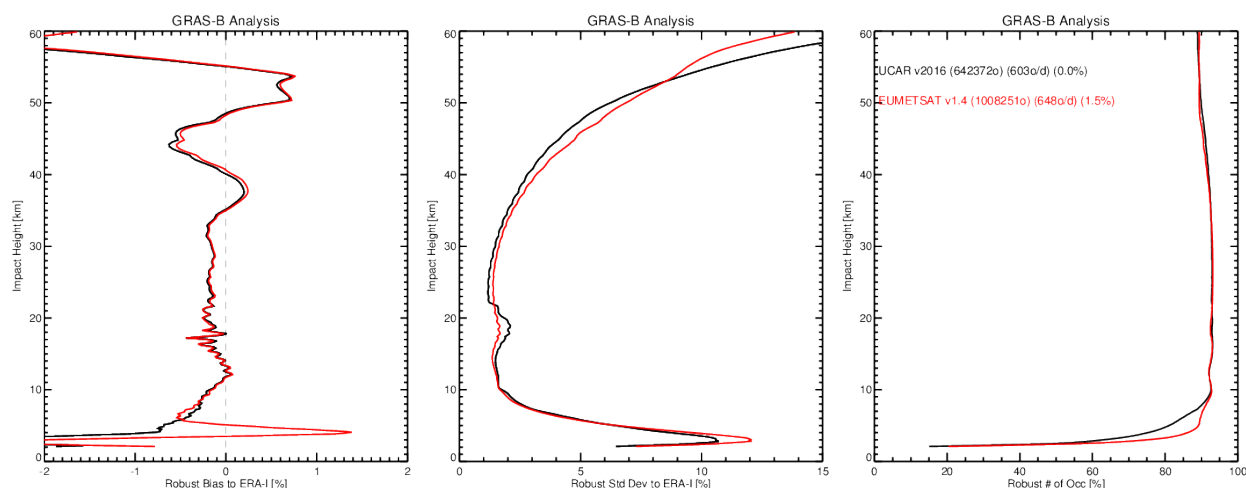


Figure 4 Metop-B GRAS reprocessed bending-angle comparison to ERA-Interim forward propagated ones for the complete Metop-B GRAS data record, by UCAR at version 2016 (black line) and EUMETSAT at Yaros v1.4. (red line). Robust bias (right), standard deviation (middle), outlier distribution (right), otherwise as Figure 2.

4.2 Direct evaluation

For validation purposes, data on the thinned levels is used (as mentioned above). These thinned levels are defined such that they represent a certain altitude above the Earth surface (actually above the WGS84 ellipsoid). Hence, by using all bending-angle data at a specific altitude level, it is possible to access the data stability over time at a specific altitude. This can be done globally or for different latitude bands.

The direct evaluation uses this dataset at a specific altitude to evaluate the time-series of the GRAS data record directly – an advantage of this method is that no other dataset is used in the validation. In order to smooth the data and remove daily variations, the actual bending-angle values at this specific altitude and latitude band are first averaged over 7 day intervals (using less than 7 days leads to more variations in the data e.g. in the number of daily observations due to data gaps, and obscure the overall message). For easier plotting, these 7 day averages are then normalized to the mean global bending angle value at that altitude (O_m), hence resulting bias and standard deviation values scatter around 1, have no unit and are more readably presented in this figure. Bias and standard deviations of these 7 day intervals are calculated and plotted for the full time series up to 2016.

Figure 5 shows this direct analysis of the complete Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR. The top 3 plots show statistics of the 7 day, normalized bending angle data around 20km, separated by latitude bands of the Northern (NH) and the Southern Hemisphere (SH). Robust statistics have again been used over the 7 day window. As mentioned above, the bias values (top plot) scatter around a value of 1.0 and have no units. The standard deviation (second plot) shows higher variability in the two mid latitude bands, a temporal shift of a few months is also visible (and contrasts to the mid latitude biases, which show a more expected 6 month annual shift). The third plot shows the quality of the data / the number of outliers for the 7 day robust statistics. This is constant throughout the whole mission, no instrument degradation is visible (at low latitudes, there is a biannual pattern visible with slight degradation, during the time period of Solar Cycle 24 which started in 2008 and peaked around 2013). The bottom plot shows the number of occultations in this 7 day interval at the respective latitude band, confirming that the GRAS instrument on Metop-A provides a very stable number of observations (except for the first few months in 2006 when the Metop-A satellite had several outages).

The same stability processing and analysis has also been applied to the UCAR COSMIC 2013 data set, as shown in Figure 6. Here, one can see the degrading performance of the instrument in the number of outliers for the 7 day robust statistics (3rd plot). In addition, the well known variations in the available number of daily occultations is visible in the bottom plot, the 6 COSMIC satellites had strongly varying performances throughout their lifetime. Otherwise, bias and standard deviations are very similar and both data sets e.g. show the pronounced higher standard deviations for NH high latitudes in early 2012.

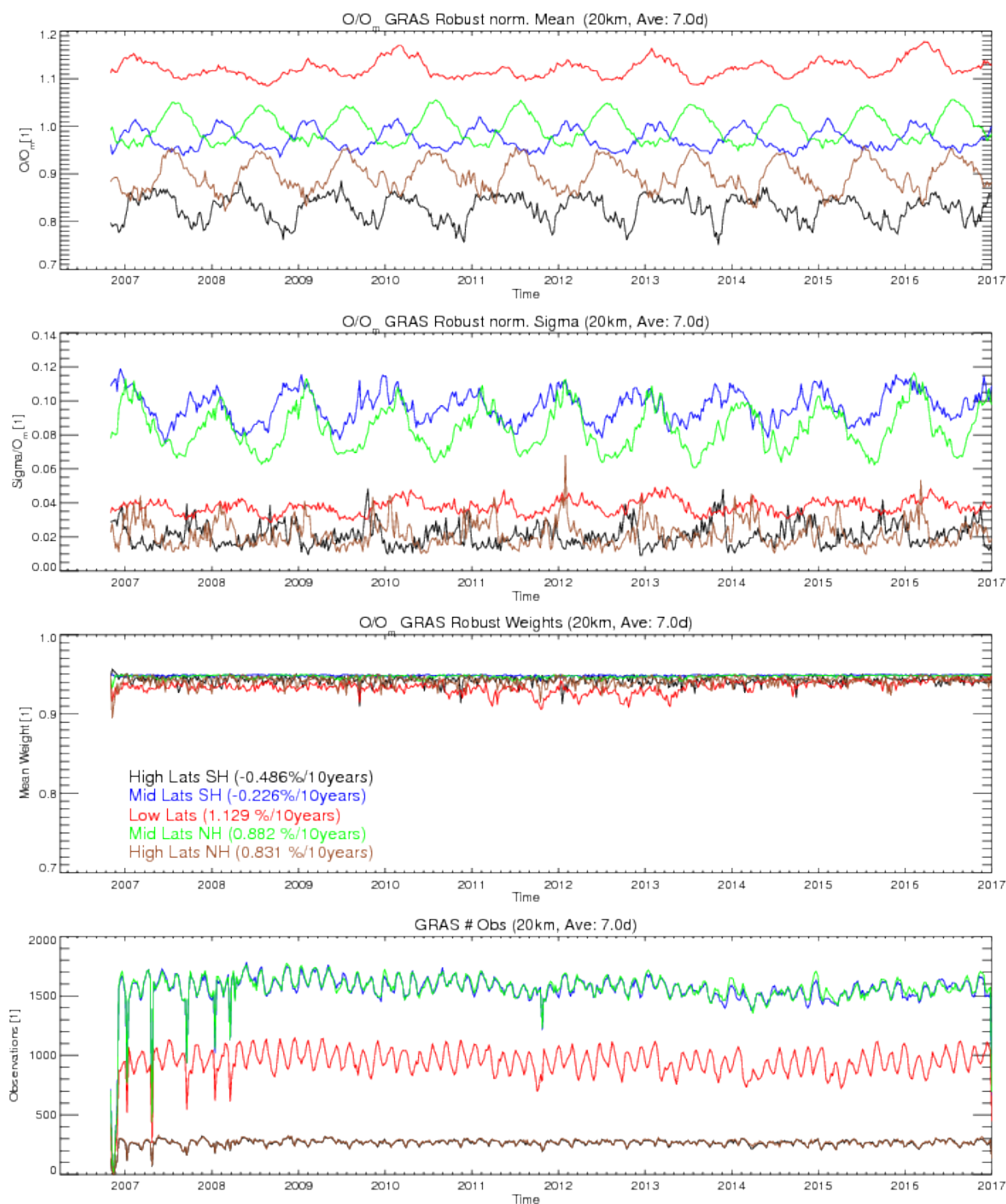
Validation Report - GRAS Level 1b Bending Angle FCDR Release 1


Figure 5 Stability of Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR bending-angle data at 20km, data averaged over 7 days using robust statistics; (top) bias, (middle top) standard deviations, (middle bottom) weight, (bottom) number of occultations per interval, separated for different latitude bands and hemispheres. Note bias, standard deviation normalized to average, global value at this altitude. A simple trends has also been fitted to the through the bias data and is given in legend.

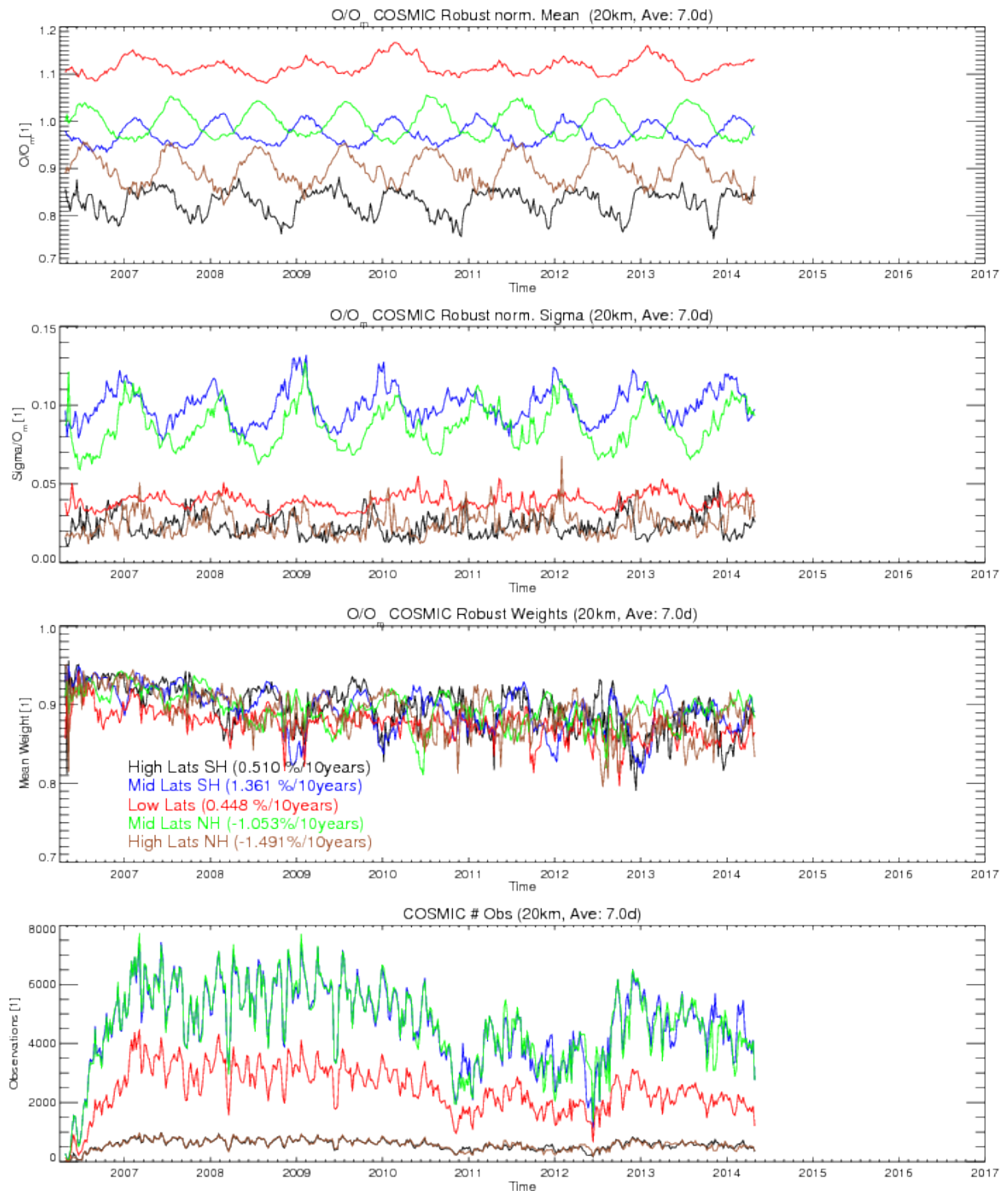
Validation Report - GRAS Level 1b Bending Angle FCDR Release 1


Figure 6 Stability of UCAR COSMIC 2013 bending-angle data at 20km, otherwise as Figure 5.

4.3 Match-up evaluation

Two types of match-up evaluations are performed here for the Metop-A Release 1 – GRAS Level 1b FCDR data from EUMETSAT:

- Match-ups against an occultation from the same instrument but from a different processing centre;
- Match-ups against an occultation from a different instrument, from the same or a different processing centre.

4.3.1 Match-ups with different processing centres

The consistency between the UCAR and EUMETSAT based GRAS/Metop-A processing is shown in Figure 7 and Figure 8. These figures show direct matches (matching the same occultation from the two data sets, thus also determining the impact of structural uncertainty). In total, about 1.8 million profiles are found, essentially almost all of the UCAR provided GRAS/Metop-A occultations are matched (see Table 1). The 0.3% missed occultations are likely not matching the geo-location criteria, thus are more than 300km apart; this can be caused by occultations that terminate higher up in the atmosphere, thus not reaching down to the nominal geo-location point of the respective processing centre. EUMETSAT in that case does not use the nominal SLTA=0km geolocation, but the lowest ray tangent location.

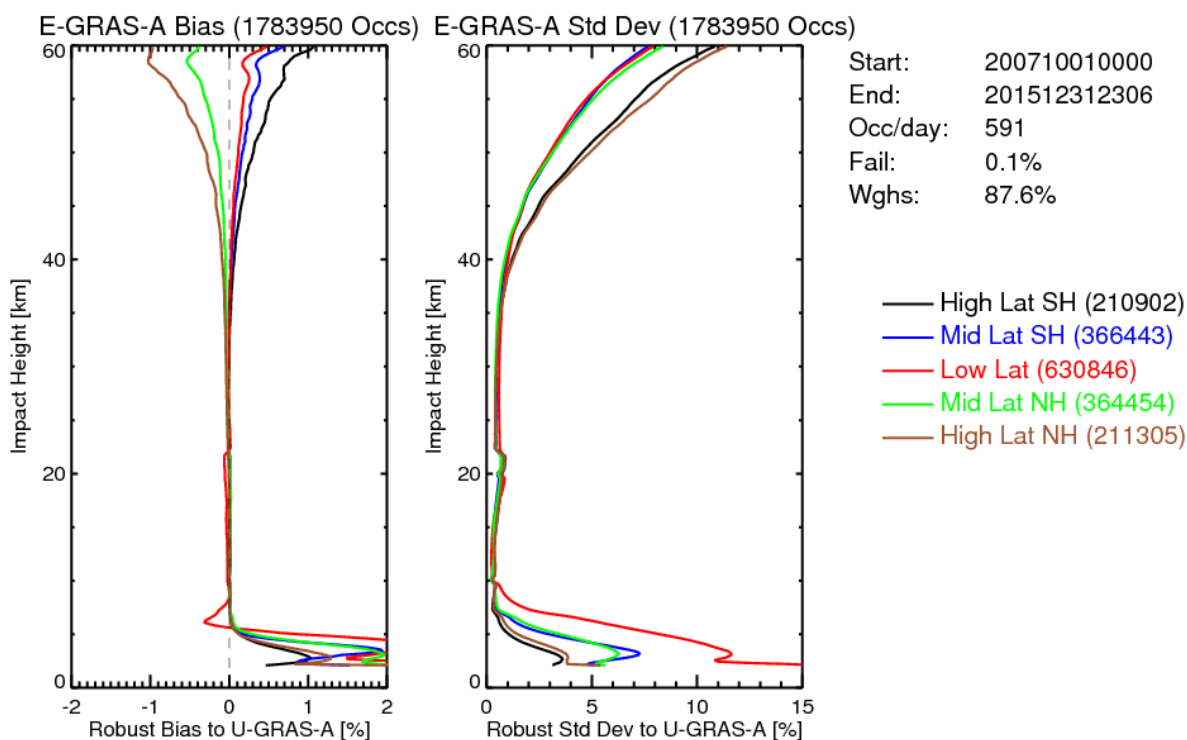


Figure 7 $(O_1 - O_2)/O_2$ matches of Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR with UCAR Metop-A 2016 data for different latitude bands on the Southern (SH) and Northern Hemisphere (NH) using robust statistics; (left) bias, (right) standard deviation, legend gives further information on the data coverage, the average number of matched occultations per day, the number of failures (e.g. if no overlapping data is found), as well as the robustness/weight of the statistics. The total number of occultations entering, as well as per latitude band, is given in brackets in title/legend.

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Figure 7 shows the agreement for all altitudes and different latitude bands and hemispheres. An ideal processing by the two centres (with a structural uncertainty of zero) would lead to a bias and standard deviation of zero, since the two processing streams yield identical results. However, in radio occultation processing, several steps are required to determine the neutral bending-angle profile, e.g. from the POD via the Geometrical Optics (GO) or WO calculation, via the ionospheric correction, different choices for the implementation are made at different processing centres. These different implementation should nevertheless lead to biases around zero, and small standard deviations. The figure shows in particular biases to be near zero for all altitudes and latitudes above about 8 km and below about 40 km. Albeit, around 22km, the switch from GO to WO processing in the UCAR data is visible in bias for low latitude data and standard deviation for all data. Above about 40km, different bias structures are visible which depend on hemisphere, the cause of this bias is under investigation, slight differences in the LEO orbit (as derived by the respective POD) is a potential cause. The bias difference is shown in bending-angle space, a rough estimate of the impact in temperature space shows agreement to be better than 0.1 K above 8 km and below 25 km, and increases above to around 0.5 K at 40 km. Below 8km, the different WO implementation can generate biases that exceed 2%, e.g. for atmospheric conditions with high humidity.

The standard deviation plot shows again in particular the different WO implementations and the transition from WO to GO around 22 km in UCAR GRAS-A data. Above about 40 km, the found increase is likely caused by the different POD and ionospheric correction implementations. Generally, the different latitude bands on the respective hemispheres do though show very similar behaviour.

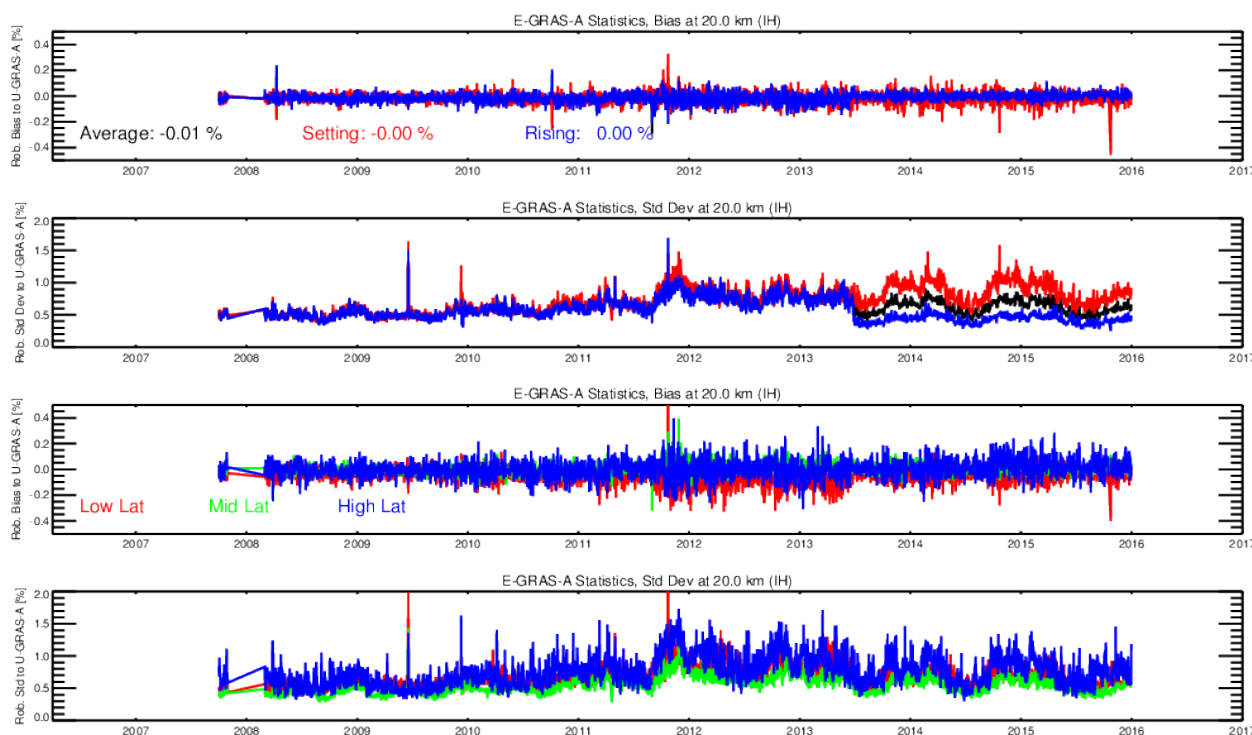


Figure 8 $(O_1-O_2)/O_2$ matches of Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR with UCAR Metop-A 2016 data at 20km, daily averaged using robust statistics; (top) bias, (middle top) standard deviations for all/setting/rising; (middle bottom) bias, (bottom) standard deviations for different latitude bands. Average bias is also given, separated for setting/rising/all.

Figure 8 shows a time-series of the bias and standard deviations from the two processing centres at 20km. The bias data (top) has also been averaged over all times to calculate a mean systematic deviation either of all data or of setting/rising data compared to the mean of all data. Both, bias and mean systematic deviation, are zero, independent of whether this is based on all data, just setting, rising, or the data is split up into latitude bands (top and bottom top plots, note that we did not further separate these kind of plots into hemispheres since the information is very similar to the presented results – albeit the feature in the bias of high latitudes towards the end of the year 2011 can be seen to be mostly driving by the NH and the SH high latitudes show slightly higher noises than NH high latitudes over all times - but the content is generally less clearly visible).

The standard deviation plots (2nd and 4th plot) show several features, the most prominent one starting in June 2013, where rising occultation standard deviations between the two processing centres decreases. This is caused by an instrument on-board software change. From June 2013 both Metop GRAS receivers no longer track the second GPS frequency in rising occultations from -35km SLTA upwards, but only from -5km. This was implemented to allow tracking gaps on the first GPS frequency in the upper troposphere to be filled. If open-loop tracking is performed up to higher SLTA, these closed-loop tracking gaps can be filled. Hence, from June 2013, the EUMETSAT and UCAR processing setup became more similar, leading to the removal of some of the noise introduced in the bending-angle from the L2 frequency processing of the rising occultations⁸ and with this, the structural uncertainty was reduced - it should be noted that this is not an improvement but rather a degradation of the overall data quality since less L2 data is available. The other standard deviation feature is an increased noise level starting in September 2011, which coincides with the Solar Cycle 24 increase. However, when the solar activity of this cycle decreased end 2015, the noise levels are not returning to the lower levels observed before.

Spikes visible in the data are likely caused by the use of daily averages and an insufficient number of available occultations on specific days.

4.3.2 Match-ups with different RO mission/processing

Figure 9 and Figure 10 show 3h / 300km ($O_1 - O_2$)/ O_2 matches between two different radio occultation instruments, the EUMETSAT Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR data and the COSMIC data record reprocessed in 2013. The data are shown either over all altitudes or as a time series at 20km height. Here, about 0.56 million matches were found, or about 200 per day.

Figure 9 shows generally less good agreement in bias between the Release 1 - GRAS Level 1b Bending Angle FCDR and UCAR COSMIC data compared to what was shown in Figure 7. RO data is generally assumed to be calibration free, thus records from different RO instruments can be combined to form a long term observation set for climate analysis. It is thus surprising to find a disagreement in bias for these match-up, since it means that a long term data set, using only UCAR processed COSMIC and GRAS data would also show these different bias characteristics (standard deviations are expected to increase with e.g. instrument errors from two ROs, collocation errors, ...). The found bias difference might be due to the different processing at UCAR (Figure 7 was using the 2016 reprocessed data, while here, only the 2013 COSMIC data is available from UCAR) and also reiterates the importance of a consistently reprocessed data set for re-analysis and climate applications. The visible opposite hemispheric biases at the same latitude band at altitudes above 40km are though still visible, but not as pronounced (e.g. at

⁸ In order to process the occultation data even without an L2 frequency, one needs to extrapolate the L1/2 information from higher up to lower altitudes.

60km, only 1% instead of 2% for high latitudes). As expected, standard deviations are increased since the data is based on different instruments and geo-locations. Otherwise, as in Figure 7, the UCAR transition from WO to GO around 20km is visible again in bias and standard deviations. It is also worth noting that the WO processing in the lower troposphere leads to different biases than found in Figure 7, indicating that the WO processing has been updated between the 2013 and 2016 UCAR versions.

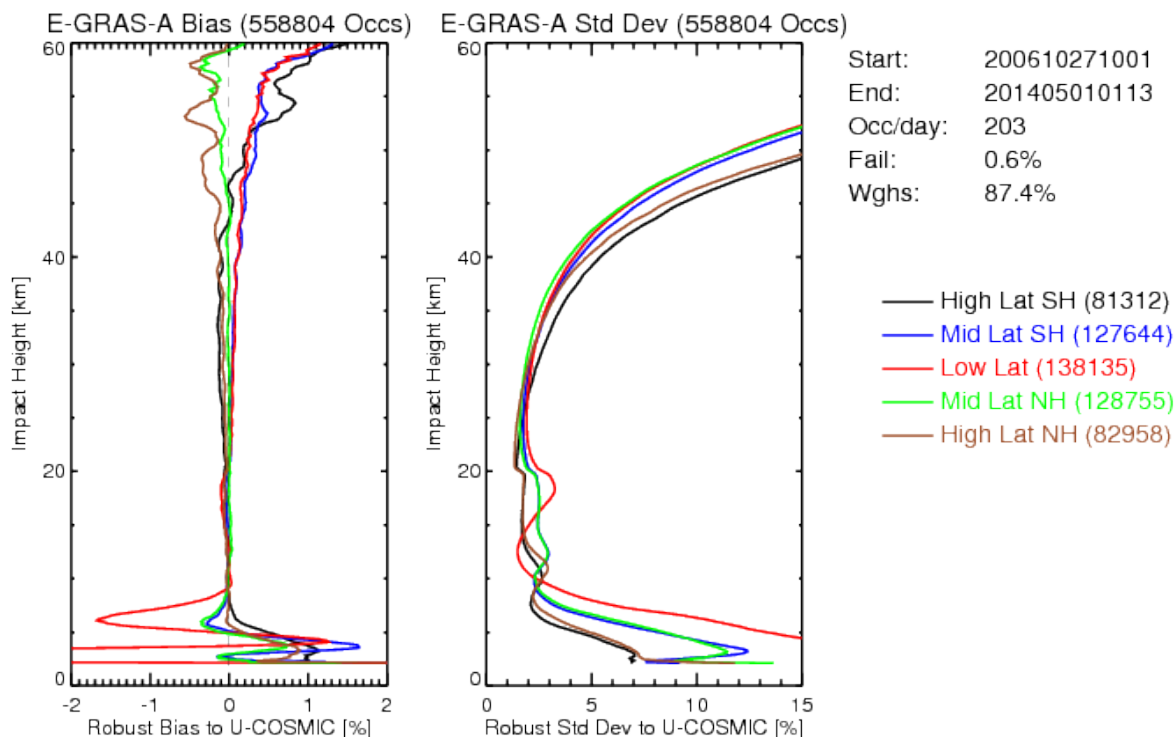


Figure 9 $(O_1-O_2)/O_2$ matches of Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR with UCAR COSMIC 2013 reprocessed data for different latitude bands on the Southern (SH) and Northern Hemisphere (NH) using robust statistics; (left) bias, (right) standard deviation, otherwise as Figure 7.

Figure 10 shows the temporal $(O_1-O_2)/O_2$ statistics for the two instruments. The bias and standard deviations are higher than for matches of the same data (see Figure 8). This might be due to the already mentioned different processing setups (see discussion on Figure 9, the UCAR COSMIC reprocessing s/w is from 2013, while the UCAR GRAS one is from 2016), but also resulting from the different instruments and the uncertainty caused by imperfect collocation. The mean systematic deviation over all times in the data is again zero/very close to zero. It is also interesting to note that the increase in standard deviation visible in Figure 8 around September 2011 is not present in these statistics (actual values are though higher for these matches). Further separation of the latitudinal data into hemispheres does not reveal additional information and was thus avoided to remove clutter.

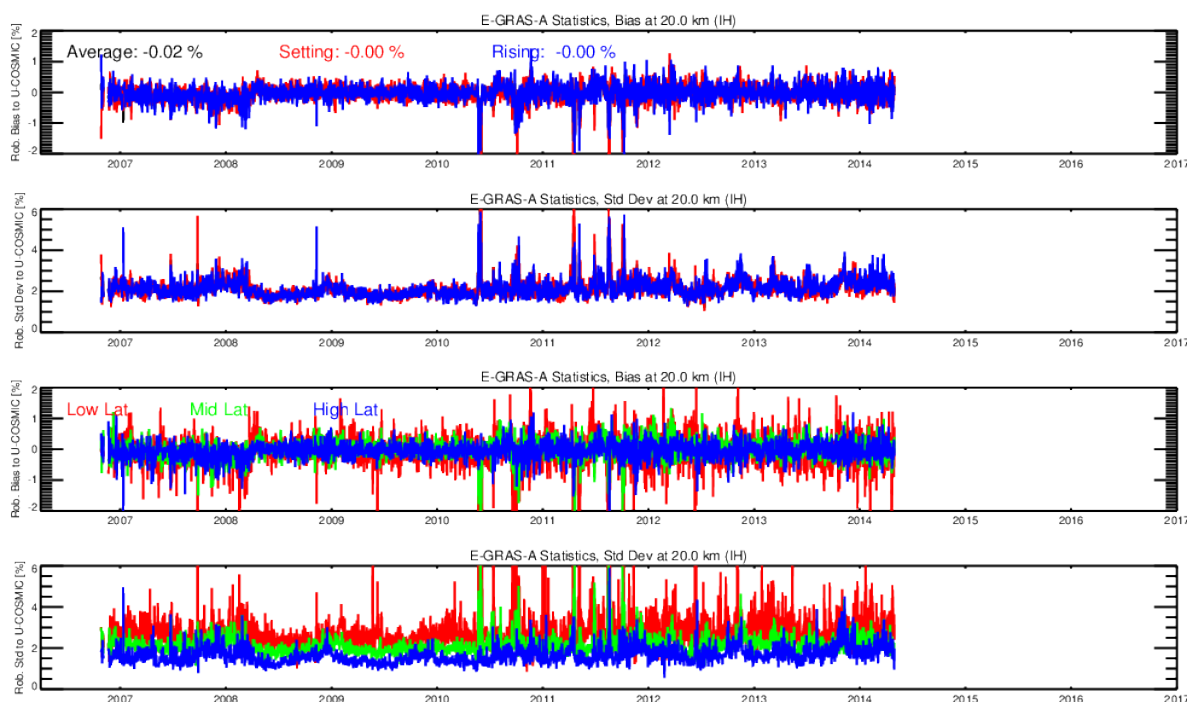


Figure 10 $(O_1 - O_2)/O_2$ matches of Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR with UCAR COSMIC 2013 data at 20km, daily averaged using robust statistics; (top) bias, (middle top) standard deviations for all/setting/rising; (middle bottom) bias, (bottom) standard deviations for different latitude bands. Average bias is also given, separated for setting/rising/all.

4.4 Re-analysis evaluation

Figure 11 and Figure 12 show more detailed $(O-B)/B$ statistics for the Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR data than shown in Figure 3, showing results separated by latitude band over hemisphere (Figure 11) and also time series (Figure 12); again compared to the ERA-Interim ECMWF background. Both plots confirm the high data quality of the GRAS instrument. The different hemispheric biases visible at the same latitude band in Figure 7 at higher altitudes are not seen here, the larger model biases are dominating. Even the very clear signature of high latitude biases in Figure 7 is not seen here, the SH and NH biases are very similar between 50km and 55km. The wiggles visible in Figure 11 bias and standard deviations are caused by the limited vertical resolution of the ERA-Interim data [RD 15].

Figure 11 also indicates in the legend the average number of occultations per day. This is, as said, slightly different to the one given in Table 1 since the statistical processing also checks other errors, e.g. double occultations - very few occultations are accidentally processed twice - whether the neutral bending-angle is available (actually the majority of errors), or whether the altitude range covered in the occultation is < 20km. The numbers in the tables above are derived directly from the coverage interval and the total available occultations.

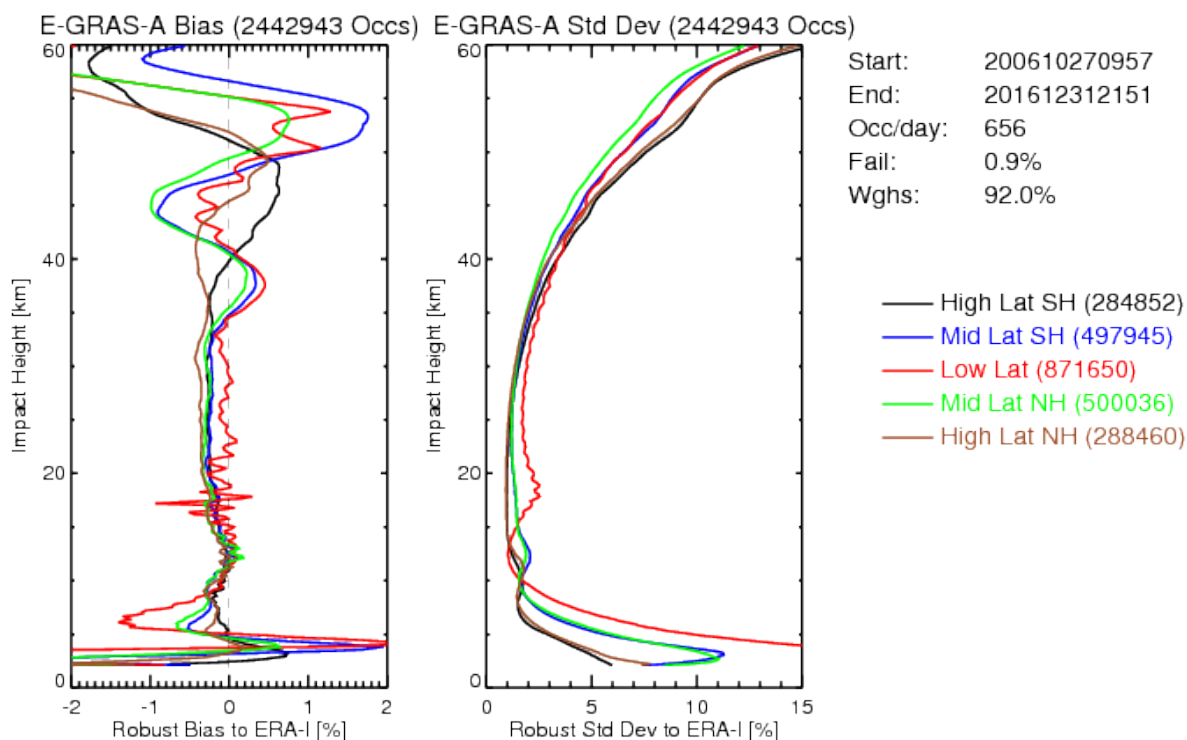


Figure 11 (O-B)/B statistics of EUMETSAT Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR with ERA-Interim data for different latitude bands on the Southern (SH) and Northern Hemisphere (NH) using robust statistics; (left) bias, (right) standard deviation. Otherwise as Figure 7.

Figure 12 shows the time series evaluation at 20km against ERA-Interim data; as expected, the bias is very small and almost constant over the 10+ years of the comparison. An improved impact of RO data (meaning reduced biases of RO vs. ERA-Interim) is though visible in October 2009, this can be traced to an update of the UCAR COSMIC processing on 01 October 2009 that removed a residual bias caused by an incorrect smoothing implementation in their processing [RD 12] - and hence led to better agreement of ERA-Interim data with Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR. Standard deviations are unaffected by this processing update. Figure 12 in addition shows the impact of the accidental removal of all RO data in ERA-Interim at the end of 2013, here in particular the mid- and high-latitude biases show a discontinuity (bottom plot, where the shown hemispheric/latitude band biases spread out more when RO data is not assimilated in late 2013 and early 2014). Again, further separation of the latitudinal data into hemispheres for the whole data period does not reveal additional information and was thus avoided to remove clutter.

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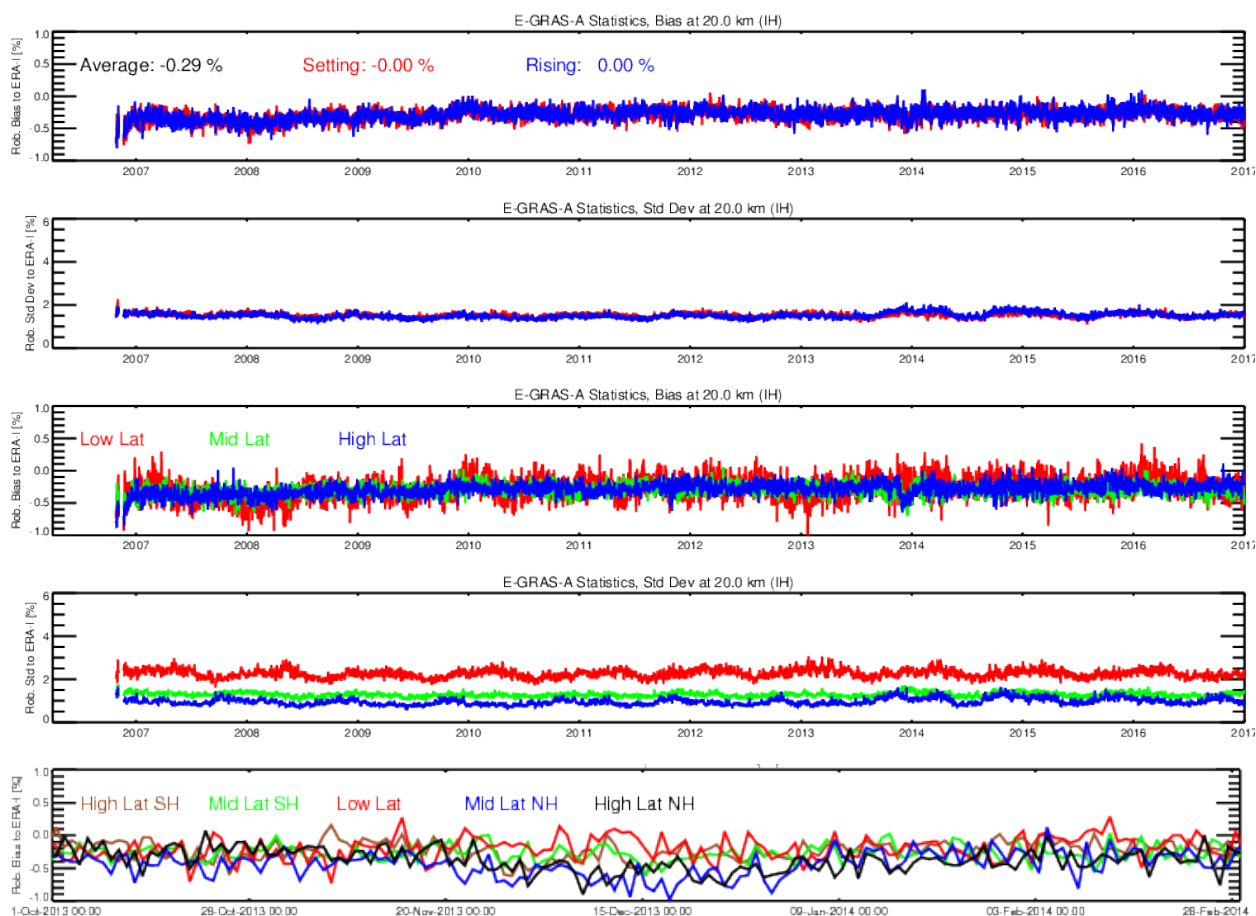


Figure 12 (O-B)/B statistics of EUMETSAT Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR against ERA-Interim data at 20km, daily averaged using robust statistics; (top) bias, (second plot) standard deviations for all/setting/rising; (third plot) bias, (fourth plot) standard deviations for different latitude bands. Average bias is also given, separated for setting/rising/all. The bottom plot shows the 3rd plot with a focus on the period where ERA-Interim did not assimilate RO data end 2013, early 2014, here separated by latitude bands and hemisphere.

5 PRODUCT EVALUATION

5.1 Simple Trend Evaluation

With more than 10 years of Metop-A GRAS data, it is also possible to evaluate bending-angle trends over altitude and different latitude bands. Trends have been calculated for every 2km altitude interval, from 4km impact height to 50km. Seasonal effects have been removed before fitting a robust trend to the data by averaging all individual months of the data set and then subtracting this average from each individual month. Though this is still not a full climate trend evaluation (e.g. the Quasi-Biennial Oscillation (QBO) is not removed from the data), it is a useful validation measure to assess the data quality.

Figure 13 shows these Metop-A GRAS bending-angle trends, expressed as percentage change over 10 years. Generally, in atmospheric regions where water vapour does not contribute much to the bending-angle / refractivity, an inverse relation to temperature changes is found – meaning an increase in temperature will lead to a decrease in bending-angle (and vice versa). The figure also shows some oscillations at lower latitudes in the upper troposphere and the stratosphere, likely the result of not removing the QBO. Within the lower tropospheric altitudes, at low latitudes, trends can be found of up to

5% in GRAS data. These trends are not covered by the shown colour range in order to focus the evaluation on altitudes where RO data has the highest quality. Note also, that neither ERA-Interim nor UCAR COSMIC data reveal such high trends here.

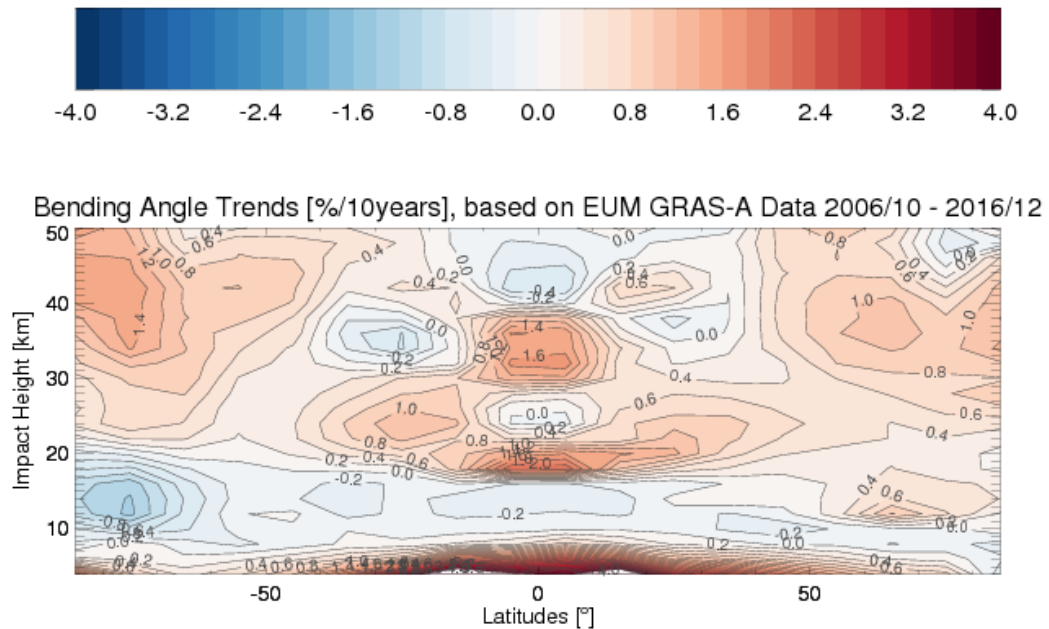


Figure 13 Bending-angle trends of EUMETSAT Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR data, expressed as percentage change over a 10-year interval. Note that low-latitude data in the lower troposphere exceeds the plotted range and is only shown as white.

For validation of the trends, the same trend processing as done for Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR data was also done on collocated ECMWF ERA-Interim bending-angle data, see Figure 14. The ERA-Interim trends are generally very similar to the Release 1 - GRAS Level 1b Bending Angle FCDR based trends, showing also the oscillation pattern at lower latitudes. There are however also slight differences, e.g. the ERA-Interim based data shows a more symmetric trend in the Northern and Southern Hemisphere at about 50° poleward than the GRAS based data. It should though be noted that an evaluation of the number of years to detect a trend within a 90% probability, using the approach outlined in [RD 19], finds that generally more than 20 years are required for altitudes above 40km, thus these numbers need to be evaluated keeping the limited coverage in time. In addition, the lower troposphere at low latitudes does not show such a strong bending-angle trend as visible in the GRAS data.

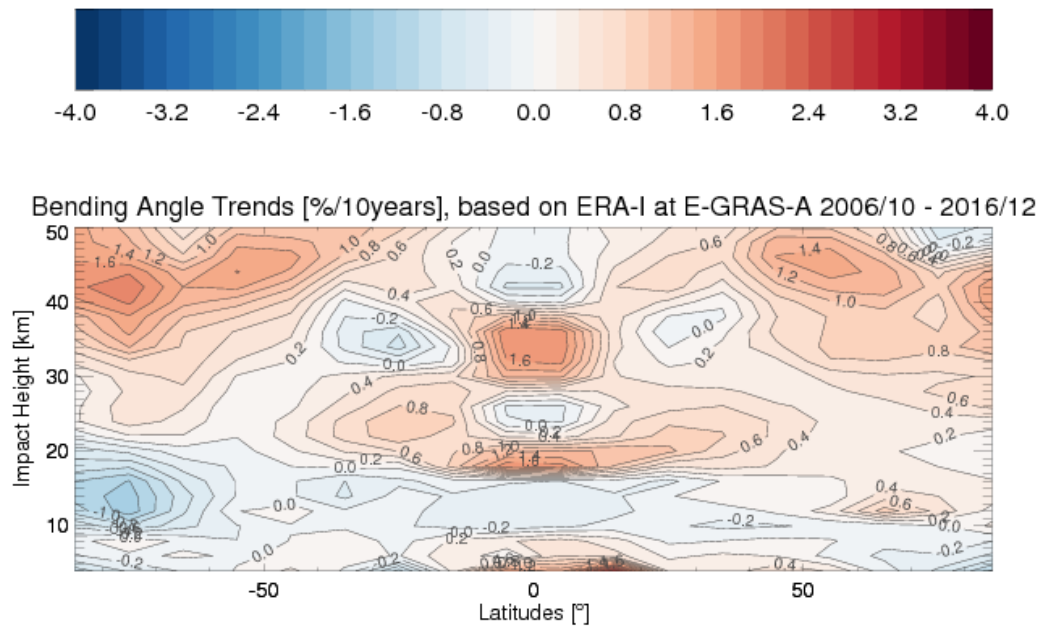


Figure 14 Bending angle trends of ECMWF ERA-Interim bending angle data collocated to the EUMETSAT Metop-A Release 1 - GRAS Level 1b Bending Angle FCDR data, expressed as percentage change over a 10 year interval.

6 SUMMARY AND CONCLUSIONS

This report describes the quality of Release 1 - GRAS Level 1b Bending Angle FCDR. The data record is based on consistent processing of GRAS data from Metop-A over the period 2006–2016. The quality of this release is verified through analysing the reprocessed data record in terms of its global and latitudinal statistics, seasonal and annual trends, inter-comparison with results from other processing centres, as well as evaluating the departures relative to ECMWF ERA-Interim. The main motivations for the generation of Release 1 - GRAS Level 1b Bending Angle FCDR are to reprocess GRAS data using the wave optics based retrieval implemented in the Yaros software, and to obtain a data record of GRAS Level 1b data that has been processed in a consistent manner using the same version of the processor (Yaros version 1.4) for the entire time-series.

The Release 1 - GRAS Level 1b Bending Angle FCDR shows highly consistent data quality for the entire data record. Comparison to UCAR based GRAS processing confirms this high quality. The validation shows that the overall coverage, the number of daily occultations, as well as the penetration to lower altitudes, from this Release is better than from the UCAR based GRAS processing. Time-series analysis revealed that the FCDR is stable in space and time. The statistics presented in section 4 confirm that GRAS level 1b product data characteristics and quality are highly consistent over the entire time-series and over different geographic regions of the Earth. Thus, from a scientific and product point of view, Release 1 - GRAS Level 1b Bending Angle FCDR is ready for official release.

Note that this Validation Report does not further discuss the outcome of the statistical comparison between Level 1b bending angles from the ROM SAF and the EUMETSAT Secretariat, which is presented in the ROM SAF Validation Report [RD 17]. Some of the findings of the ROM SAF Validation Report are though presented here, in particular the different hemispherical biases at the same latitude band when comparing the Release 1 - GRAS Level 1b Bending Angle FCDR against UCAR processed data. The ROM SAF statistical comparison has actually been performed for Level 1b data

from Metop-A and Metop-B. Since Release 1 - GRAS Level 1b Bending Angle FCDR only covers Metop-A data, it was decided to include the more detailed finding of that statistical comparison in the future Validation Report for Release 2 - GRAS Level 1b FCDR. This Release is planned for Q2 2019 and will include GRAS Level 1b data from both Metop-A and Metop-B for the period 2006-2017.

7 ACKNOWLEDGEMENTS

The generation of this data record was partly funded by the ERA-CLIM2 project under the EU-FP7 (Grant Agreement No. 607029).

8 REFERENCES

Reference documents contain additional information related to this document.

<i>Number</i>	<i>Document Name, Reference</i>
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