The EUMETSAT Network of Satellite Application Facilities

ROM SAF

Radio Occultation Meteorology

ROM SAF CDOP-2

Algorithm Theoretical Baseline Document: Level 2A refractivity profiles

Version 1.2

12 August 2016

Danish Meteorological Institute (DMI)
European Centre for Medium-Range Weather Forecasts (ECMWF)
Institut d'Estudis Espacials de Catalunya (IEEC)
Met Office (METO)

Ref: SAF/ROM/DMI/ALG/REF/001

DOCUMENT AUTHOR TABLE

	Author(s)	*Function*	*Date*	*Comment*
Prepared by:	Stig Syndergaard	ROM SAF Scientist	12/08/2016	
Reviewed by (internal):				
Approved by:	Kent B. Lauritsen	ROM SAF Project Manager	12/08/2016	

DOCUMENT CHANGE RECORD

Issue/Revision	*Date*	*By*	*Description*
1.0	28/02/2013	SSY	First version of ATBD for refractivity
1.1	16/03/2016	SSY	Version for PCR-RE1 review. New parts are Sections 2, 3.1, 3.3, 4, 5, 6, and 7.
1.2	12/08/2016	SSY	Updated version after PCR-RE1 review, taking into account RIDs #2, #7, #10, #11, #21, #22, #23, #26, #27, #28, #29.

ROM SAF

The Radio Occultation Meteorology Satellite Application Facility (ROM SAF) is a decentralised processing center under EUMETSAT which is responsible for operational processing of GRAS radio occultation (RO) data from the Metop satellites and radio occultation data from other missions. The ROM SAF delivers bending angle, refractivity, temperature, pressure, humidity, and other geophysical variables in near-real time for NWP users, as well as reprocessed data (Climate Data Records) and offline data for users requiring a higher degree of homogeneity of the RO data sets. The reprocessed and offline data are further processed into globally gridded monthly-mean data for use in climate monitoring and climate science applications.

The ROM SAF also maintains the Radio Occultation Processing Package (ROPP) which contains software modules that aids users wishing to process, quality-control and assimilate radio occultation data from any radio occultation mission into NWP and other models.

The ROM SAF Leading Entity is the Danish Meteorological Institute (DMI), with Cooperating Entities: i) European Centre for Medium-Range Weather Forecasts (ECMWF) in Reading, United Kingdom, ii) Institut D'Estudis Espacials de Catalunya (IEEC) in Barcelona, Spain, and iii) Met Office in Exeter, United Kingdom. To get access to our products or to read more about the ROM SAF please go to: http://www.romsaf.org

Intellectual Property Rights

List of Contents

1. Introduction

1.1 Purpose

This ATBD document describes the algorithms used to derive the refractivity products produced by the Radio Occultation Meteorology (ROM) Satellite Application Facility (SAF). The complete list of products covered by this ATBD is provided in Table 1.1. The current operational status of all these and all other ROM SAF data products is available at the website: http://www.romsaf.org

The product requirements baseline is the PRD version 2.3 [AD.3]. The ATBD software package is based on the ROPP [RD.1].

Table 1.1 List of products covered by this ATBD

Product ID	Product name	Product acronym	Product type	Operational satellite input	Dissemination means	Dissemination format
GRM-01	NRT Refractivity Profile	NRPMEA	NRT Product	Metop-A/ GRAS	GTS EUMETCast Web	BUFR BUFR/netCDF BUFR/netCDF
GRM-09	OFL Refractivity Profile	ORPMEA	Off-line Product	Metop-A/ GRAS	Web	BUFR/netCDF
GRM-29-L2-R-R1	Reprocessed Refractviity Profile	RRPMET	Data Record	Metop Level 1A data from EUM Secretariat	Web	BUFR/netCDF
GRM-30-L2-R-R1	Reprocessed Refractviity Profile	RRPCO1	Data Record	COSMIC Level 1A data from CDAAC	Web	BUFR/netCDF
GRM-32-L2-R-R1	Reprocessed Refractivity Profile	RRPCHA	Data Record	CHAMP Level 1A data from CDAAC	Web	BUFR/netCDF
GRM-33-L2-R-R1	Reprocessed Refractivity Profile	RRPGHA	Data Record	GRACE Level 1A data from CDAAC	Web	BUFR/netCDF
GRM-40	NRT Refractivity Profile	NRPMEB	NRT Product	Metop-B/ GRAS	GTS EUMETCast Web	BUFR BUFR/netCDF BUFR/netCDF
GRM-47	OFL Refractivity Profile	ORPMEB	Off-line Product	Metop-B/ GRAS	Web	BUFR/netCDF

1.2 Applicable and reference documents

1.2.1 Applicable Documents

The following list contains documents with a direct bearing on the contents of this document:

[AD.1] CDOP-2 Proposal: Proposal for the Second Continuous Development and Operations Phase (CDOP-2); Ref: SAF/GRAS/DMI/MGT/CDOP2/001 Version

1.1 of 21 March 2011, approved by the EUMETSAT Council in Ref. EUM/C/72/11/DOC/10 at its 72nd meeting on 28-29 June 2011

[AD.2] CDOP-2 Cooperation Agreement: Agreement between EUMETSAT and DMI on the Second Continuous Development and Operations Phase (CDOP-2) of the Radio Occultation Meteorology Satellite Applications Facility (ROM SAF), approved by the EUMETSAT Council; Ref: EUM/C/72/11/DOC/15 at its 72nd meeting on 28-29 June 2011 and signed on 29 June 2011 in Copenhagen

[AD.3] ROM SAF CDOP-2 Product Requirements Document, Ref. SAF/ROM/DMI/MGT/PRD/001

1.2.2 Reference Documents

The following documents provide supplementary or background information, and could be helpful in conjunction with this document:

[RD.1] The Radio Occultation Processing Package (ROPP) User Guide, Part III: Pre-processor module, Ref. SAF/ROM/METO/UG/ROPP/004

[RD.2] Gorbunov ME (2009) Upgrading of OCC code for operational processing of GRAS raw sampling data. ROM SAF CDOP Visiting Scientist Report 6, Ref: SAF/GRAS/DMI/MGT/CVS06/003

[RD.3] Gorbunov ME (2002) Canonical transform method for processing radio occultation data in the lower troposphere. Radio Sci. 37:1076, doi:10.1029/2000RS002592

[RD.4] Scherllin-Pirscher B, Syndergaard S, Foelsche U, and Lauritsen KB (2015) Generation of a bending angle radio occultation climatology (BAROCLIM) and its use in radio occultation retrievals. Atmos. Meas. Tech. 8:109-124, doi:10.5194/amt-8-109-2015.

[RD.5] Syndergaard S (2012) Deriving bending angle, refractivity, temperature, and pressure using GRAS SAF software. Technical report (WP-2) of Assessment of the Structural Uncertainty of GRAS Products from Level 1B (bending angles) up to Level 2 (temperatures), Danish Meteorological Institute, EUMETSAT Contract No. EUM/CO/10/4600000745/AvE.

[RD.6] Gorbunov ME (2002) Ionospheric correction and statistical optimization of radio occultation data. Radio Sci. 37:1084, doi:10.1029/2000RS002370

[RD.7] Gorbunov ME, Shmakov AV, Leroy SS, Lauritsen KB (2011) COSMIC radio occultation processing: Cross-center comparison and validation. J Atmos Ocean Technol 28:737–751.

[RD.8] Hedin AE (1991) Extension of the MSIS thermosphere model into the middle and lower atmosphere. J. Geophys. Res. 96:1159-1172

[RD.9] Lauritsen KB, Syndergaard S, Gleisner H, Gorbunov ME, Rubek F, Sørensen MB, Wilhelmsen H (2011) Processing and validation of refractivity from GRAS radio occultation data. Atmos. Meas. Tech. 4:2065-2071, doi:10.5194/amt-4-2065-2011

[RD.10] Algorithm Theoretical Baseline Document: Level 1B bending angles, Ref. SAF/ROM/DMI/ALG/BA/001

[RD.11] Algorithm Theoretical Baseline Document: Level 2A dry temperature profiles,

Ref. SAF/ROM/DMI/ALG/TDRY/001
[RD.12] The Radio Occultation Processing Package (ROPP) User Guide, part I: Input/Output module, Ref. SAF/ROM/METO/UG/ROPP/002
[RD.13] WMO FM94 (BUFR) Specification for Radio Occultation Data, Ref. SAF/ROM/METO/FMT/BUFR/001
[RD.14] Syndergaard S, Kursinski ER, Herman BM, Lane EM, Flittner DE (2005) A Refractive Index Mapping Operator for Assimilation of Occultation Data. Mon. Wea. Rev. 133:2650-2668. doi: http://dx.doi.org/10.1175/MWR3001.1
[RD.15] Syndergaard S (2012) Assessment of the Structural Uncertainty of GRAS Products from Level 1B (bending angles) up to Level 2 (temperatures), Final Report, Danish Meteorological Institute, EUMETSAT Contract No. EUM/CO/10/4600000745/AvE.
[RD.16] ROM SAF CDOP-2 Validation Report: Near Real-Time Level 2a Refractivity Profiles: Metop-A (GRM-01, NRPMEA) and Metop-B (GRM-40, NRPMEB), Ref: SAF/ROM/DMI/RQ/REP/001
[RD.17] Gorbunov ME, Lauritsen KB, Rhodin A, Tomassini M, Kornblueh L (2006) Radio holographic filtering, error estimation, and quality control of radio occultation data. J. Geophys. Res. 111:D10105, doi:10.1029/2005JD006427
[RD.18] Zeng Z, Sokolovskiy S (2010) Effect of sporadic E clouds on GPS radio occultation signals. Geophys Res Lett 37:L18817, doi:10.1029/2010GL044561
[RD.19] Sokolovskiy SV (2001) Tracking tropospheric radio occultation signals from low Earth orbit. Radio Sci 36:483-498
[RD.20] Sokolovskiy SV, Schreiner W, Rocken C, and Hunt D (2009) Optimal noise filtering for the ionospheric correction of GPS radio occultation signals. J. Atmos. & Oceanic Tech. 26:1398-1403, doi:10.1175/2009JTECHA1192.1
[RD.21] Algorithm Theoretical Baseline Document: Level 3 gridded data, Ref. SAF/ROM/DMI/ALG/GRD/001

1.3 Acronyms and abbreviations

ATBD	Algorithm Theoretical Baseline Document
BA	Bending Angle
BAROCLIM	Bending Angle Radio Occultation Climatology
CDAAC	COSMIC Data Analysis and Archive Center
CDOP-2	Second Continuous Development and Operations Phase
COSMIC	Constellation Observing System for Meteorology, Ionosphere, and Climate
CL	Closed Loop
DMI	Danish Meteorological Institute
ECF	Earth Centered Fixed
ECI	Earth Centered Inertial
ECMWF	European Center for Medium-range Weather Forecast
EDC	EUMETSAT Data Centre (former UMARF)
EGM96	Earth Gravitational Model
EPS	EUMETSAT Polar satellite System
EUMETSAT	EUropean organisation for the exploitation of METeorological SATellites

GMST	Greenwich Mean Sidereal Time
GNSS	Global Navigation Satellite System
GO	Geometric Optics
GPS	Global Positioning System (US)
GRAS	GNSS Receiver for Atmospheric Sounding (Metop instrument)
IEEC	Institut d'Estudis Espacials de Catalunya (Spain)
LEO	Low Earth Orbit
Metop	Meteorological Operational Polar satellite (EPS/EUMETSAT)
MSIS	Mass Spectrometer and Incoherent Scatter
MSL	Mean Sea Level
NCO	Numerically Controlled Oscillator
NIMA	National Imagery and Mapping Agency
NRT	Near-Real Time
NWP	Numerical Weather Prediction
OL	Open Loop
OLC	Optimal Linear Combination
RMS	Root Mean Square
RO	Radio Occultation
ROM SAF	Radio Occultation Meteorology SAF (EUMETSAT), former GRAS SAF
ROPP	Radio Occultation Processing Package
RS	Raw Sampling
SAF	Satellite Application Facility (EUMETSAT)
SLTP	Straight-Line Tangent Point
SNR	Signal-to-noise ratio
UKMO	The UK Meteorological Office (aka: Met Office)
WGS84	World Geodetic System
WMO	World Meteorological Organisation
WO	Wave Optics

1.4 Definitions

RO data products from the GRAS instrument onboard Metop and RO data from other missions are grouped in *data levels* (level 0, 1, 2, or 3) and *product types* (NRT, Reprocessed, or Offline). The data levels and product types are defined below. The lists of variables should not be considered as the complete contents of a given data level, and not all data may be contained in a given data level.

Data levels:

Level 0: Raw sounding, tracking and ancillary data, and other GNSS data before clock correction and reconstruction;

Level 1A: Reconstructed full resolution excess phases, total phases, pseudo ranges, SNR's, orbit information, I, Q values, NCO (carrier) phases, navigation bits, and quality information;

Level 1B: Bending angles and impact parameters, tangent point location, and quality information;

Level 2: Refractivity, geopotential height, "dry" temperature profiles (level 2A), pressure, temperature, specific humidity profiles (level 2B), surface pressure, tropopause height, planetary boundary layer height (level 2C), ECMWF model level coefficients (level 2D); quality information;

Level 3: Gridded or resampled data, that are processed from level 1 or 2 data, and that are provided as, e.g., daily, monthly, or seasonal means on a spatiotemporal grid, including metadata, uncertainties and quality information.

Product types:

NRT product: Data product delivered less than 80 min (95%; EPS-SG Global), 40 min (95%; EPS-SG Regional) and 3 hours (EPS) after measurement;

Reprocessed product: Climate Data Record (CDR) covering an extended time period of several years, generated using a fixed set of processing software in order to provide a homogeneous data record appropriate for climate usage;

Offline product: Data product which typically extends a CDR from a reprocessing, thus providing an "interim" CDR; delivered from less than 5 days to up to 6 months after measurement depending on the requirements.

2. Algorithm overview

RO data may potentially have benchmarking quality for climate analyses because of the all-weather capability of the technique and because there is no need for calibration (as opposed to many other remote sensing instruments). However, RO processing is generally complex, not the least because different RO missions have different problems (such as low SNR, poor L2 tracking, data gaps, spikes, etc). Thus, besides the processing steps that can be easily described by equations, it is necessary to also have algorithms that can cope with a number of problematic issues. The algorithms in the Radio Occultation Processing Package (ROPP) have been developed over many years to do just that.

ROPP contains a module designed to compute ionospheric corrected bending angle, refractivity, and dry temperature profiles either from excess phase or L1 and L2 channel bending angle data measured during a radio occultation. A flow chart illustrating the ROPP pre-processor module is given in Figure 2.1. The main aspects of the algorithm for the level 2A refractivity are described in the ROPP pre-processor user guide [RD.1].

The algorithm description in this ATBD complements the ROPP user guide by focusing on details not described in the user guide or elsewhere. References to equations and sections in the user guide are provided when appropriate. Many of the algorithms in the ROPP pre-processor module are also described in [RD.2]. References to original work on which algorithms are based are provided in the relevant sections.

In the descriptions in the following, the specific choices of parameters that affect the outcome of the processing is mentioned, such as filter widths, intermediate and output vertical grids, limits and parameters determining specifics in the processing at various stages, interpolation methods, etc. The values mentioned in this ATBD are the values that are either hard-coded in the software or set in a configuration file in the ROM SAF processing. Although these choices have influence on the results, and contribute to the structural uncertainty of the products, they are not considered to have any negative impact on the products and they do not compromise the benchmarking quality of the data.

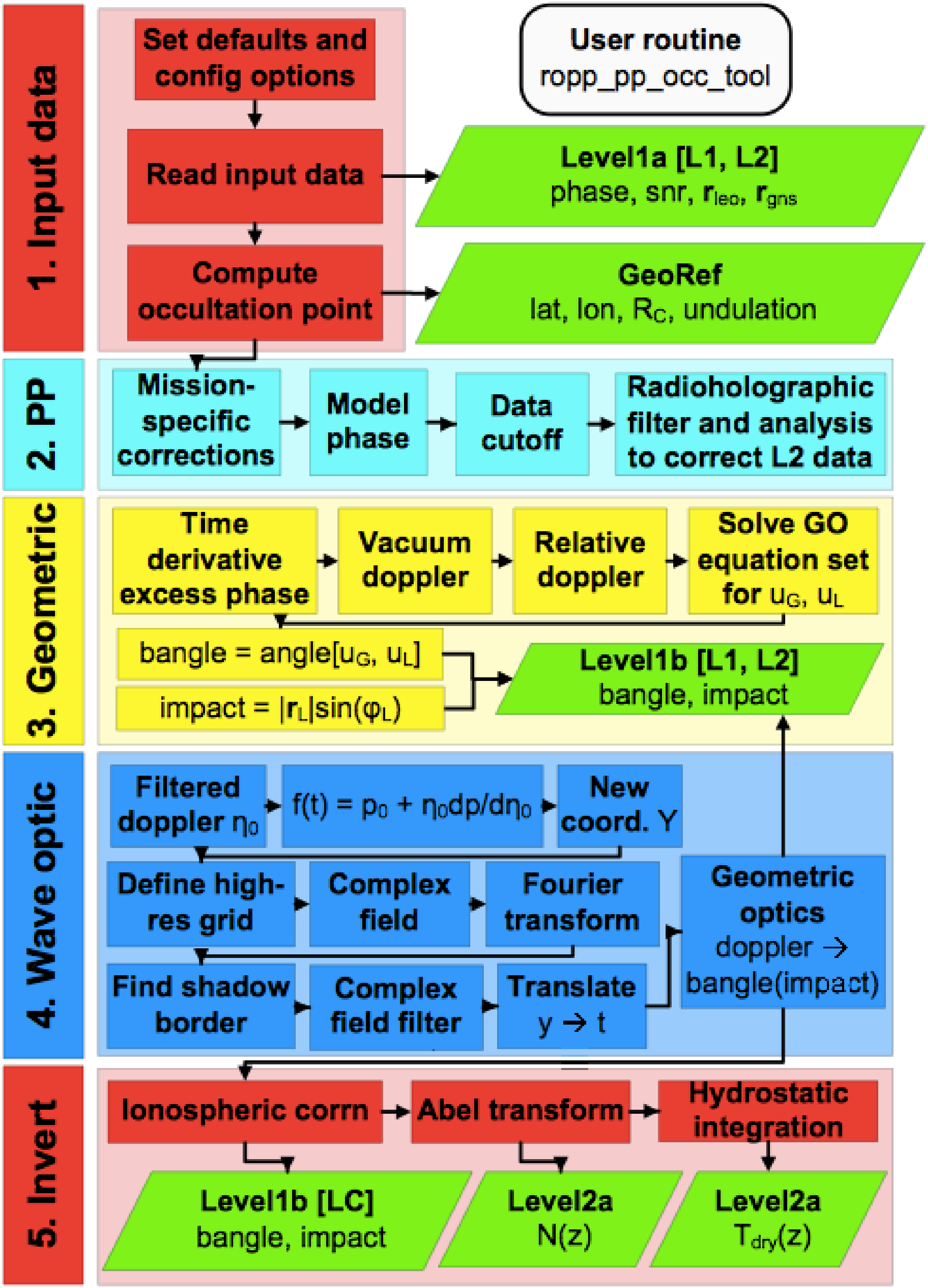

Figure 2.1 Flow chart illustrating calling tree of the ROPP pre-processor occ tool to compute ionospheric corrected bending angle, refractivity, and dry temperature profiles from input L1 and L2 channel amplitude and phase measurements [RD.1].

3. Algorithm description

3.1 Physics of the problem

3.1.1 Fundamental observables

The fundamental observables measured by an RO instrument are the phase, L_i, and amplitude, A_i, of the Doppler-shifted incoming signal. Index i denotes one of the two GNSS frequencies L1 (1575.42 MHz) and L2 (1227.60 MHz). Each occultation measurement is a time-series of measured phases and amplitudes as well as precise position information for the transmitter (GNSS) satellite and the receiver (LEO) satellite.

3.1.2 Doppler-shift and derived quantities

The received signal will be Doppler-shifted due to the motion of the transmitter and receiver satellites. With known satellite positions and velocities this Doppler-shift may be calculated to high precision for the vacuum case. When the ray bends in the atmosphere the angles between the ray path and the directions of motion change both for the transmitting and the receiving satellite. This leads to a change in the observed Doppler-shift. From observed signal phases the observed Doppler-shift may be found and from this the bending of the ray path through the atmosphere may be derived. This leads to a profile of bending angles as a function of impact parameter. Via the Abel transform the profile of bending angles as a function of impact parameter is converted to a profile of atmospheric refractive index as a function of altitude. For convenience results are given in terms of the refractivity N instead of the refractive index n, with refractivity defined by $N = 10^6(n\text{-}1)$.

3.1.3 Ionospheric correction and statistical optimization

The bending of a ray passing through the atmosphere consists of a contribution from free electrons in the ionosphere, and a contribution from neutral species in the denser stratosphere and troposhere. The ionospheric contribution has a well-understood dependence on frequency whereas the neutral-atmospheric bending is approximately the same for the L1 and L2 frequencies. Therefore the presence of both the L1 and L2 signals allows one to disentangle the ionospheric contribution from the ionosphere-free or neutral-atmosphere contribution to the bending. The neutral-atmosphere contribution is the signal of interest in the present application, but in principle the algorithm also delivers the ionospheric signal as output. Because of measurement noise and residual ionospheric disturbances it is necessary to merge the measured bending angle with a very smooth background profile (usually from a climatology) at high altitudes (above some 40 km). This is referred to as statistical optimization.

3.2 Mathematical description of the algorithm

Given profiles of high-resolution L1, L2, and LC bending angles at equidistant impact parameter levels (cf. Section 3.2 in [RD.10]), the following subsections describe the steps taken to obtain the refractivity as a function of altitude above the geoid.

3.2.1 Background profile for statistical optimization

As a first step toward determining a background profile for the statistical optimization (cf. Section 3.1.3), a global search through a spectral representation of bending angles constructed from the BAROCLIM model [RD.4] is performed. The search goes through every month and every 10° latitude in the model (a total of 12x18=216 profiles). Each of these BAROCLIM bending angle profiles are compared with a smooth version (smoothed with a window corresponding to about 3 km; on a 100 m equidistant vertical grid) of the ionospheric corrected bending angle between 40 and 60 km. The BAROCLIM bending angle profile with the best least squares fit (smallest RMS residual) is chosen to be modified to fit the ionospheric corrected bending angle even better (described in the next paragraph).

As a second step toward determining a background profile for the statistical optimization, the chosen BAROCLIM bending angle profile as a function of impact height is scaled by slightly different factors below 40 km and above 60 km, with a gradual transition in between. The mathematical details are described in [RD.5]. The resulting profile will in the following be referred to as the background profile. The scaling factors are found by linear regression as those which results in the closest fit between 40 and 60 km. Usually the scaling factors are close to unity, but in cases of erroneous data, they can be off by large factors, and are therefore used as an additional quality check.

3.2.2 Dynamical error estimation

The principles of the dynamic error estimation for the statistical optimization are outlined in [RD.6] (cf. Section 4.5.2 in [RD.1]). The error estimation is based on certain vertical intervals. The upper limit that is used for the error estimation is determined as follows: First, the mean, μ, and standard deviation, σ, of the L1 and L2 bending angle difference between 12 and 50 km is computed. The L1-L2 bending angle difference, ε, at any point above 50 km is considered too large if it is more than six standard deviations from the mean:

- if $\varepsilon - \mu > 6\sigma$ is found above 75 km, the upper limit is set to 70 km;
- if $\varepsilon - \mu > 6\sigma$ is found between 70 and 75 km, but not above, the upper limit is set to 65 km;
- if $\varepsilon - \mu > 6\sigma$ is found between 65 and 70 km, but not above, the upper limit is set to 60 km;
- if none of the above, the limit is set to 80 km;

The background profile is subtracted from the L1 and L2 bending angles, and the a priori ionospheric bending angle (smooth difference between L1 and L2 bending) is calculated using a sliding polynomial filter of degree three, and with a window width of about 2 km (Eq. 4.7 in [RD.1]).

The L1 and L2 bending angle noise (observation error) at high altitudes is estimated as the mean between 50 km and the upper limit, again using a sliding polynomial filter of degree three, and with a window width of about 2 km (Eq. 4.8 in [RD.1]). The estimate of the error of the a priori ionospheric bending angle is also based on a mean between 50 km and the upper limit (Eq. 4.9 in [RD.1]). The estimate of the error of the background profile is based on a mean between 12 and 35 km (Eq. 4.10 in [RD.1]).

3.2.3 Correction for L2 outliers below 12 km

The L2 bending angle is dismissed below a given height if the ionospheric bending angle starts becoming excessively large somewhere below 12 km. The particular threshold is that the difference between the ionospheric bending angle below 12 km and a smoothed version of the ionospheric bending angle taken at 14 km must not become larger than ten times the standard deviation of mean ionospheric bending angle noise estimated between 12 and 35 km. If it does (which probably happens rarely), the L2 bending angle is effectively dismissed below the point where this happens. Additionally, the lowest 3 km of the L2 bending angle is dismissed. Below the (new) lowest point, the ionospheric corrected bending angle, coming out of the OLC algorithm (see next paragraph), is augmented with the L1 bending angle corrected for the ionospheric bending taken at the (new) lowest point (equivalent to L2 extrapolation maintaining a constant offset between L1 and L2 bending angles below).

3.2.4 Optimal Linear Combination (OLC)

The neutral atmospheric (statistically optimized) bending angle is given by optimal linear combination (OLC) [RD.6]. The OLC is solving a set of linear equations involving the L1 and L2 bending angles, the background profile, and the a priori ionospheric bending as determined above, as well as the estimated variances (Eqs. 2.40 - 2.41 in [RD.1]). The outcome is referred to as the OLC bending angle.

Above the top of the profile (uppermost data point), the OLC bending angle is augmented by the background profile up to 150 km. The combined profile is used later in the processing to refractivity, and will be referred to as the augmented OLC bending angle profile.

3.2.5 Abel Transform

The augmented OLC bending angle profile is put through the Abel transform (Eq. 2.45 in [RD.1]) to obtain the refractive index and subsequently the refractivity as a function of impact parameter. With the Abel transform, the refractive index profile, $n(r)$, is given by

$$n(r) = \exp\left[\frac{1}{\pi}\int_x^\infty \frac{\alpha(a)}{\sqrt{a^2 - x^2}}\,da\right],$$

where α is the bending angle, a is the impact parameter, and $r = a/n(r)$. The Abel transform is implemented as a sum of contributions, assuming that bending angle varies linearly in between impact parameter levels (Eqs. 4.13 - 4.14 in [RD.1]). The level separation is equidistant and ~100 m.

3.2.6 Upper boundary condition

Above 150 km, the contribution to the Abel integral is determined by an expression assuming that the bending angle falls off exponentially to infinity with a constant scale height (Eq. 4.15 in [RD.1]). This is referred to as asymptotic correction. The scale height is determined from the uppermost 3/4 of the profile by a simple difference between the logarithm of the bending angle at 150 and 115 km (equivalent to the mean slope of the logarithm of bending angle in this interval).

3.2.7 Conversion to Mean Sea Level (MSL) altitude

The altitude above the WGS84 ellipsoid is determined by the refractive index at a given impact parameter and the Earth's radius of curvature in the occultation plane (Eq. 2.3 in [RD.1]). The Mean Sea Level (MSL) altitude is calculated by subtracting the undulation. The undulation is based on the NIMA EGM96 geoid coefficients with respect to the WGS84 ellipsoid. These are in the form of geoid potential and correction coefficients to order and degree 360. The coefficients are expanded as Legendre polynomials and applied to the reference location of the occultation.

3.3 Error sources

As a general consideration, the radio occultation signal consists of an excess phase and an amplitude. High-quality data is data with high SNR both in terms of amplitude and in terms of excess phase.

Amplitude noise is dominated by instrument noise under quiet ionospheric conditions. However, in the presence of ionospheric disturbances, or tilted sporadic E-layers, it can be severely affected by scintillations [RD.18]. Under quiet conditions the SNR is generally high except in the middle to lower troposphere, where the denser atmosphere leads to loss of signal intensity. This is particularly true when the humidity is high, which typically occurs in the tropics [RD.19]. This results in degraded bending angle data quality in the lower to middle troposphere, particularly in the tropics.

Besides instrument noise, the measured excess phase is affected by residual ionospheric noise [RD.20]. The ionospheric contribution to the signal is not fully removed by the linear combination of the L1 and L2 signals due to short timescale ionospheric variation and other higher order effects. Since the measured excess phase signal is a function of atmospheric density it falls off approximately exponentially with impact height and so the noise comes to dominate the signal at high altitudes in the upper stratosphere and above. In the lower troposphere the tracking of the L2 signal becomes difficult and for that reason only the L1 signal is useful. This limits the accuracy of derived products.

The highest data quality is therefore found at intermediate altitudes of the higher troposphere to lower stratosphere, where the signal is strong both in terms of amplitude and in terms of excess phase.

Above a certain altitude in the upper stratosphere to lower mesosphere (depending on the noise level) the retrieved refractivity is based on a merge between observations and a climatology (see also [RD.21]). The implementation of the global search and fitting procedure (Section 3.2.4) should ensure a very little bias influence from the climatology.

4. Practical considerations

4.1 Validation method

As a whole, the algorithms will be used to process a number of occultation observations, which are then compared to the corresponding profiles extracted from ECMWF analyses and forecasts (forward modelled to refractivity as a function of altitude above the geoid). The refractivity profiles based on input data from CDAAC will also be compared to the corresponding refractivity profiles produced by CDAAC.

As the refractivity is derived from the bending angle, the validation of all parts of the processing chain from bending angle to refractivity is relevant to ensure the quality of the refractivity. Many parts of the algorithms described here together with those described in [RD.10] and [RD.11], have been validated over many years, as similar versions of the algorithms have been used to produce results for scientific publications and reports (see [RD.2], [RD.3], [RD.7], [RD.9], [RD.15], and [RD.17]).

Certain parts have been modified over the past few years in the version of ROPP at DMI. These parts include an improvement to the search and fitting strategy to find a suitable background for the statistical optimization and the development and inclusion of the BAROCLIM model (Section 3.2.4). These modifications were validated by comparisons to data produced by the unmodified code, comparisons against ECMWF analyses, and comparisons to corresponding profiles from CDAAC. The algorithms have also been validated by comparing 'raw' and optimized bending angles. The latter approach is an efficient way to evaluate to which extent a potential bias from the climatology affects the retrievals. The generation and the validation of BAROCLIM for its use in radio occultation retrievals (though with a different search and fitting strategy than the one used here) can be found in [RD.4].

4.2 Quality control and diagnostics

The following quality control parameters are used to ensure the quality of the refractivity products:

L2 quality score:

> Measures the quality of the L2 signal. This score is defined as the maximum of an L2 penalty function over the interval 15 km - 50 km (see [RD.10]).

SO quality score:

> This is based on the estimated profile of error variances of the bending angle solution (see section 2(e) of [RD.7]), and is estimated after the performance of statistical optimization. This variance estimate has two terms: One term is from the statistical optimization and ionospheric correction procedure and measures the quality of the match between the data and the fitted background profile. The second term is a radioholographic error variance on the L1 signal (from the CT2 wave-optics processing; see [RD.10]), which is a measure of the noisyness of the L1 signal. The SO quality score is constructed as the maximum over the entire profile of the square root of the solution bending angle variance estimate taken as a percentage of the solution bending angle.

Both quality scores are constructed such that a low value means high quality data.

Scaling factors:

The fitting of the background profile to the data at high altitudes results in two scaling factors. Usually the scaling factors are close to unity, but in cases of erroneous data, they can be off by large factors, and are therefore used as an additional quality check.

Quality scores and scaling factors are generated at different places in the code when the relevant parameters to generate them are readily available. The quality scores and scaling factors are output together with the data and are common to bending angle, refractivity, and dry temperature products. If any of the quality scores or scaling factors exceeds defined thresholds, all three products are considered to have poor quality and marked as non-nominal.

As a final sanity check, the refractivity is compared to the corresponding profile extracted from the ECMWF analysis (forward modeled to refractivity as a function of altitude above the geoid). If the refractivity fails this sanity check (if the difference is outside defined thresholds), the level 2A data is marked as non-nominal.

4.3 Exception handling

N/A

4.4 Outputs

The output of the processing to refractivity is a ROPP NetCDF file containing the following profile variables:

- Altitude above the geoid
- Geopotential height
- Refractivity

The same NetCDF file contains the output from the bending angle [RD.10] and dry temperature [RD.11] processing. A more complete and technical description of the output to the NetCDF file can be found in [RD.12].

The above-mentioned variables are also written to a BUFR file [RD.13].

5. Assumptions and limitations

5.1 Assumptions

5.1.1 Spherical symmetry

Radio occultation data are generally processed under the assumption of spherical symmetry. However, in principle this is only an apparent assumption because it depends on the interpretation of the retrieved profiles. If profiles are interpreted as representing the vertical structure in the atmosphere at a given fixed location, then the spherical symmetry assumption gives rise to a real error because the atmosphere is only approximately spherically symmetrical. If, on the other hand, retrieved profiles are interpreted as being weighted averages of the 3-dimensional (3D) atmosphere (primarily in the 2-dimensional (2D) occultation plane), the spherical symmetry assumption does not in principle give rise to any errors. This is why it could be an advantage to assimilate occultation data with 2D or 3D observation operators. A 3D observation operator for refractivity assimilation has been developed in [RD.14].

5.2 Algorithm limitations

The following subsections discuss limitations in the algorithms described in the corresponding subsections with the same titles in Section 3.2.

5.2.1 Dynamical error estimation

The dynamical error estimation results in a different weighting of the observations versus background in the statistical optimization for different occultations, which in turn gives differences in how far down into the stratosphere the background profile (climatology) is weighted significantly. An alternative approach (though not implemented in ROPP) would be to use a fixed (common for all observations) height interval for the transition between the observation and the background profile.

Retrieved refractivity profiles may occasionally (probably only a few times a month per satellite) be very bad with very large errors at high altitudes, with the error in some cases propagating all the way down to the surface. This is most likely related to the dynamical error estimation in combination with ionospheric scintillations at high altitudes (see RD.15]).

5.2.2 Optimal Linear Combination (OLC)

Vertical error correlations in observations and a priori are neglected in the statistical optimization.

6. Description of differences for NRT, Offline and Reprocessing

This chapter describes the parts of the algorithm which are different for NRT, Offline and Reprocessed products.

6.1 NRT

The processing starts from level 1b bending angles by transferring input files to a particular directory in the NRT operational system. The input bending angles are provided by EUMETSAT and are in the operational system pre-screened for cases with no or very few data points. Such input bending angles are then dismissed and not processed further.

Currently the statistical optimization is performed using MSIS [RD.8] instead of BAROCLIM, and the fitting and scaling approach follows that outlined in [RD.9] instead of that outlined in Section 3.2.4. A so-called MSIS bending angle profile is obtained for every month (one representative day), every 10° latitude, and every 20° longitude. A future upgrade of the NRT processing system will use BAROCLIM and the approach outlined in Section 3.2.4.

Currently the code used in the NRT processing is not ROPP, but is a different set of Fortran libraries called OCC. However, the parts of ROPP used for processing radio occultation data was coded from OCC, and the two sets of algorithms and configuration parameters are mostly the same (except for the differences used in the NRT processing as mentioned in this section). In a future upgrade the NRT processing will use the algorithms in ROPP as described in Section 3.

Since the NRT processing is based on input bending angles from EUMETSAT, the quality control (QC) in NRT is different from that described in Section 4.2 (see [RD.16] for a detailed account of the QC in NRT). In a future upgrade of the NRT processing system, the QC for NRT will become more in line with the QC described in Section 4.2.

6.2 Offline

The algorithms used in offline are the same as the algorithms used in reprocessing; it is the algorithms as described in Section 3.

6.3 Reprocessing

The algorithms used in reprocessing are the same as the algorithms used in offline; it is the algorithms as described in Section 3.

7. Appendices

7.1 Description of how to run the code

The code is run by the following command (for offline and reprocessing):

```
ropp_pp_occ_tool <input_file> --no-ranchk -o <output_file> -c
<config_file>
```

The input file is a ROPP NetCDF file containing high-resolution level 1a data. The output file is a ROPP NetCDF file containing high-resolution level 1b and 2a data. An example of a configuration file is given in Section 7.2.

The generation of a BUFR file is done by the following commands:

```
ropp2ropp <input_file> --no-ranchk -o <output_file> -p
<thin_file>
ropp2bufr <input_file> -o <output_file>
```

The input file to the `ropp2ropp` command is a ROPP NetCDF file containing level 1b and 2a data (the high-resolution output of the retrieval). The output file of the `ropp2ropp` command is a ROPP NetCDF file containing thinned level 1b and 2a data. The thinning file is the one provided by EUMETSAT (`ropp_thin_eum-247.dat`). The input file to the `ropp2bufr` command is the NetCDF file containing thinned level 1b and 2a data and the output file is a BUFR file.

7.2 Configuration files

An example of a ROPP PP configuration file is given below. The values of parameters are not necessarily the final ones that will be set in the offline and reprocessing of refractivity.

```
# $Id: $

#****c* Configuration Files/cosmic_pp.cf *
#
# NAME
#    default_pp.cf - COSMIC data configuration file for pre-processor
#                    implementations in ROPP
#
# SYNOPSIS
#    <pp_program> ... -c cosmic_pp.cf ...
#
# DESCRIPTION
#    This file reflects the configuration for the PP
#    implementations within ROPP suitable for use with COSMIC data.
#
# NOTES
#
# AUTHOR
#   Met Office, Exeter, UK.
#   Any comments on this software should be given via the ROM SAF
#   Helpdesk at http://www.romsaf.org
#
# COPYRIGHT
#   (c) EUMETSAT. All rights reserved.
#   For further details please refer to the file COPYRIGHT
```

```
#   which you should have received as part of this distribution.
#
#****

#-------------------------------------------------------------------------------
# 0. Output options
#-------------------------------------------------------------------------------
output_lev1a = .false.      # Flag to output (modified) level 1a data

output_lev1b = .true.       # Flag to output level 1b data

output_lev2a = .true.       # Flag to output level 2a data

output_diag = .false.       # Flag to output additional diagnostics

#-------------------------------------------------------------------------------
# 1. Excess phase to bending angle processing
#-------------------------------------------------------------------------------

# 1.1 Occultation processing method
# ---------------------------------

# GO - use GEOMETRIC OPTICS processing to derive bending angle as a function of
#      impact parameter from excess phase as a function of time.
# WO - use WAVE OPTICS (CT2 algorithm) processing to derive bending angle as a
#      function of impact parameter from excess phase as a function of time.

occ_method = WO

# 1.2 Filtering method
# --------------------

# optest - use OPTIMAL ESTIMATION: solution of integral equation
# slpoly - use SLIDING POLYNOMIAL

filter_method = slpoly

# 1.3 Smoothing bending angle profile
# -----------------------------------


fw_go_smooth = 3000.0   # Filter width for smoothed GO bending angles (m)

fw_go_full  = 3000.0    # Filter width for full resolution GO bending angles (m)

fw_wo = 2000.0           # Filter width for wave optics bending angle above 7
km(m)

fw_low = -1000.0           # Filter width for wave optics bending angle below 7
km (m)

# 1.4 Maximum height for wave optics processing
# ---------------------------------------------

hmax_wo = 25000.0      # Maximum height for wave optics processing (m)

# 1.5 Data cut-off limits
# ----------------------

Acut     = 0.0        # Fractional cut-off limit for amplitude

Pcut     = -2000.0        # Cut-off limit for impact height

Bcut     = 0.1       # Cut-off limit for bending angle
```

```
Hcut     = -250000.0     # Cut-off limit for straight-line tangent altitude

# 1.6 CT2 options
# ---------------

CFF      = 3        # Complex field filter flag (CFF = 'Pa')

dsh      = 200.0    # Shadow border width (m)

# 1.7 Degraded L2 data flag
# -------------------------

opt_DL2  = .true.

# 1.8 Compute and output spectra flag
# -----------------------------------

opt_spectra = .false.

# 1.9 Paths to EGM96 geoid model coefficients and corrections file
# ----------------------------------------------------------------

egm96 = ../data/egm96.dat                # EGM96 coefficients file

corr_egm96 = ../data/corrcoef.dat        # Correction coefficients file

#--------------------------------------------------------------------------------
# 1. Ionospheric correction processing
#--------------------------------------------------------------------------------

# 1.1 Ionospheric correction method
# ---------------------------------

# GMSIS - use MSIS climatology bending angle (searching global MSIS profiles
#          for best fit profile to obs) in ionospheric correction,
#          statistical optimization and bending angle to refractivity inversion.
#
# MSIS - use MSIS climatology bending angle in ionospheric correction,
#         statistical optimization and bending angle to refractivity inversion.
#
# GBARO - use BAROCLIM bending angle (searching global BAROCLIM profiles
#          for best fit profile to obs) in ionospheric correction,
#          statistical optimization and bending angle to refractivity inversion.
#
# BARO - use BAROCLIM bending angle in ionospheric correction,
#         statistical optimization and bending angle to refractivity inversion.
#
# BG   - use climatology from a specified input file containing
#         background temperature, pressure and humidity
#         (e.g. from an NWP analysis). The input filename can be specified
#         using the '-bfile' command line argument or setting 'bfile' (see 1.5).
#
# NONE - linear combination of L1 and L2 bending angles in ionospheric
#       correction, no additional information above observed profile top
#         in the inverse Abel to compute refractivity.

method  = GMSIS                 # Ionospheric correction method

# 1.2 Abel integral method
# ------------------------

# LIN  - assume linear variation of bending angle and ln(n) between
#         observation levels. This algorithm is used in ROM SAF NRT processing
#
# EXP  - assume exponential variation of bending angle and ln(n) between
```

```
#         observation levels. This algorithm is used in ropp_fm module.

abel = LIN

# 1.3 Statistical optimisation method
# -----------------------------------

# SO   - statistical optimisation.
# LCSO  - linear combination plus statistical optimisation.

so_method = so

# 1.4 Climatology model coefficients files
# --------------------------------

msisfile = MSIS_coeff.nc       # MSIS model coefficients file
mfile    = MSIS_coeff.nc       # Model coefficients file for stat.opt.

# 1.5 Background model temperature, humidity, pressure file
# ---------------------------------------------------------

bfile    = BG_file.nc       # Background meteorology profile file (method=BG)

#-------------------------------------------------------------------------------
# 2. Impact parameter grid
#-------------------------------------------------------------------------------

# The ionospheric correction interpolates L1 and L2 bending angle profiles onto a
# standard grid.

dpi = 100.0         # Step of standard impact parameter grid (m)

#-------------------------------------------------------------------------------
# 3. Smoothing bending angle profile
#-------------------------------------------------------------------------------

# A smoothed bending angle profile is derived compute the fit of observed bending
# angles to the model bending angle profile.

np_smooth = 3       # Polynomial degree for smoothing regression

fw_smooth = 1000.0      # Filter width for smoothing profile

#-------------------------------------------------------------------------------
# 4. Model bending angle profile fit to observations
#-------------------------------------------------------------------------------

# To avoid systematic deviations from the observed profile with climatology,
# the model profile is scaled to the observed profile by a fitting method.

sf_method = convoluted  # Search and fit method (convoluted or regular)

nparm_fit = 2           # Number of parameters for model fit regression

hmin_fit  = 20000.0     # Lower limit for model fit regression

hmax_fit  = 70000.0     # Upper limit for model fit regression

omega_fit = 0.3         # A priori standard deviation of regression factor

#-------------------------------------------------------------------------------
# 5. Ionospheric correction and statistical optimization
#-------------------------------------------------------------------------------

# The method described by Gorbunov (2002) is implemented to perform ionospheric
```

```
# correction with statistical optimization.

f_width = 2000.0    # Ionospheric correction filter width

delta_p = 20.0             # Step of homogeneous impact parameter grid

s_smooth = 2000.0   # External ionospheric smoothing scale

z_ion = 50000.0            # Lower height limit of ionospheric signal

z_str = 35000.0            # Lower height limit of stratospheric signal

z_ltr = 12000.0            # Lower height limit of tropospheric signal

n_smooth = 11       # Number of points for smoothing (must be odd)

model_err = 0.5         # A priori model error std.dev. (dyn.est. if negative)

#--------------------------------------------------------------------------------
# 6. Bending angle inversion to refractivity
#--------------------------------------------------------------------------------

# The Abel inversion is computed to retrieve refractivity from corrected
# bending angles. The corrected bending angle profile is extended
# using MSIS or BAROCLIM data above the observed profile top.

ztop_invert = 150000.0     # Height of atmosphere top for inversion

dzh_invert = 50.0   # Step of inversion grid above observation top

dzr_invert = 20000.0       # Interval for regression in inversion

#--------------------------------------------------------------------------------
# 7. Tangent point lat-lons
#--------------------------------------------------------------------------------

# Set tp_bending=.true. to update lat-lons accounting for bending

tp_bending = .false.
```