ROM SAF CDOP-2

Validation Report: NRT Level 2b and 2c 1D-Var products (Metop-A: GRM-02,03,04,05) (Metop-B: GRM-41,42,43,44)

Version 1.8

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Danish Meteorological Institute (DMI)
European Centre for Medium-Range Weather Forecasts (ECMWF)
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Met Office (METO)

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DOCUMENT CHANGE RECORD

Issue/Revision	***Date***	***By***	***Description***
Version 1.0	15 Maj 2009	KMK	Initial release for ORR-B. This document serves as validation test result for the cases 2 (see VPR)
Version 1.1	27 Aug 2009	KMK	Intermediate (non-released) version following ORR-B. Implemented RID's: 060, 105, 012, 018, 020, 076, 077, 107, 111, 112, 023, 024, 025, 026, 027, 029, 122, 123, 124, 083, 084, 085, 086, 089, 090, 091, 108.
Version 1.2	08 Mar 2011	SSY	Version for ORR-B closeout February 2011. Updated with figures corresponding to the NRT refractivity upgrade on 01/02/10 (GRM-01 version 1.3); Implemented RID's: 022, 028, 110.
Version 1.3	13 Apr 2011	JKN	Informal non-released version. Implemented Action 2, editorial remarks from ORR-B part 1 close-out.
Version 1.4	30 Apr 2014	JKN	Version submitted for ORR4 and ORR-B-Backlog review.
Version 1.5	20 May 2014	JKN	Version updated prior to ORR4 and ORR-B-Backlog review, according to romsaf_prd_v22-draft.
Version 1.6	23 June 2014	JKN	Updated for ORR4 & ORR-B-Backlog review. Implemented RIDs 019, 022, 024, 025, 026, 034, 035 and 038.
Version 1.7	12 October 2016	JKN	Version updated prior to ORR-8 review, introduction of Wave Optics, based on GS2 test data from September, 2016
Version 1.8	21 October 2016	JKN	Updated version from ORR-8 review. Implemented RIDs 004, 007, 008, 009 and 010. Added discussion about pressure bias under "Open Issues"

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.

List of Contents

1 Introduction

1.1 Purpose of document

This document describes the validation results for the following ROM SAF NRT level 2b and 2c products:

GRM-02	NRT Temperature profile (Metop-A)	NTPMEA
GRM-03	NRT Specific humidity profile (Metop-A)	NHPMEA
GRM-04	NRT Pressure Profile (Metop-A)	NPPMEA
GRM-05	NRT Surface Pressure (Metop-A)	NSPMEA
GRM-41	NRT Temperature profile (Metop-B)	NTPMEB
GRM-42	NRT Specific humidity profile (Metop-B)	NHPMEB
GRM-43	NRT Pressure Profile (Metop-B)	NPPMEB
GRM-44	NRT Surface Pressure (Metop-B)	NSPMEB

The product version number is 1.3. These products are all outputs from the ROM SAF 1DVAR processing using as input the ROM SAF NRT Refractivity Profiles together with ancillary information from ECMWF forecasts. The 1D-Var products are validated against ECMWF analysis. The validation presented in this document is based on NRT refractivity profiles (GRM-01 (Metop A) and GRM-40 (Metop B)) version 1.5. The 1DVAR processing is performed using ROPP software version 8.1 and ROM SAF 1DV code version number 3.1

1.2 Applicable & 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: 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.

[AD.4] ROM SAF CDOP-2 Service Specification, Ref. SAF/ROM/DMI/RQ/SESP/001.

1.2.2 Reference Documents

[RD.1] ECMWF, http://www.ecmwf.int/products/data/technical/model_levels/index.html and http://www.ecmwf.int/research/ifsdocs/DYNAMICS/Chap2_Discretization4.html#961180, -.

[RD.2] Healy, S. B. and Eyre, J. R., Retrieving temperature, water vapor and surface pressure information from refractive–index profiles derived by radio occultation: A simulation study, *Quart. J. Roy. Meteorol. Soc.*, *126*, 1661–1683, 2000.

[RD.3] Healy, S. B., Jupp, A., and Marquardt, C., Forecast impact experiment with GPS radio occultation measurements, *Geophys. Res. Lett.*, *33*, doi: 10.1029/2004GL020 806, 2005.

[RD.4] Holm, E. V. and Kral, T., Flow-dependent, geographically varying background error covariances for 1D-VAR applications in MTG-IRS L2 Processing, ECMWF Technical Memorandum No. 680, 2012.

[RD.5] Kursinski, E. R., Healy, S. B., and Romans, L. J., Initial results of combining GPS occultations with ECMWF global analyses within a 1DVar framework, *Earth Planets Space*, *52*, 885–892, 2000.

[RD.6] Press, W., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P., *Numerical recipes in Fortran – The Art of Scientific Computing*, Cambridge University Press, Cambridge, New York, 2nd edn., 1992.

[RD.7] Randel, W. J., Wu, F., and Gaffen, D. J., Interannual variability of the tropical tropopause derived from radiosonde data and NCEP reanalysis, *J. Geophys. Res.*, *105*, 15.509–15.523, 2000.

[RD.8] ROM SAF, Algorithm Theoretical Baseline Document: 1D-Var Algorithm, SAF/ROM/DMI/RQ/REP/002, -.

[RD.9] ROM SAF, Validation Report: Near Real-Time Level 2a Refractivity Profiles: Metop-A (GRM-01, NRPMEA) and Metop B (GRM-40, NRPMEB), SAF/ROM/DMI/RQ/REP/001, -.

[RD.10] ROM SAF, Report: Levenberg-Marquardt minimisation in ROPP, SAF/GRAS-/METO/REP/GSR/006, 2008.

1.3 Acronyms and abbreviations

API	Application Programming Interface
BG	Background
COSMIC	Constellation Observing System for Meteorology, Ionosphere & Climate
DMI	Danish Meteorological Institute
ECMWF	The European Centre for Medium-Range Weather Forecasts
EPS	EUMETSAT Polar System
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GNSS	Global Navigation Satellite Systems (generic name for GPS, GLONASS and the future GALILEO)
GPS	Global Positioning System (US)
GRAS	GNSS Receiver for Atmospheric Sounding (onboard Metop)
GRAS SAF	Consortium formed to define and prepare the Operational GRAS SAF. Members are DMI (leader), UKMO and IEEC.

GRM	GRAS Meteorology
GO	Geometrical Optics
LEO	Low Earth Orbited
METOP	Meteorological Operational polar satellites (EUMETSAT)
N/A	Not Applicable or Not Available
NRT	Near Real Time
NWP	Numerical Weather Prediction
PFS	Product Format Specifications
PCD	Product Confidence Data
Q/C	Quality Control
RO	Radio Occultation
ROM SAF	The EUMETSAT Satellite Application Facility responsible for operational processing of radio occultation data from the Metop satellites. Members are DMI (leader), UKMO, ECMWF and IEEC.
ROPP	Radio Occultation Processing Package
SAF	Satellite Application Facility (EUMETSAT)
SAG	Scientific Advisory Group
sG	Data set processed with geometrical optics.
STDV	Standard Deviation
sW	Data set processed with wave optics.
TP	Tangent Point
UKMO	United Kingdom Meteorological Office
UTC	Universal Time Coordinated
VAR	Variational analysis; 1D, 2D, 3D or 4D versions (NWP data assimilation technique)
VT	Validation or Verification Time
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 Background

2.1 Refractivity profiles

The starting point for the ROM SAF NRT 1D-Var processing is vertical profiles of atmospheric refractivity as function of geopotential height provided in ROM SAF data products GRM-01 and GRM-40 (level 2a). The validation in this report is based on EUMETSAT PPF 4.4.0 data from the Metop A and Metop B satellites, retrieved in the time period September 1-5 2016 [RD.12]. EUMETSAT PPF 4.4.0 is identical to EUMETSAT PPF 4.4.2, except for some changes in the thinned data. Since the ROM SAF processes un-thinned data the validation is also valid for PPF 4.4.2. Bending angle profiles (level 1b) are received at DMI, and processed to refractivity profiles (level 2a). The NRT refractivity data has undergone a Quality Control (QC) of several steps, all described in [RD.9]. Profiles failing to pass the refractivity QC are received with a refractivity PCD flag set to non-nominal, and this status is inherited in the proceeding 1D-Var process. The non-nominal refractivity profiles are however processed if possible, and disseminated with a non-nominal meteorology PCD flag.

2.2 Background Data

The background state is taken from an ECMWF global forecast from the standard dissemination stream, currently Cycle Cy41r2, and currently on 137 model levels. Future changes from ECMWF's side will be implemented in the ROM SAF NRT production immediately.

Each occultation has latitude, longitude, and time associated with it. For the background, we interpolate the newest ECMWF forecast from the two closest 6-hourly time step (i.e. at UTC 0, 6, 12 or 18) taking care to avoid forecasts which already have assimilated the observed RO profile. The ECMWF forecasts ("oper" stream) starts from the analysis at 0 UTC and 12 UTC. The 6 hour 4D-Var analysis windows ranges from 3 UTC to 9 UTC and from 21 UTC to 3 UTC. Hence the forecasts used in the nominal situation are as shown in table 2.1.

0:00 UTC	-	3:00 UTC:	forecast valid at	0 UTC (step 12 of forecast started at	12 UTC*)
3:00 UTC	-	9:00 UTC:	forecast valid at	6 UTC (step 6 of forecast started at	0 UTC)
9:00 UTC	-	15:00 UTC:	forecast valid at	12 UTC (step 12 of forecast started at	0 UTC)
15:00 UTC	-	21:00 UTC:	forecast valid at	18 UTC (step 6 of forecast started at	12 UTC)
21:00 UTC	-	24:00 UTC:	forecast valid at	0 UTC next day (s. 12 of f. st. at	12 UTC)

Table 2.1: *The table shows how forecast times are attributed to occultation times. The term "step" refers to number of hours after the analysis time when the forecast where initiated. (*) Here the forecast is initiated on the day before.*

No time interpolation is performed. The model fields are linearly interpolated to the same geographic location as the observed profile. For each observed profile we thus obtain a corresponding model profile which provides the a priori information that is required for the 1D-Var analysis.

2.3 1D-Var processing

Atmospheric refractivity can be considered as a state variable that is dependent on temperature, pressure and specific humidity. In a dry atmosphere the ambiguity between temperature and pressure can be resolved via the hydrostatic equation combined with the equation of state, and so vertical profiles of temperature and pressure can be uniquely determined from the refractivity profile. When water vapour is present there is no way to uniquely determine profiles of pressure, temperature and humidity from the observed refractivity profiles without introducing some ancillary information. In the 1D-Var procedure [RD.2, RD.5] statistically optimal profiles for pressure, temperature and humidity are determined from the observed refractivity profile with error estimates together with 'background' profiles of pressure, temperature and humidity with error estimates.

The ROM SAF 1D-Var processing software 1DV generates a co-located background profile for each RO observation from an ECMWF forecast. The 1DV algorithm and processing framework is described in full detail in [RD.8].

2.3.1 The cost function

The purpose of the 1D-Var processing is to find a maximum likelihood estimate of a vertical atmospheric profile $\boldsymbol{x}$, given a set of m observations $\boldsymbol{y}^o$ of the refractivity and some a priori knowledge $\boldsymbol{x}^b$, also referred to as a background. The atmospheric profile, $\boldsymbol{x}$, is a n-component vector containing surface pressure and for each of the $(n-1)/2$ atmospheric levels, temperature and humidity. Both the observations and the background have associated uncertainties described by an observational error covariance matrix $\boldsymbol{R}(m,m)$ and background error covariance matrix $\boldsymbol{B}(n,n)$. In the case of Gaussian error distributions, the statistically optimal solution that simultaneously fits both the observation and the background to within their respective errors, is obtained by minimising the cost function

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}^b)^T\boldsymbol{B}^{-1}(\boldsymbol{x}-\boldsymbol{x}^b) + \frac{1}{2}(\boldsymbol{y}^o - H(\boldsymbol{x}))^T\boldsymbol{R}^{-1}(\boldsymbol{y}^o - H(\boldsymbol{x})) \tag{2.1}$$

with respect to the state $\boldsymbol{x}$. Here, $H(\cdot)$ is the forward operator mapping the atmospheric state $\boldsymbol{x}$ into measurement space. In practice this means converting a vertical profile of pressure, temperature, and humidity given on the 1D-Var levels into a corresponding profile of refractivity given on the observed refractivity levels.

The state $\boldsymbol{x}$ and the background $\boldsymbol{x}^b$ are given on the 1D-Var levels, defined as a set of ECMWF model levels ([RD.1]). Hence, the first term in the cost function $J(\boldsymbol{x})$ is evaluated on the 1D-Var levels, whereas the second term is evaluated on refractivity levels which are expressed in terms of geopotential heights. It may be noted that the minimisation of the cost function J is effectively a least-square fitting procedure with $2J$ approximately having a χ^2 distribution with m degrees of freedom. The 1DV- package employs the Levenberg-Marquardt minimiser which was recommended in [RD.10] to determine the best solution by minimising J. The minimiser outputs both $2J/m$ and the number of iterations used. These quantities are used to evaluate the quality of the solution (see section 2.4)

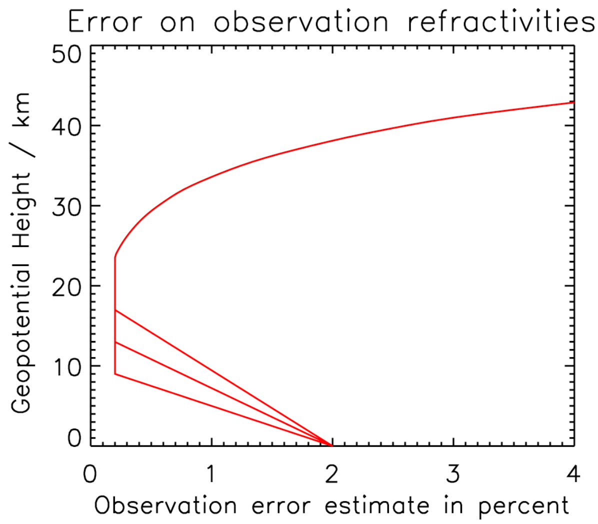


Figure 2.1: Fractional refractivity error estimates for 3 different tropopause heights (9km, 13km, 17km).

2.3.2 Observation error covariance

Radio occultation errors in the troposphere are dominated by horizontal gradients and the presence of water vapour (see for example [RD.5]). In the stratosphere, the circulation is nearly zonally symmetric and there's no water vapour, so RO measurements are generally good in this part of the atmosphere. Errors increase below the tropopause because stratospheric conditions change into tropospheric ones, and specific humidity increases. Thus, the tropopause as boundary between stratosphere and troposphere is also the natural boundary between two different error regimes of radio occultation data. The error model employed in 1DV reflects this [RD.3]. Figure 2.1 shows the observational error model that is implemented in 1DV. The refractivity error estimate is 2% at the surface, decreasing linearly to 0.2% at the tropopause. Above the tropopause, the fractional errors are 0.2% or 0.02 N-units, whichever is greatest.

The altitude of the tropopause is determined from the background profile using the standard definition of the tropopause as the lowest level at which the lapse rate decreases to 2 K/km or less, provided that the average lapse rate between this level and all higher levels within 2 km does not exceed 2 K/km. This dynamically-determined tropopause height is then compared to a climatological value [RD.7]. If the pressure at the dynamically-determined tropopause height differs by more than a factor of 2 from the climatological value, the climatological value will be used instead of the dynamically-determined value.

The observational error covariance matrix $\boldsymbol{R}$ used in 1DV is derived from the error estimates given above by the expression:

$$\boldsymbol{R}_{kl} = \sigma_k \sigma_l e^{\frac{-|z_k - z_l|}{h}} \tag{2.2}$$

where σ_k and σ_l are the error estimates at two points k and l along a vertical profile, z_k and z_l are the geopotential heights and h is a characteristic scale height. A uniform scale height of 3 km is assumed [RD.2]. The refractivity correlation matrix is plotted in figure 2.2 (right).

2.3.3 Background Error Covariance

The 1D-Var processing also needs as input a background error covariance matrix $\boldsymbol{B}$. As was the case for the observation error covariances, this matrix is constructed from one dimensional profiles of error estimates combined with an error correlation matrix $\boldsymbol{C}$:

$$B_{kl} = \sigma_k \sigma_l C_{kl} \tag{2.3}$$

The used error correlation matrix, provided by ECMWF ([RD.4]), is plotted in figure 2.2 (left).

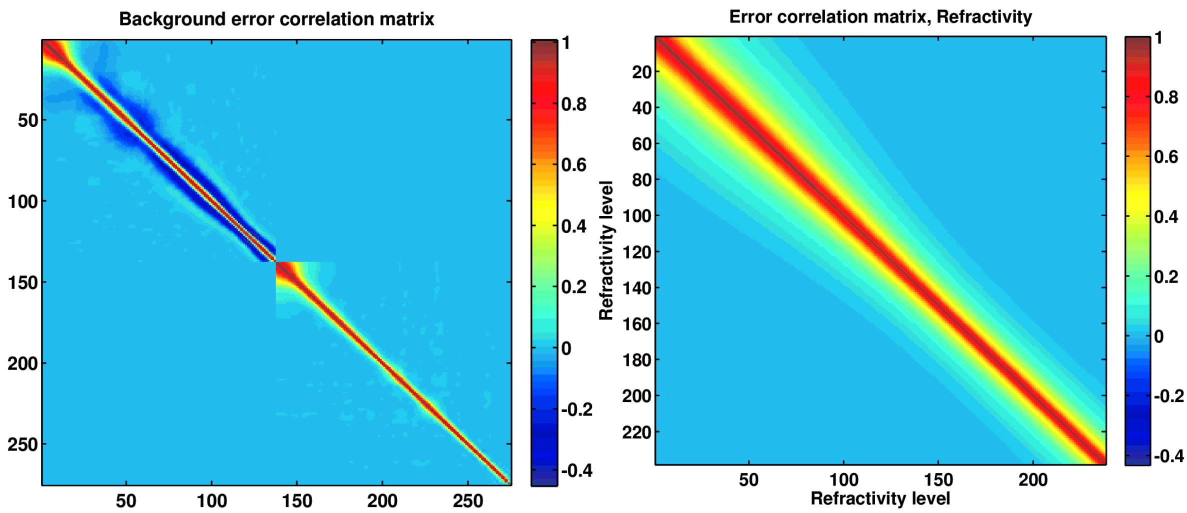


Figure 2.2: Left: Error correlation matrix between 275 state-vector entries. Index 1-137; temperature error correlations. Index 138-274; specific humidity error correlations. Last row and column (index 275) shows surface pressure error correlations (zeros except for the diagonal). Right: Refractivity error correlation matrix.

The error estimates for temperature and humidity are based on the "Scaled Ensemble Standard Deviation" ("**ses**") variable[1] [RD.4]. The specific humidity background error profile and the surface pressure error are calculated individually for each occultation, assuming a constant relative error of specific humidity and surface pressure, while a constant temperature background error profile is used. A detailed description of the background error covariance construction can be found in [RD.8]. The resulting temperature error and the effective error of specific humidity as function of levelnumber is plotted in figure 2.3. For reference we also plot previous background error assumtions which has been used in earlier 1DV versions in figure 2.3.

[1] Specifically, the data type "**ses**" (stream=enda, class=od) disseminated by ECMWF, representing the estimated error of the forecast at 0900 UT and 2100 UT.

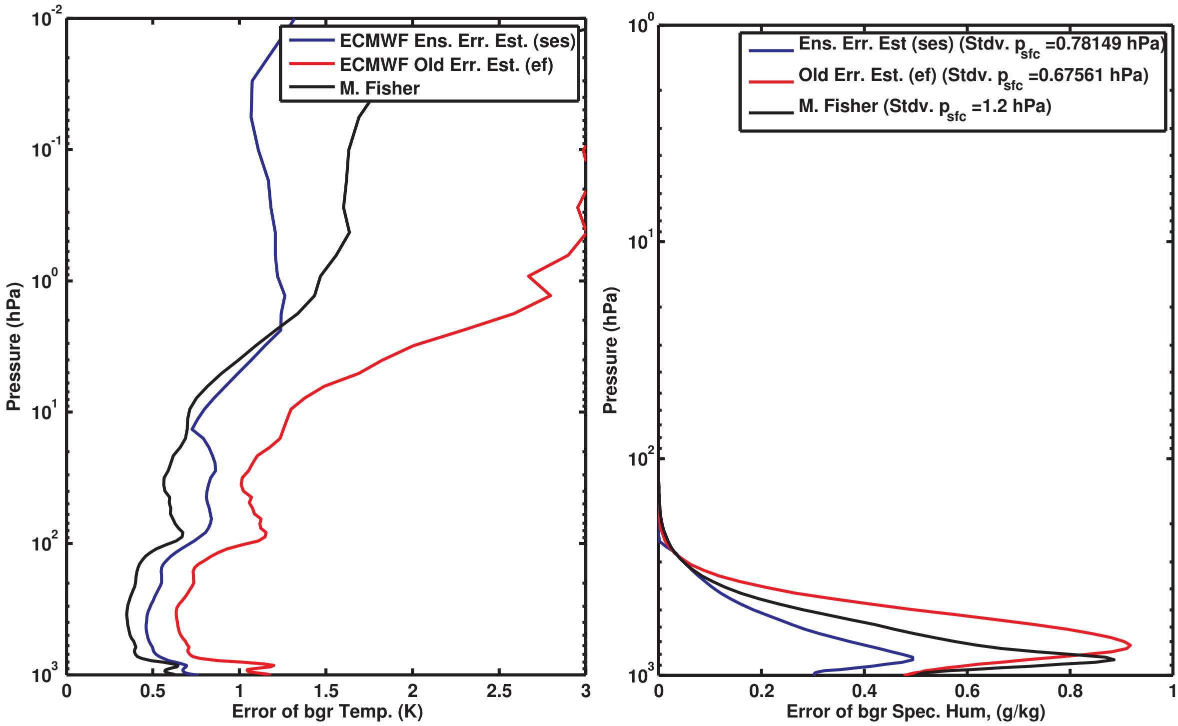


Figure 2.3: Temperature background error profile (left) and specific humidity background error profile (right). (See caption for surface pressure background error). The figure also shows some previous background error assumptions based on the socalled "ef" (error of first guess) fields and an old error estimate originally received from M. Fisher (ECMWF, 2004).

2.4 Quality Control

After 1D-Var processing a number of solution profiles are rejected based on diagnostics of the minimiser. In data version 1.3, the 1D-Var solutions are disseminated as non-nominal if:

a) The $2J/m$ quality score of the solution is above 13.0.

b) The Levenberg-Marquardt minimiser used more than 25 iterations to find the solution.

c) The ingoing refractivity profile was marked non-nominal (see section 2.1).

3 Validation

The retrieved state vectors are validated against ECMWF analysis, i.e. a data set which has assimilated Metop A and Metop B RO data. For comparison we show equivalent validation figures based on profiles produced from geometrical optics, from the same set of occultations. Figures in this section are based on two different versions (sets) of all data from the validation period:

sG Data version 1.2, Geometrical Optics, 1-5 September 2016 with background and analysis profiles from ECMWF IFS Cycle 41r2; total of 6731 profiles.

sW Data version 1.3, Wave Optics,1-5 September 2016 with background and analysis profiles from ECMWF IFS Cycle 41r2; total of 6759 profiles.

The validation results presented in this document are based on version 1.5 of the NRT refractivity profiles (GRM-01 and GRM-40). Primary 1D-Var variables, obtained through the 1D-Var processing, are profiles of temperature and specific humidity as well as surface pressure given on ECMWF model levels. The validation is however done on geopotential height coordinates. The nomenclature S = 1D-Var Solution, B = Background, A = ECMWF analysis and O = Observation is adopted throughout this chapter.

3.1 QC performance

3.1.1 Iteration count

Figure 3.1 shows time series and histograms of the number of iterations needed to find a solution. A vast majority of occultations are in the range 3-5 iterations. Only one profile of the examined 6759 WO profiles exceeds the 25 iterations limit.

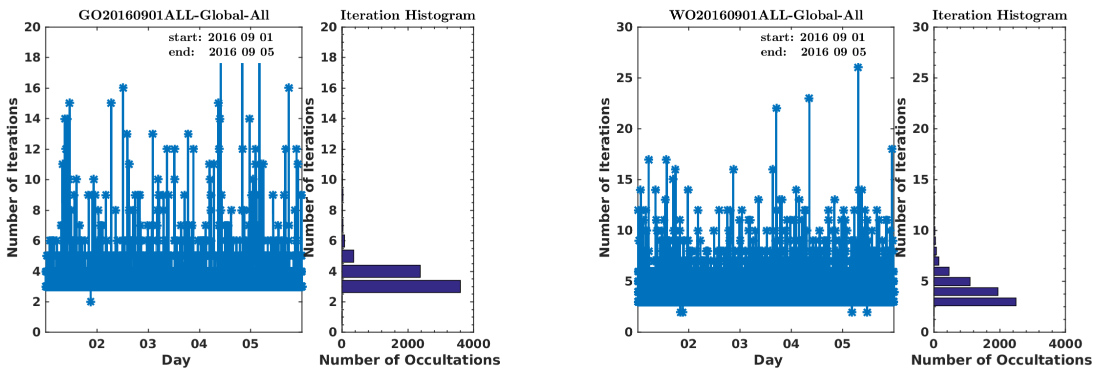


Figure 3.1: Number of iterations of the minimiser needed to find a solution. Time series and histogram. Left: sG, right: sW.

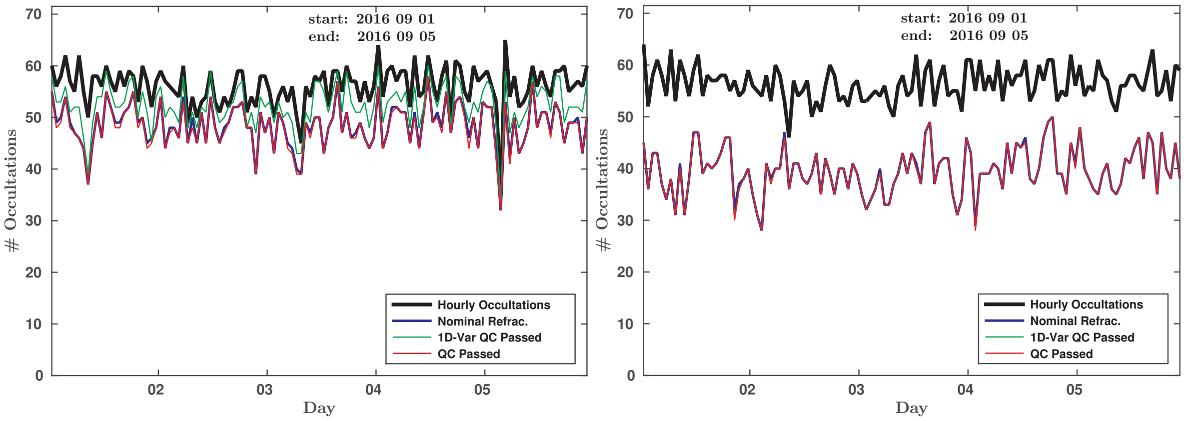


Figure 3.2: QC performance time series plotted as hourly occultations. Total number of occultations (black), occultations with nominal refractivity (blue), occultations with nominal 1D-Var result (green) and the final number of successful profiles (red)). Left: sG, right: sW.

Figure 3.2 shows the 4 key numbers (total number of occultations, occultations with nominal refractivity, occultations with nominal meteorology and the combined number final number of completely successful profiles) illustrating the performance of 1D-Var as function of time through the 5 days period wich is focus of the analysis. The sG dataset is subject to QC version 1.2 while sW is subject to QC version 1.3. In version 1.2 the threshold for the cost function $2J/m$ was set to 4.0, while in version 1.3 it was raised to 13.0. Another difference is that in version 1.2 the QC's at different levels of processing were independent, while in version 1.3 a non-nominal product status is inherited to the next processing level. This is why the number of nominal 1D-Var result is identical to the number of fully nominal profiles in sW.

The QC performance is summarized in table 3.1.

The right panel shows the QC performance for the version 1.3 data set which is under validation. A big part, 4,8%, of the total number of profiles pass the refractivity QC but fails to be processed through 1D-Var. Only few of these, (1.2 %), are actually caught by he 1D-Var QC, the rest fails before an output is produced. This is generally because these profiles do not meet the criteria for starting the 1D-Var, either because they contain too few refractivity data points below 60 km or does not reach below 20 km.

QC performance; GO20160901ALL-Global-All

Total # of profiles:	6731	100.0 %
Nominal refractivity:	5829	86.6%
Passing 1D-Var QC:	5799	86.2%
$\frac{2J}{m} \geq 4$	214	3.2%

QC performance; WO20160901ALL-Global-All

Total # of profiles:	6759	100.0 %
Nominal refractivity:	4756	70.4%
Passing 1D-Var QC:	4745	70.2%
$\frac{2J}{m} \geq 13$	80	1.2%

Table 3.1: *QC summary for sG (left) and sW (right). "Nominal refractivity" means that the refractivity is declared nominal and that an 1D-Var run was attempted.*

3.1.2 $2J/m$ quality measure

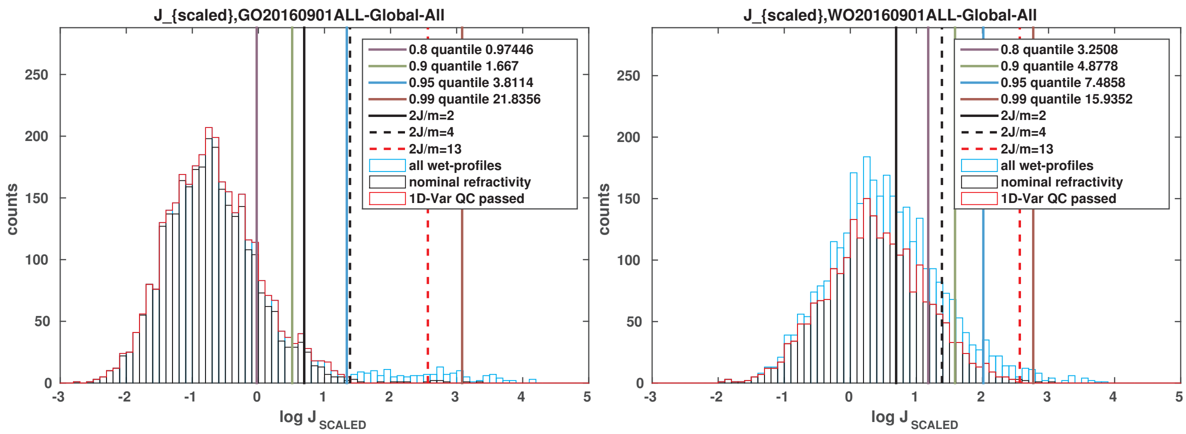


Figure 3.3: $2J/m$ time series and histograms. Left: sG, right: sW.

If the errors specified by the $\boldsymbol{R}$ and $\boldsymbol{B}$ matrices are in accordance with the actual errors then $2J$ is expected to follow a χ^2_m (chi-squared distribution with m degrees of freedom) where m is the dimension of observation space, i.e. m is the number of refractivity values used in the 1D-Var processing [RD.6]. Thus the expected value of $2J$ at convergence is m with a standard deviation of $\sqrt{2m}$. Figure 3.3 shows a histogram of $2J/m$ values and figure 3.4 shows the latitude dependence of the $2J/m$ mean value. It is assumed that the increase of the cost function $2J/m$ is due to inconsistent assumptions on the errors in the troposphere. The tuning of the error covarainces $\boldsymbol{B}$ and $\boldsymbol{R}$ will be assessed in the future.

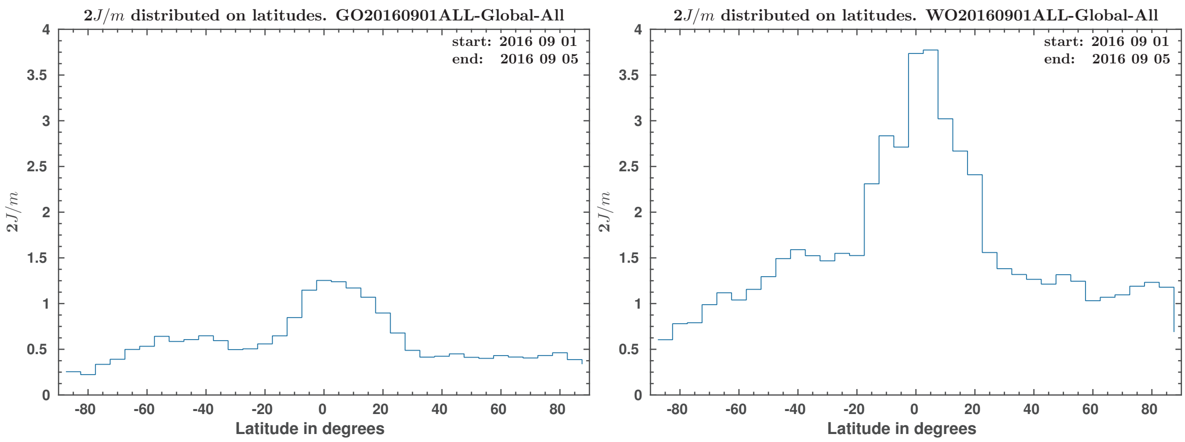


Figure 3.4: Mean $2J/m$ as a function of latitude. Left: sG, right: (validation data set) sW.

The latitude dependence of $2J/m$ is also illustrated with histograms in figure 3.5. It is seen that even though the cost function distribution varies with latitude, it is reasonable to have a common threshold value for all latitudes.

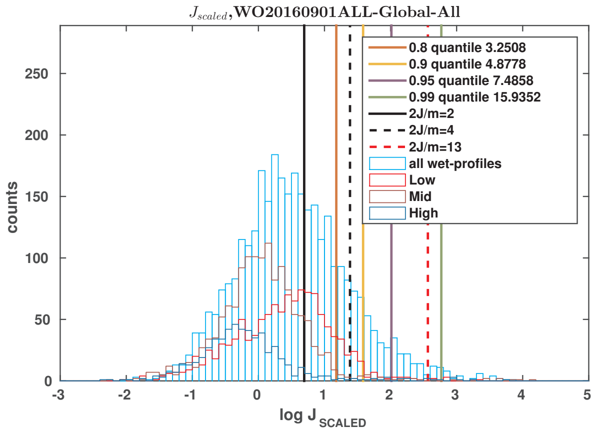


Figure 3.5: Wave Optics, $J_{scaled} = \frac{2J}{m}$ distribution for sW, partitioned on different latitude bands; Low < 30 deg ≤ Mid < 60 deg ≤ High.

The great majority of occultations have $2J/m$ larger than 1.0 while in version 1.2 the values were mainly below 1.

3.2 Error estimates

In addition to the solution state vector calculated by 1D-Var the error estimates for the state varariables is also disseminated in the 1DV products. By comparing this error with the background error estimate one can get an indicator of how much information was gained from the observation.

3.2.1 Temperature, specific humidity and pressure error estimates

Figure 3.6 (left panel) shows the background and solution error estimate profiles for temperature. The temperature solution error estimates show a potential for improvement with respect to the background, roughly in the range 8 km to 35 km. There are also some small improvements at higher altitudes. The minimum value that the solution error estimates approach in the region 15 km to 25 km reflects the 0.2 % minimum refractivity error (see figure 2.1). The specific humidity solution error estimates are shown in figure 3.6 (right panel).

Likewise the pressure errors are plotted before and after 1D-Var has been applied in figure 3.7. Since the 1D-Var output is given on ECMWF model levels, which are constant pressure levels above 75 hPa, there are no pressure errors above above this level. The pressures below 75 hPa are uniquely determined by the surface pressure through a linear form. The pressure error is largest at surface and falls rapidly to zero a 75 hPa. The effective pressure error, however, arises from interpolation to specific geopotential height levels. The geopotential height is found from integration of the hydrostatic equation, thus the errors arising from this integration are inherited in the pressure profiles and causes a discrepancy between ECMWF analysis pressures and 1D-Var pressures even at high altitude.

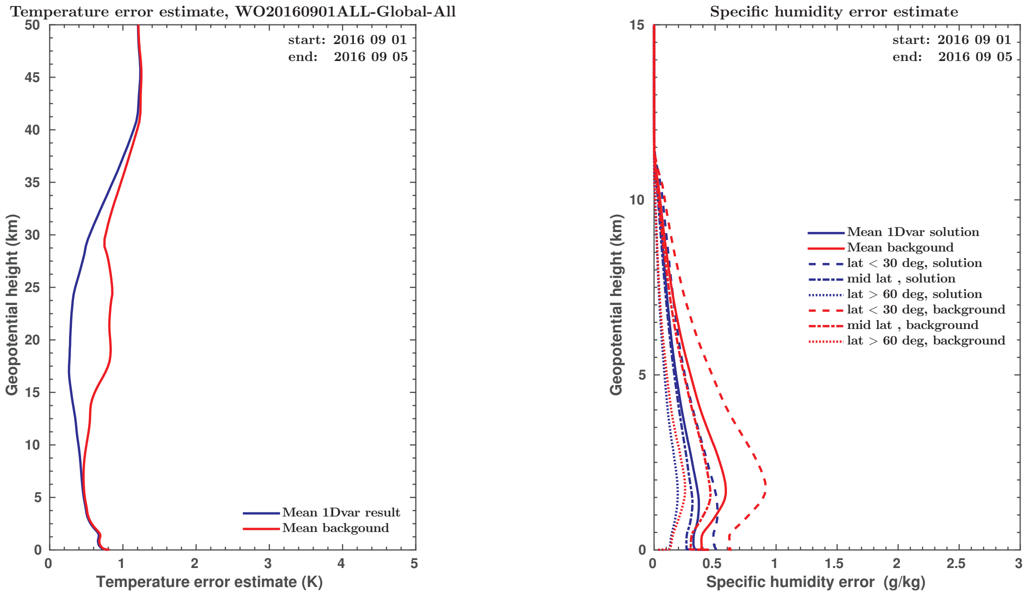


Figure 3.6: Background (red) and solution (blue) error estimates for temperature (left) and specific humidity (right) sW.

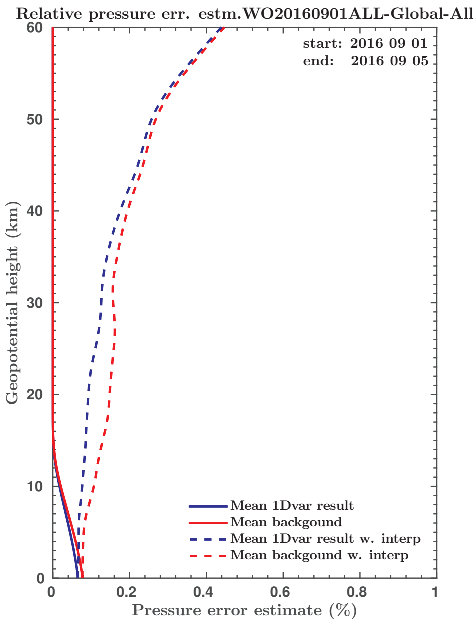
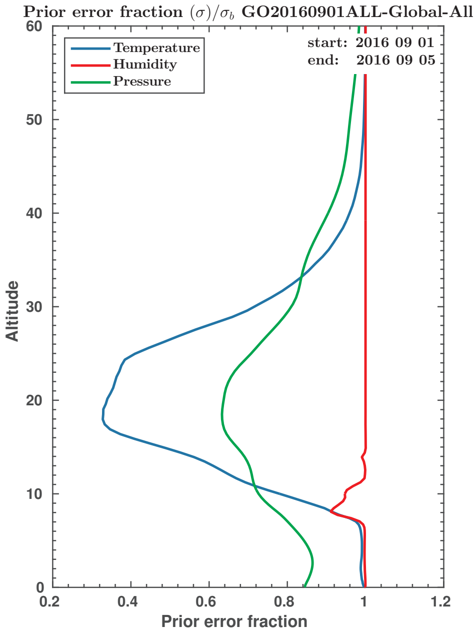


Figure 3.7: Background (red) and solution (blue) error estimates for pressure. The solid branches represents the error of the pressure disseminated at model levels, and the dashed branches represents the effective error arising from interpolation to geopotential height levels. Left: sG, right: sW.

Prior fractions

The introduction of open-loop processing and wave-optics algorithms in GRAS data processing has improved the quality of refractivity data at low altitude in areas of high atmospheric humidity.

The solution error estimates are smaller than the background errors at levels where observation data are actually used in the 1D-Var retrieval. So a way to summarize the theoretical improvement of 1D-Var is to plot the prior fractions of the retrieved variables, i.e. σ_S/σ_B, as is done in figure 3.8. This figure illustrates at which altitudes to expect improvement of the retrieved variables; where the prior fraction is less than unity, data from measurement have been used in 1D-Var to narrow the prior uncertainty. It is seen in Figure 3.8 that especially the



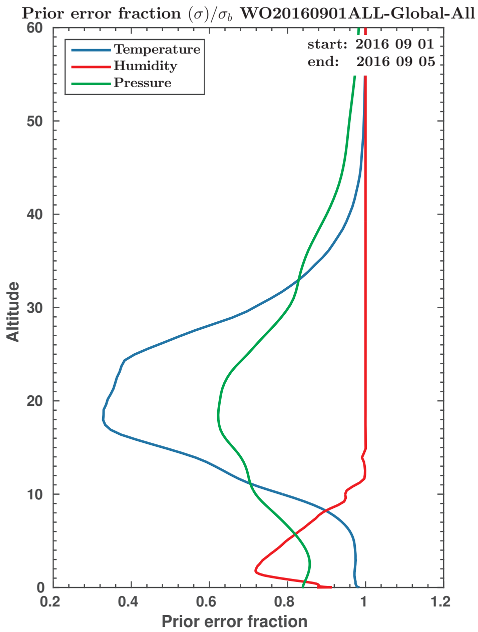


Figure 3.8: Prior reduction vectors for temperature, specific humidity and pressure. Left: sG, right: sW.

water vapour precision is improved in data version 1.3 compared to version 1.2. The "prior fraction" σ_S/σ_B shown in figure 3.8 reflects the choice of background error covariance matrix and observation covariance matrix. The prior fraction σ_S/σ_B is the square root of the ratio between the diagonals of $\boldsymbol{S}$ and $\boldsymbol{B}$ matrices. This is reflected in Figure 3.9, where the specific humidity prior fraction turns out to be smaller, with a minimum around 0.6, at low (tropical) latitudes than at high (arctic) latitudes. This may be attributed to the larger background specific humidity error at low latitudes. It is also observed that the temperature prior fraction is decreased near the tropopause at mid-latitudes, compared to the tropics, because the refractivity error is assumed to be at minimum (0.2 %) down to the tropopause.

3.3 Comparison to ECMWF analysis

Validation data consist of summary statistical information on the reliability and quality of the sounding products. Validation is done globally and on the full vertical domain of the product. In this section we validate the 1D-Var solutions by comparison with co-located profiles from ECMWF, IFS Cycles Cy41r2 4D-Var analyses, at the closest synoptic hour. Since we use an ECMWF forecast (not analysis) as background for the 1D-Var processing we are comparing each 1D-Var result against a different ECMWF field than was the basis for the 1D-Var calculation.

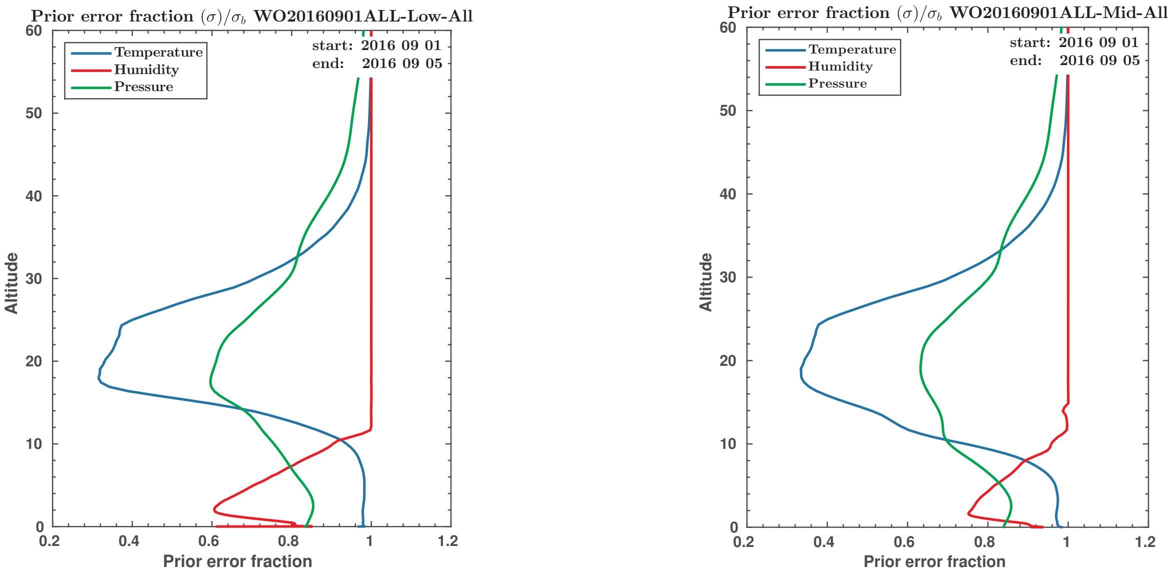


Figure 3.9: Prior reduction vectors for temperature, specific humidity and pressure. Left: Low latitudes. Right: High latitudes. The positive prior fraction around 9 km altitude at high latitudes is attributed to numerical uncertainty in determination of the solution error.

The plots in this section are attributed with target (dashed orange curve) and threshold error profiles (dashed red curve). The quantile, $r = \frac{1}{2}(1 - \mathrm{erf}\,\sqrt{2})$, corresponds to the standard deviation if the data obeys a Gaussian distribution. Therefore the r-quantile is calculated from the data at each level and plotted with a green dashed line. This serves to indicate if the error distributions are non-Gaussian, which is detected as ranges where the standard deviation of a given property is larger than the r-quantile. At the end of this section there is a comparison between rising and setting occultations.

3.3.1 Temperature

Figure 3.10 shows comparisons of the 1D-Var temperature solution profiles against ECMWF analysis (S-A statistics) together with the PRD specifications. The following may be noted:

- Temperatures are unbiased up to 35 km.
- Temperature S-A standard deviations complies with the target value.
- The S-A temperature distribution is close to a Gaussian distribution up to 35 km.
- There is little difference in the overall temperature statistics between geometric optics (sG) and wave optics (sW).

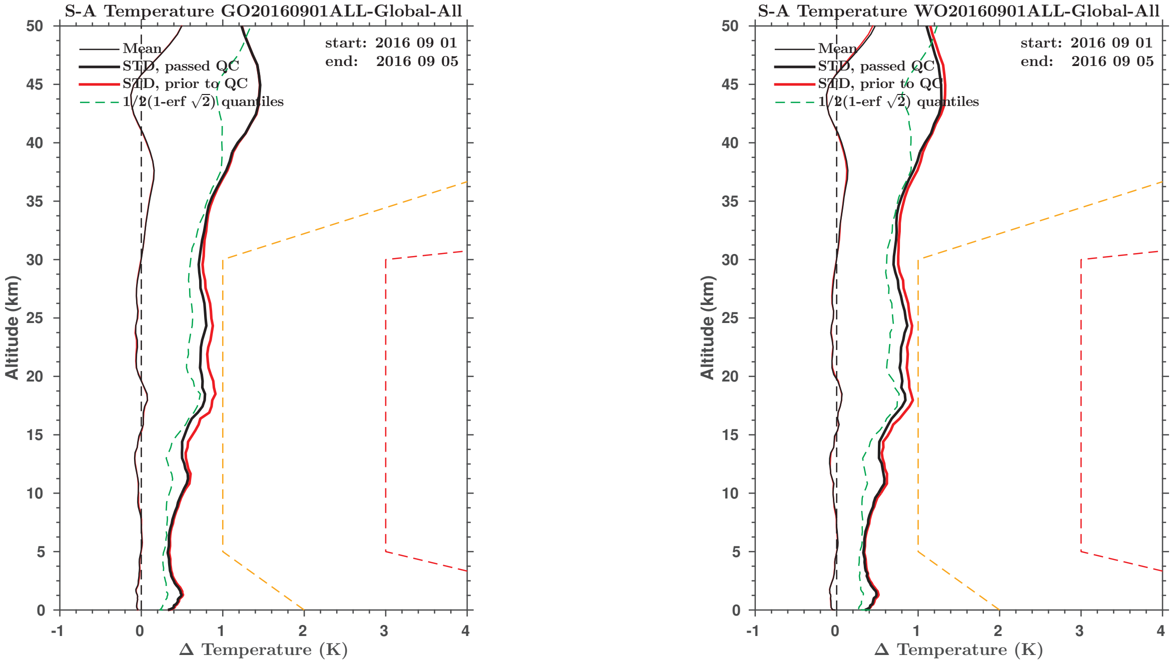


Figure 3.10: Temperature; 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias ± STDV. Also shown; the formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]) and the quantile corresponding to 1 STDV in a Gaussian distribution (green). I.e, if the distribution had been gaussian the green line would be on top of the black line. Left: sG, right: sW.

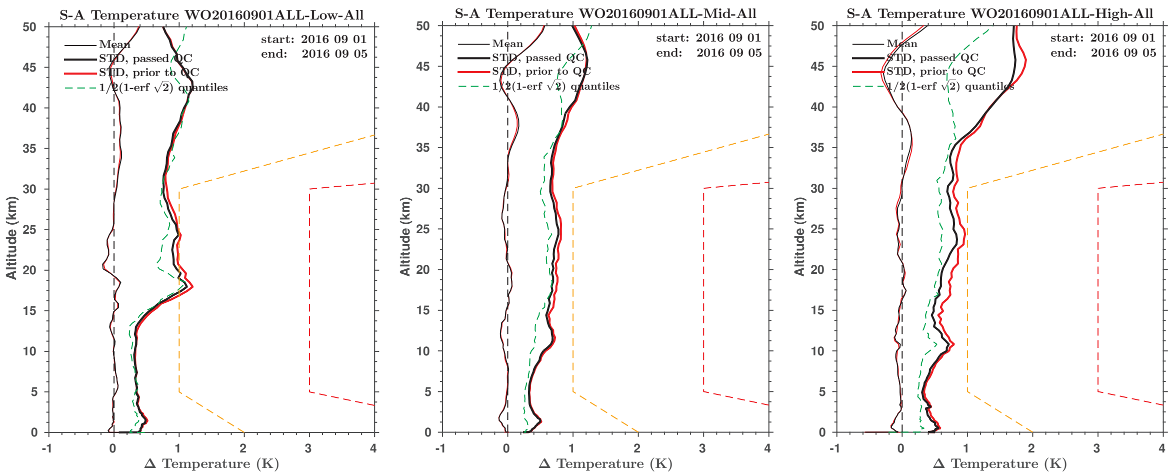


Figure 3.11: Temperature; 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias ± STDV. As in figure 3.10. Left: 0 to 30 deg latitude; Mid 30 to 60 deg latitude; Right: 60 to 90 deg latitude.

1D-Var temperature in different latitude bands

In figure 3.11 the difference between profiles in different latitude bands is shown. Fewer tropical occultations reach below 16 km and therefore 1D-Var falls back on the background which is relatively close to the analysis, hence the STDV narrows below 16 km in the tropics. The variability of the tropical tropopause seems to be hard to capture either for the model or the RO instruments (or for both). In any case the temperature STDV exceeds the target between 16 and 26 km at low latitudes.

3.3.2 Specific humidity

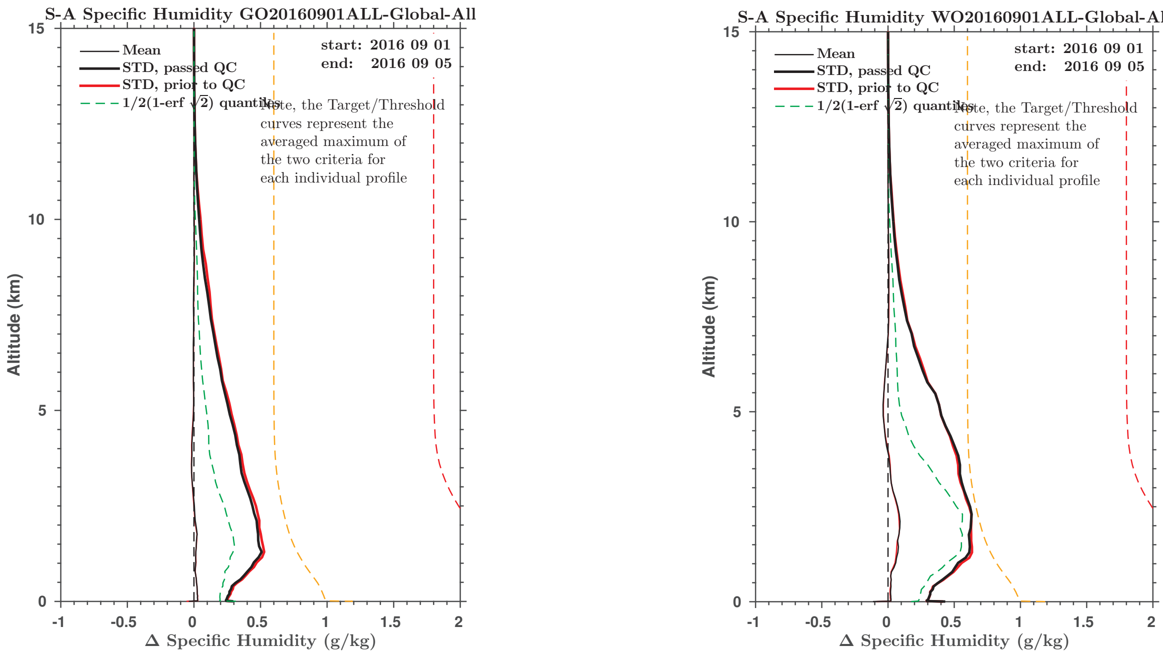


Figure 3.12: Specific humidity; 1D-Var specific humidity minus ECMWF 4D-Var analysis (S-A). Also shown: The formal ‘Threshold’ (red) and ‘Target’ (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a Gaussian distribution (green). Left: sG, right: sW.

Figures 3.12 and 3.13 shows comparisons of 1D-Var specific humidity solution profiles against ECMWF analyses. The specific humidity errors complies with the product requirements, though the S-A standard deviation has increased considerably in data version 1.3 compared to version 1.2. It may be noted that the specific humidity S-A distribution is more non-Gaussian than it is the case for temperature S-A distribution.

3.3.3 Pressure profile and surface pressure

The relative deviations of 1D-Var result pressure from ECMWF analyses are shown in Figures 3.14, 3.15 and 3.16. It should be kept in mind that the statistics are based on a short time interval of 5 days and therefore the may be subject to some uncertainty.

- The pressure shows a negative bias of around 0.1 % throughout the altituderange sG. This bias appears to be slightly more pronounced in sW.

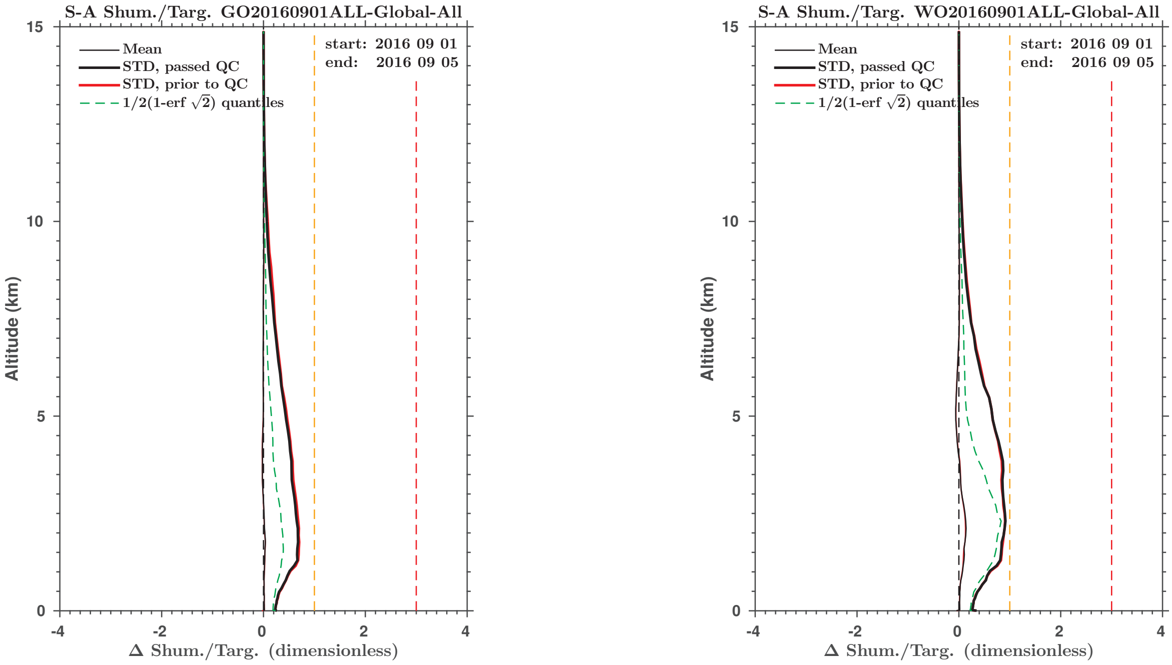


Figure 3.13: Specific humidity; 1D-Var specific humidity minus ECMWF 4D-Var analysis relative to the target value. Also shown: The formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a gaussian distribution (green). Left: sG, right: sW.

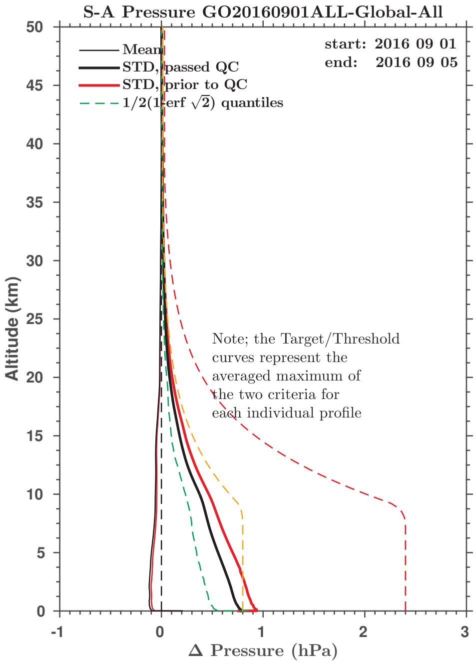
- Pressure standard deviations increase from about 0.1 % at the ground to around 0.25 % at 40 km and increase more rapidly above this.

- The pressure profile PRD requirements are met everywhere. At high latitudes the target value is touched around 35 km.

- S-A surface pressure bias is 0.1 hPa in sG and -0.14 hPa in sW. The S-A surface pressure standard deviation is 0.75 hPa in sG and 0.79 hPa in sW. So the validation as a whole does meet the PRD target value (0.8 hPa). However, the introduction of wave optics has not led to a decrease of surface pressure STDV. See further discussion in 3.5.

- The surface pressure bias is largest at mid latitudes (-0.27 hPa), while the surface pressure SDV is largest, 0.97 hPa, at high latitudes.

Table 3.2 shows the bias and standard deviations of surface pressure. Also shown are the previous similar quantities from two older data sets, COSMIC and Metop A/B from 2013. The surface pressure S-A statistics have improved since the previous operational Metop A/B data from 2013, where STDV S-A were 0.99, but are slightly worse than the geometrical optics (STDV S-A = 0.75) and the COSMIC data from 2013 (STDV S-A = 0.71).



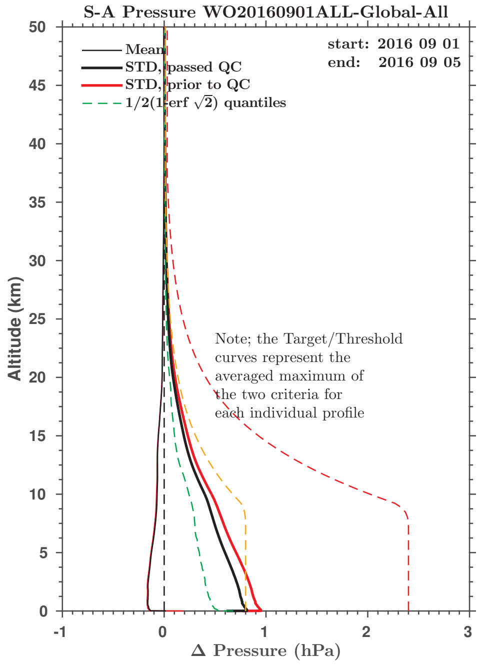


Figure 3.14: 1D-Var pressure minus ECMWF 4D-Var analysis pressure. Also shown: The formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a gaussian distribution (green). Left: sG, right: sW.

1D-Var for setting and rising occultation.

In figure 3.17 we show a comparison between the sW 1D-Var results and ECMWF analysis for rising and setting occultations for all latitudes. There is a larger pressure standard deviation for the setting than for rising occultations. It is remarkable that the setting occultation, which penetrates deeper into the troposphere has reduced pressure STDV. In the refractivity the setting occultations has the largest standard deviations in the lower stratosphere as shown in [RD.9]. The retrieved surface pressure depends on refractivities at all levels, so the results suggest the setting occultations as a whole have lesser statistical errors. The temperature show only modest difference between rising and setting occultations. The sW data set has been quality controlled in this plot.

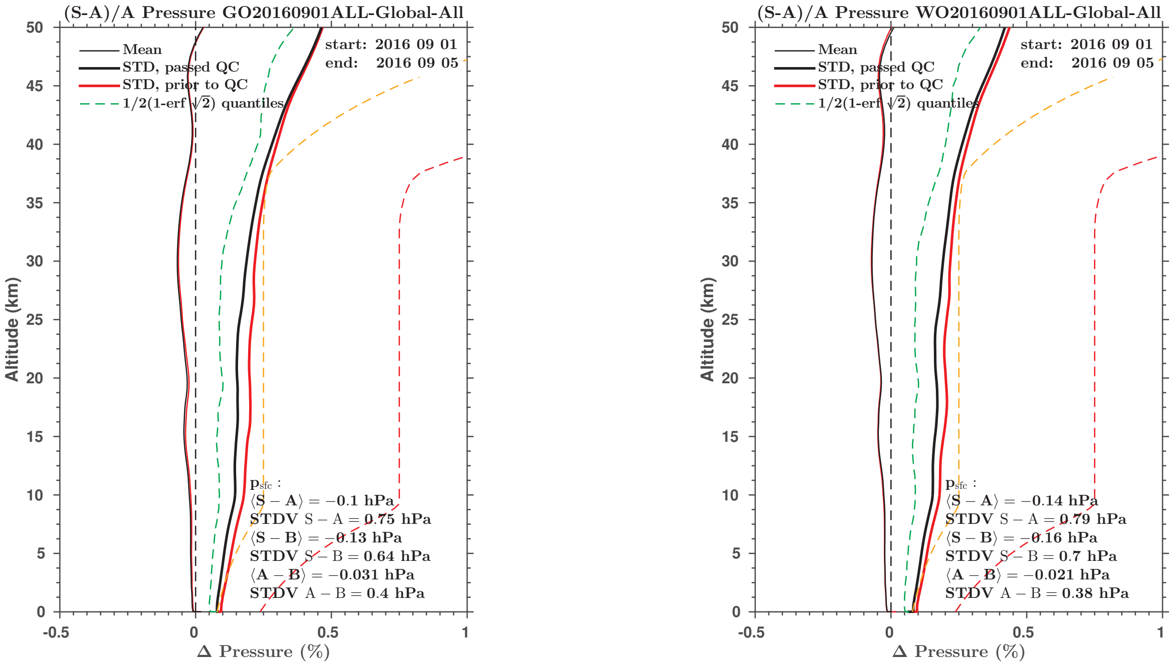


Figure 3.15: Relative pressure deviations (S-A)/A . Also shown: The formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a gaussian distribution (green). Left: sG, right: sW.

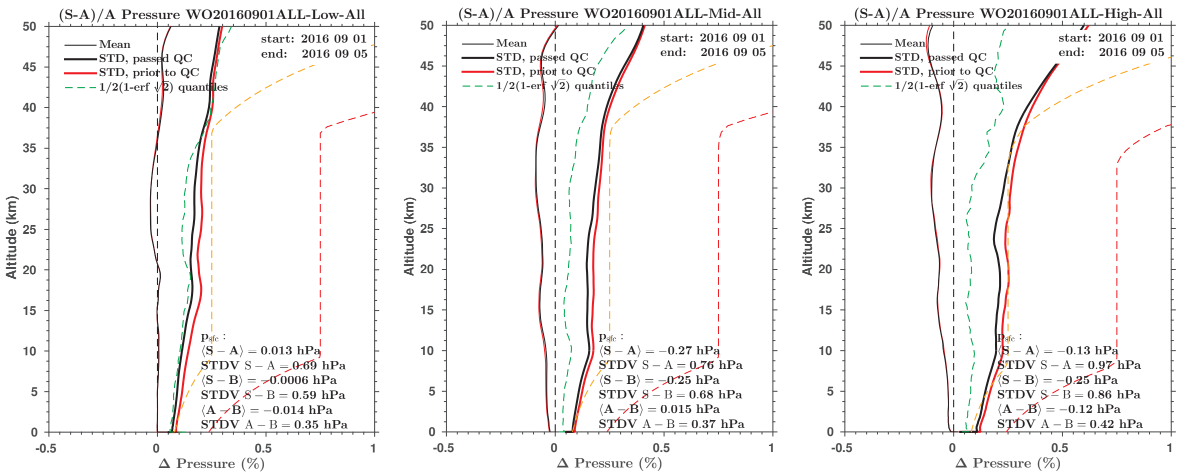


Figure 3.16: sW, (wave optics) 1D-Var pressure minus pressure of ECMWF 4D-Var analysis pressure divided with analysis pressure. Also shown are: The formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a Gaussian distribution (green). Statistics for surface pressure are inserted in lower right corners. Left: Low, Mid: MId, Right: High - latitude

Table 3.2: *Summary of surface pressure statistics. S: 1D-Var solution, A: ECMWF analysis and B: ECMWF background.*

		Bias (hPa)	STDV (hPa)
COSMIC 2013	S-A	-0.08	0.71
	S-B	-0.09	0.60
	A-B	-0.01	0.38
Metop 2013	S-A	-0.11	0.99
	S-B	-0.04	0.74
	A-B	-0.07	0.71
sG	S-A	-0.1	0.75
	S-B	-0.13	0.64
	A-B	-0.03	0.4
sW	S-A	-0.14	0.79
	S-B	-0.16	0.7
	A-B	-0.02	0.38

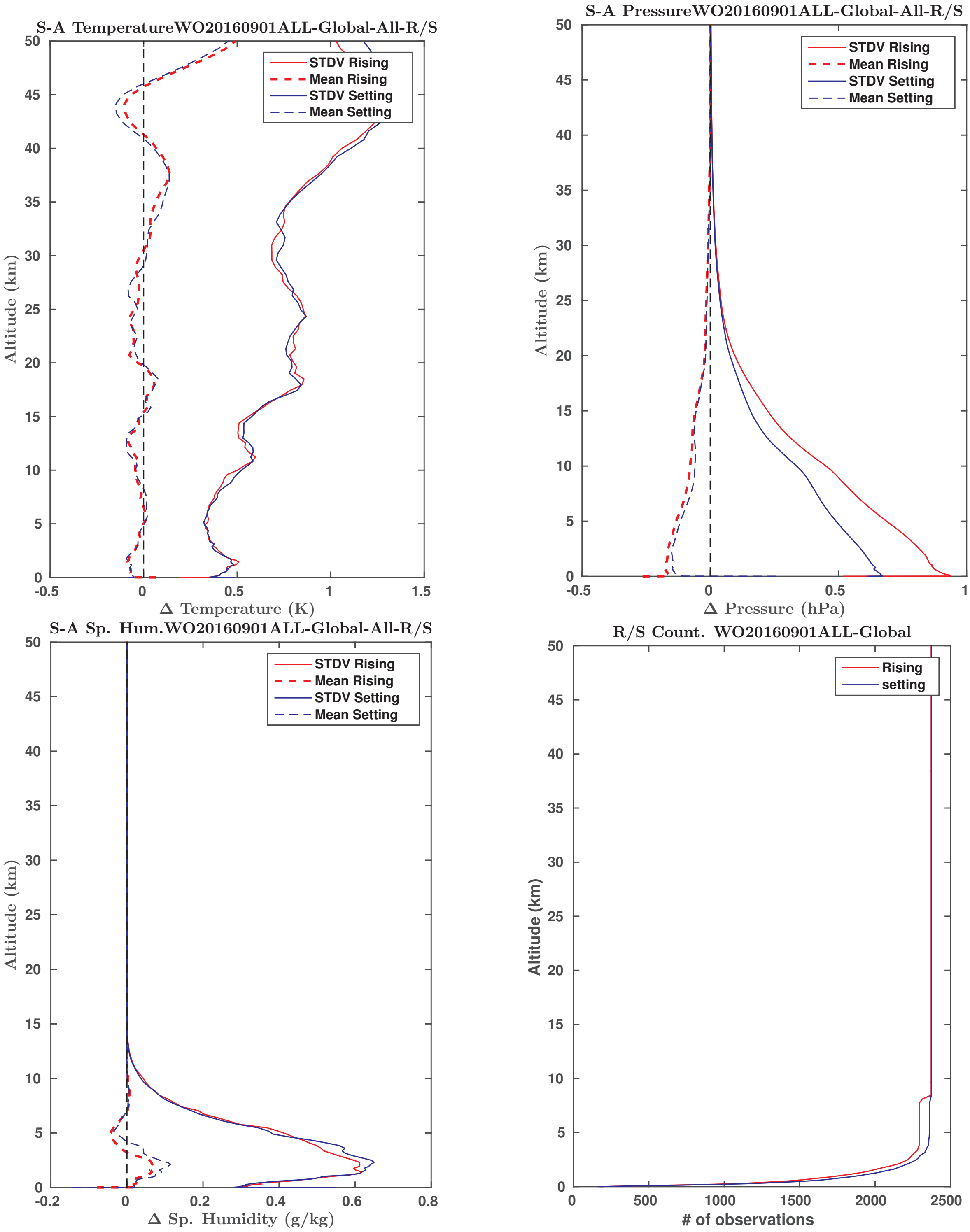


Figure 3.17: Temperature, Sp. Humidity and Pressure, sW (Wave optics); 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias STDV.

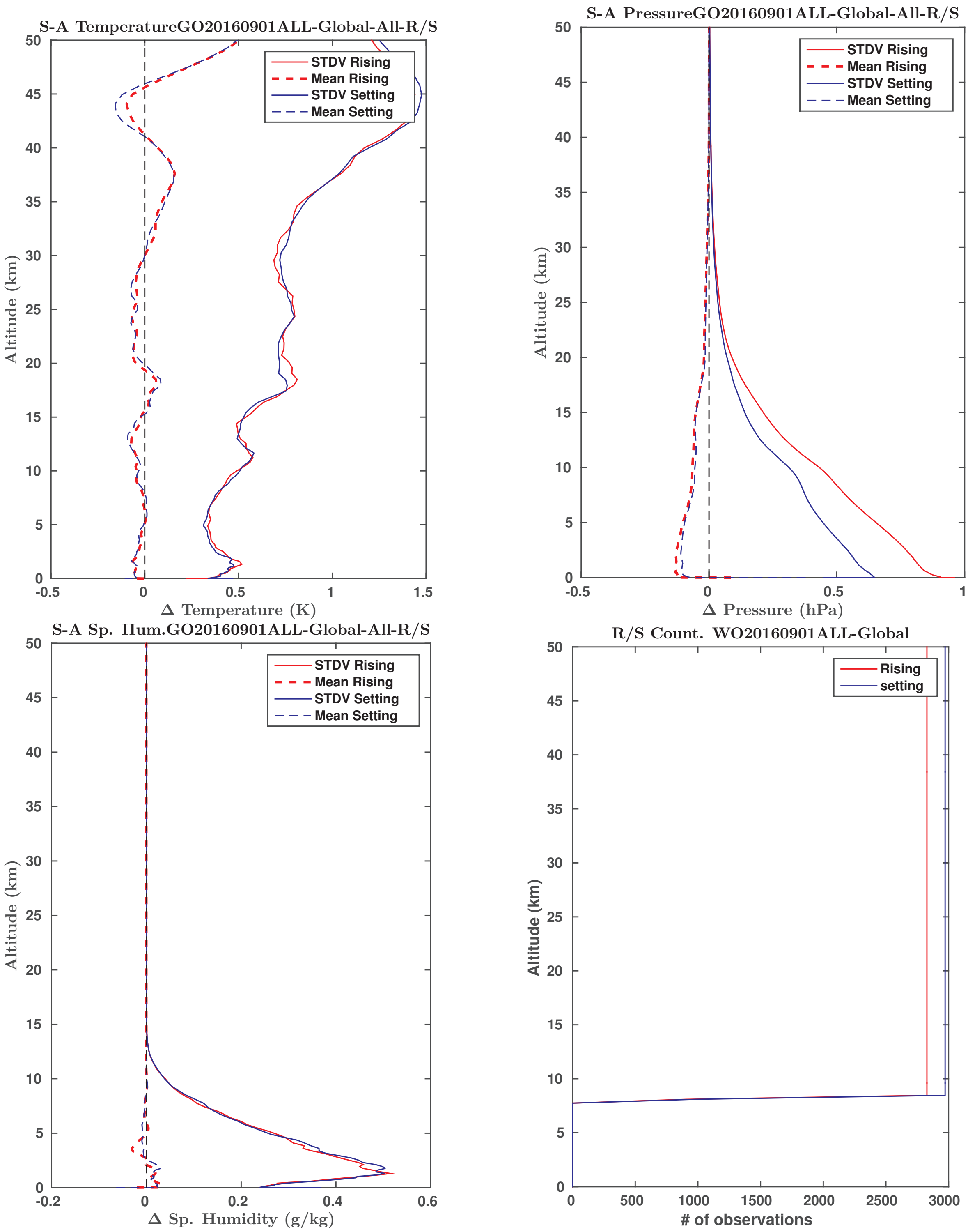


Figure 3.18: Temperature, Sp. Humidity and Pressure, sG (Geometric optics); 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias STDV.

3.4 Refractivity statistics

Figures 3.19 and 3.20 shows statistics of the observation versus background (solid) and solution (dotted) refractivity, normalized with the assumed observation error. As expected the solution is closer to the observation than to the background and approaches the background at high altitudes. There is no pronounced difference between the biases of the two periods sG and sW, except for the fact that sG contains no data below 8 km.

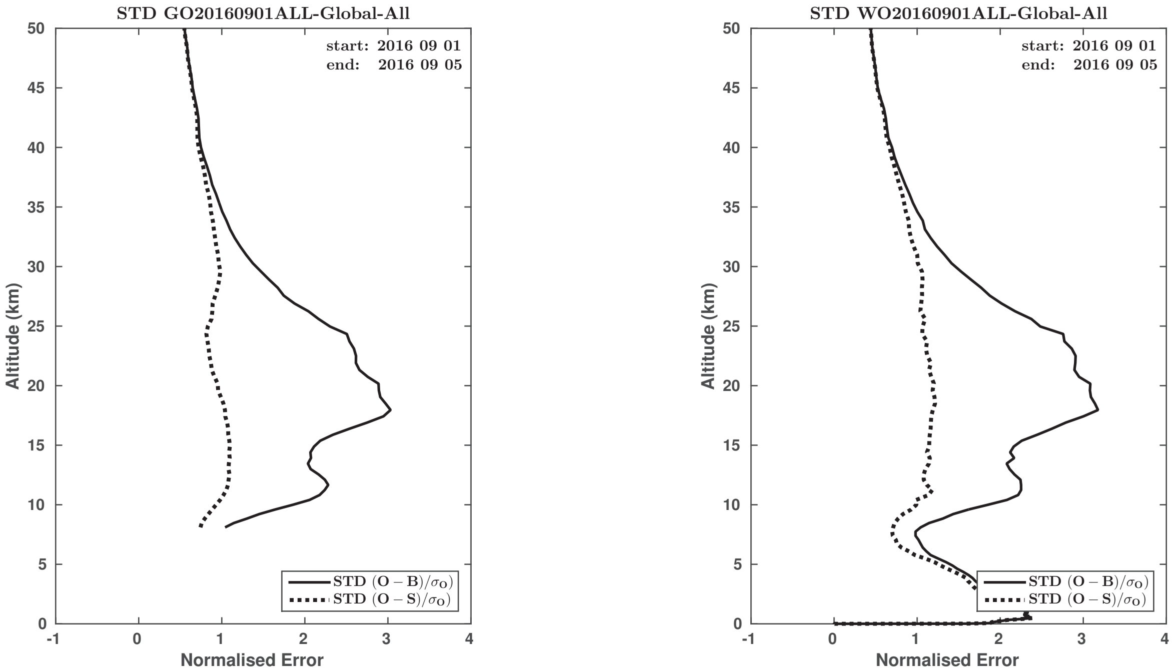


Figure 3.19: Refractivity errors. Standard deviation of $(O-B)/\sigma_O$ (solid) and $(O-S)/\sigma_O$ (dotted). Left: sG, right: sW.

3.5 Compliance with requirements

For the 1D-Var products the accuracy is defined as follows: Standard deviation of the difference of (1D-Var product - model analysis) where “model analysis” is the time interpolated analysis from ECMWF The formal requirements for the ROM SAF data products are given in the Products Requirements Document [AD.3]. The threshold and target requirements are shown in figure 3.10, 3.11, 3.12, 3.13, 3.14 and 3.16 as dashed red and orange curves. I.e. the QC requirements are interpreted as standard deviations of the S-A values. Table 3.3 is summarizing the QC requirements for the 1D-var products.

Standard deviations of observed temperature deviations from the ECMWF analysis (figure 3.10) are within target specifications globally, but fails in the tropical tropopause.

Pressure profiles standard deviations (S-A) are within target values. The pressure profile standard deviation touches the target values around 35 km (figure 3.16), and exceeds the target slightly below 1 km (but not on ground level).

Specific humidities also meet target values (figures 3.12 and 3.13).

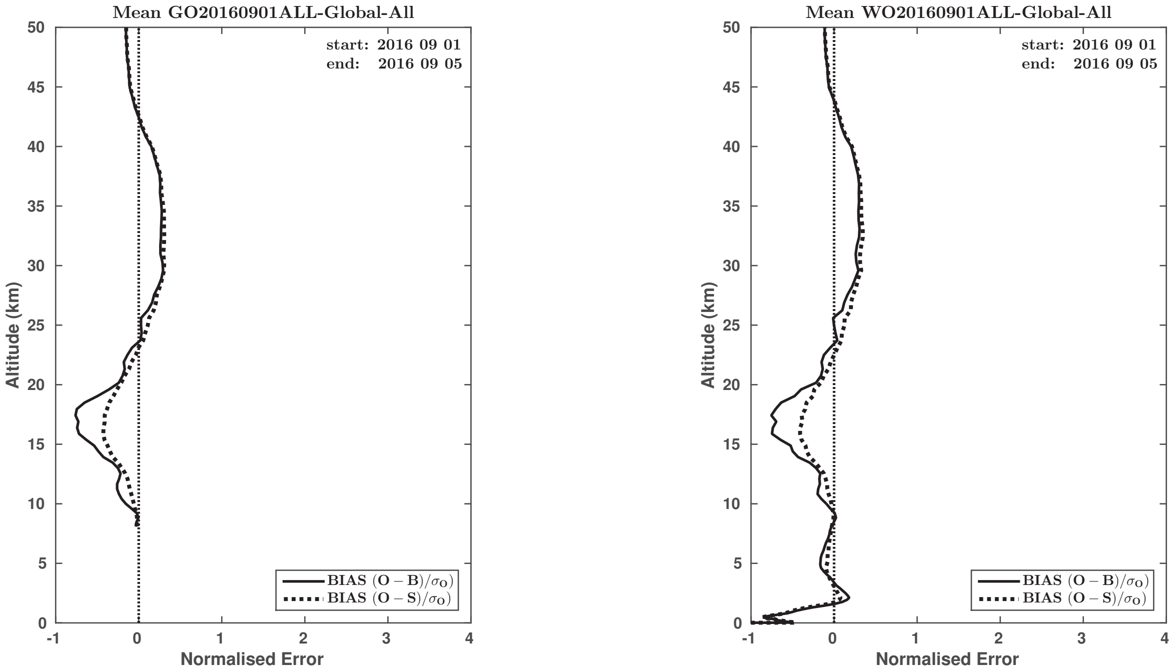


Figure 3.20: Refractivity errors. Mean of $(O-B)/\sigma_O$ (solid) and $(O-S)/\sigma_O$ (dotted). Left: sG, right: sW.

Table 3.3: *Threshold, Target, and Optimal accuracies according to the PRD v. 2.3 [AD.3]*

Threshold	Target	Optimal
GRM-02/41		
0-5 km: 6-3 K 5-30 km: 3 K 30-50 km: 3-30 K	0-5 km: 2-1 K 5-30 km: 1 K 30-50 km: 1-10 K	0-5 km: 1-0.5 K 5-50 km: 0.5 K 30-50 km: 0.5-5 K
GRM-03/42*		
max of 1.8 g/kg or 30 %	max of 0.6 g/kg or 10 %	max of 0.3 g/kg or 10 %
GRM-04/43		
max of 0.03 hPa or 0.75 % but less than 2.4 hPa	max of 0.01 hPa or 0.25 % but less than 0.8 hPa	max of 0.005 hPa or 0.1 % but less than 0.7 hPa
GRM-05/44		
2.4 hPa	0.8 hPa	0.7 hPa

*) Only specific humidity up to 12 km is considered.

3.6 Service specifications

The Service Specifications [AD.4] describes the commitments by the ROM SAF related to the services and products provided to the users. These commitments include a set of operational accuracy targets that should be met by the level 2b and 2c 1D-Var products, and which is monitored regularly and documented as a part of normal operations. In the case of 1D-Var the service specifications (table 3.4) are identical to the target values of product requirements. The target values of table 3.4 should be understood as an average over a running time interval. Compliance to the service specifications will be reported in the biannual operations report.

Table 3.4: *Service specifications for NRT 1D-Var*

Mean of S-A standard deviation
GRM-02/41
0-5 km: 2-1 K 5-30 km: 1 K 30-50 km: 1-10 K
GRM-03/42*
max of 0.6 g/kg or 10 %
GRM-04/43
max of 0.01 hPa or 0.25 % but less than 0.8 hPa
GRM-05/44
0.8 hPa
Notes: Current version of the products may have reduced information content below 8-10 km due to limitations in the input data;

*) Only specific humidity up to 12 km is considered.

4 Open Issues

4.1 GRAS data processing in the lower troposphere

The negative pressure bias in both WO and GO profiles is not fully understood and is therefore a topic for ongoing investigations. In figure 4.1 the pressure biases and standard devi-

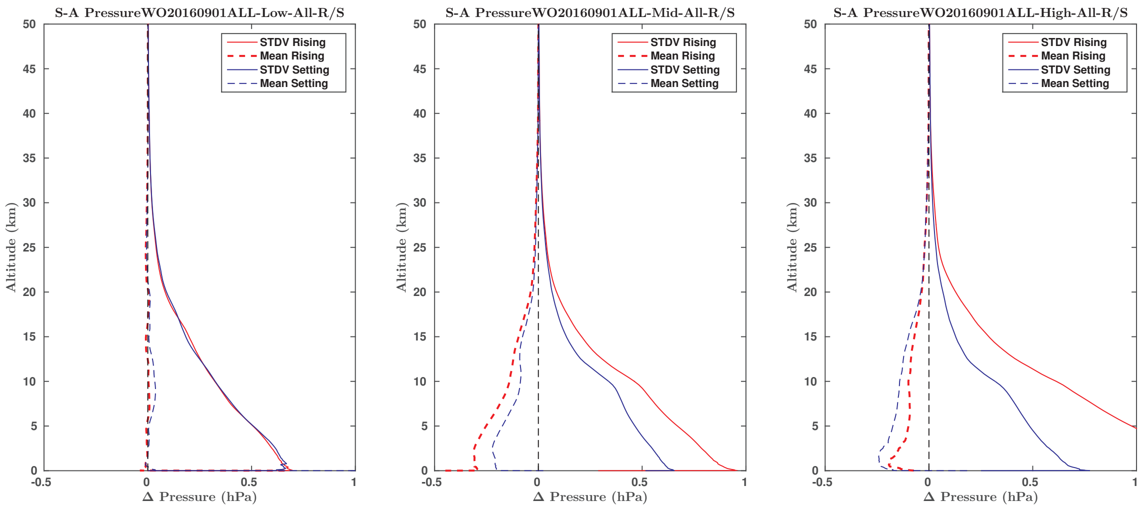


Figure 4.1: Rising (red) setting (blue) pressure (S-A) statistics for tree low(left), mid (mid) high (right)latitudes

ations are broken down in rising/setting occultations for three latitude bands. In addition to the bias which is mostly present at mid and high latitudes, there is also an increased pressure STDV at mid and high latitudes for rising occultations. We speculate that the increased errors are related to an increased refractivity STDV at higher latitudes in rising occultations, between 10 and 30 km. This a subject for future work.

Impact of Background fields

In the ROM SAF 1D-Var ECMWF forecast data are used as background, and therefore the integrity of the occultation data is "compromised". Great care has been taken to reduce the errors of the 1D-Var products through quality control and product validation. The S-A validation scheme seeks to minimize the solutions departure from the ECMWF analysis, but in climate applications one might want to look at the trend of a certain derived parameter, and our validation method does not ensure that possible unphysical trends in the daily analysis are minimized. So for that reason it is not recommended to use the NRT 1D-Var products for climate trend studies. Furthermore, the NRT products are subject to operational updates which may change biases and therefore possibly corrupt trend calculations.

The ROM SAF also produces climate products that are processed with the same configuration throughout the whole GNSS RO era, and re-analysis data are used for such products. The ECMWF reanalysis products are based on homogeneous assimilation procedures, and the quality of 1D-Var based climate products is at least expected to match the reanalysis at which they will be based.

Impact of error assumptions

There is still an issue with the error assumptions that users should be aware of, namely the handling of the water vapour / temperature ambiguity. The handling of this weighting between water and temperature impact on the refactivity is determined by the $\boldsymbol{B}$ matrix. As it is at the moment, $\boldsymbol{B}$ is constructed from the reported errors and error correlations of the IFS model which happens to put all the weight on the humidity in the lower troposphere as seen in Figure 3.8. This reflects that the model has relatively large specific humidity errors in the troposphere. It means that effectively the ROM SAF 1D-Var produces a specific humidity estimate in the troposphere while the temperature is basically a copy of the ECMWF temperature.

5 Conclusions

About 950 refractivity profiles are processed in NRT every day via the 1D-Var procedure into profiles of temperature, pressure and specific humidity. About 1.2 % of the profiles subsequently fail a quality check based on diagnostics of the 1D-Var algorithm.

The tropics generally have higher $2J/m$ scores in the range 2-4, while mid and high latitudes are closer to unity. It is assumed that the increase of the cost function $2J/m$ is due to inconsistent assumptions on the errors in the troposphere. The tuning of the error covarainces $\boldsymbol{B}$ and $\boldsymbol{R}$ will be assessed in the future.

Temperature profiles show a significant reduction in the error estimate in the range 9 km - 35 km (see figure 3.6) indicating that information from the observed profile contributes to the 1D-Var result in this range. Humidity profiles show a considerable reduction in the error estimate in the troposphere between 1 and 8 km.

Validating against co-located ECMWF analyses the 1D-Var temperatures show little or no bias globally and standard deviations increasing from roughly around 0.5 K and staying within 1.0 K below 30 km. Specific humidity S-A standard deviation stays within target values.

The mean bias of surface pressure is -0.1 hPa in sG and -0.14 hPa in sW with a standard deviation of 0.75 hPa and 0.79 respectively. Pressure S-A standard deviations increase from below 0.1 % at the ground to about 0.24 % at 40 km and increase more rapidly above this.

The refractivity errors in figure 3.19 show a clear improvement from the background to the 1D-Var solution when compared to the observed refractivity.

Temperature statistics are within target requirements. Pressure profile statistics are close to or within target requirements, except below 1 km and at the surface. Pressure profiles and surface pressures are still within threshold.

Specific humidities are within target requirements.

It should be noted that the 1D-Var NRT products have limited applicability as climate products. The products depends on the applied background profiles which are subject to occasional updates from ECMWF.