Validation Report: NRT Level 2B and 2C 1D-Var products: Metop-C (GRM-61, 62, 63, 64)

Version 1.1

8 February 2019

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European Centre for Medium-Range Weather Forecasts (ECMWF)
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DOCUMENT CHANGE RECORD

Version	*Date*	*By*	*Description*
1.0	30 Nov 2018	JKN	First version of validation report for NRT Metop-C, prepared for EUMETSAT PVRB on 7 December 2018. (The structure is based on a previous validation report for Metop-A and Metop-B: Removed all discussion to geometric optics versus wave optics; Renewed all figures in Ch. 3 to include Metop-A, Metop-B and Metop-C validation; Ch 3: Rewrote everything to focus on Metop-C differences; Removed section 3.4, refractivity plots)
1.1	8 Feb 2019	JKN	Updated version prepared for EUMETSAT PVRB on 11 February 2019: - p5,17: Validation based on 77 days rather than 10 days - p5: Comment about 10 % drop in nominal refractivity - p15-33: Changed all validation plots - p31: Remeoved sentence; “It is a bit early” - p37: 400 -> 360 - p37: The bias of surface pressure... (slightly modified)

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 Climate Data Records (CDRs) and Interim Climate Data Records (ICDRs) for users requiring a higher degree of homogeneity of the RO data sets. The CDRs and ICDRs 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 aid 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`.

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List of Contents

Executive Summary

NRT Metop-C data has been validated based on a 77 days period (November 16 2018 to January 31 2019). The Metop-C GRAS data meets the product requirements, but the comparison to ECMWF analysis contains an apparent slightly enhanced stochastic noise in the tropical tropopause region compared to Metop-A and Metop-B (when compared to ECMWF analysis). This is presumably due to the fact that Metop-C was not assimilated by the ECMWF during the validation period. The effect of Metop-C assimilation at ECMWF will be monitored by the ROM SAF.

1 Introduction

1.1 Purpose of document

This document describes the validation results for the ROM SAF NRT level 2B and 2C products based on Metop-C. The product version number in this report is 1.3 to match the already existing version numbers for Metop-A and B, and indicating that all three 1D-Var products are processed with the same software. These products are all outputs from the ROM SAF 1D-Var 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 data presented in this document is produced from the NRT refractivity profiles GRM-01 (Metop-A), GRM-40 (Metop-B) and GRM-60 (Metop-C). The product version number of the GRM-60 product validated in this report is 1.6 to match the already existing version numbers for GRM-01 and GRM-40, and indicating that all three products are processed with the same software. The 1D-Var processing is performed using ROPP software version 8.1 and ROM SAF 1DV code version number 3.1.

1.1.1 List of products being validated in this report

Table 1.1: *List of products covered by this Validation Report.*

Product ID	Product name	Product acronym	Product type	Operational satellite input	Dissemination means	Dissemination format
GRM-61	NRT Temperature profile	NTPMEC	NRT	Metop Level 1A/1B data from EUM Secretariat	GTS EUMETCast Web	BUFR netCDF
GRM-62	NRT Specific humidity profile	NHPMEC	NRT	Metop Level 1A/1B data from EUM Secretariat	GTS EUMETCast Web	BUFR netCDF
GRM-63	NRT Pressure Profile	NPPMEC	NRT	Metop Level 1A/1B data from EUM Secretariat	GTS EUMETCast Web	BUFR netCDF
GRM-64	NRT Surface Pressure	NSPMEC	NRT	Metop Level 1A/1B data from EUM Secretariat	GTS EUMETCast 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-3 Proposal: Proposal for the Third Continuous Development and Operations Phase (CDOP-3); Ref: SAF/ROM/DMI/MGT/CDOP3/001 Version 1.2 of 31 March 2016, Ref: EUM/C/85/16/DOC/15, approved by the EUMETSAT Council at its 85th meeting on 28-29 June 2016.

[AD.2] CDOP-3 Cooperation Agreement: Agreement between EUMETSAT and DMI on the Third Continuous Development and Operations Phase (CDOP-3) of the Radio Occultation Meteorology Satellite Applications Facility (ROM SAF), Ref. EUM/C/85/16/DOC/19, approved by the EUMETSAT Council and signed at its 86th meeting on 7 December 2016.

[AD.3] ROM SAF 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] ECMWF, http://www.ecmwf.int/products/data/technical/model_levels/index.html and http://www.ecmwf.int/...
research/ifsdocs/DYNAMICS/Chap2_Discretization4.html#961180, 2018.

[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] Poli, P., Joiner, J., and Kursinski, E. R., 1DVAR analysis of temperature and humidity using GPS radio occultation refractivity data, *J. Geophys. Res.*, *107*, doi:10.1029/2001JD000 935, 2002.

[RD.7] 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.8] 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.9] ROM SAF, Validation Report: Reprocessed Level 2B and 2C 1D-Var CDR v1.0 products (Short title: Validation Report: Reprocessed 1D-Var products), SAF-/ROM/DMI/REP/1DVAR/001, -.

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

[RD.11] ROM SAF, Validation Report: NRT Level 2A and 2C 1D-Var products (Metop-A: GRM-02,03,04,05) (Metop-B: GRM-41,42,43,44), Version 1.8, SAF/ROM/DMI-/RQ/REP/002, 2016.

[RD.12] 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, Version 1.6, 2016.

[RD.13] ROM SAF, Algorithm Theoretical Baseline Document: Level 2B and 2C 1D-Var products, SAF/ROM/DMI/ALG/1DV/002, 2018.

[RD.14] ROM SAF, Algorithm Theoretical Baseline Document: Level 2B and 2C 1D-Var products, Versoin 3.0, SAF/ROM/DMI/ALG/1DV/002, 2018.

[RD.15] ROM SAF, Validation Report: NRT Level 2A Refractivity Profiles: Metop-C (GRM-60), Version 1.0, Ref: SAF/ROM/DMI/RQ/REP/003, 2018.

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)
GRM	Product id.
GO	Geometrical Optics
IFS	Integrated Forecast System
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	Radio Occultation Meteorology Satellite Application Facility
ROPP	Radio Occultation Processing Package
SAF	Satellite Application Facility (EUMETSAT)
SAG	Scientific Advisory Group
STDV	Standard Deviation
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, offline, CDR, or ICDR). The data levels and product types are defined below[1]. 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, SNRs, 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:

[1] Note that the level definitions differ partly from the WMO definitions: `http://www.wmo.int/pages/prog/sat/dataandproducts_en.php`

NRT product: Data product delivered less than: (i) 3 hours after measurement (SAF Level 2 for EPS); (ii) 80 min after measurement (SAF Level 2 for EPS-SG Global Mission); (iii) 40 min after measurement (SAF Level 2 for EPS-SG Regional Mission);

Offline product: Data product delivered from less than 5 days to up to 6 months after measurement, depending on the requirements. The evolution of this type of product is driven by new scientific developments and subsequent product upgrades;

CDR: Climate Data Record generated from a dedicated reprocessing activity using a fixed set of processing software[2]. The data record covers an extended time period of several years (with a fixed end point) and constitutes a homogeneous data record appropriate for climate usage;

ICDR: An Interim Climate Data Record (ICDR) regularly extends in time a (Fundamental or Thematic) CDR using a system having optimum consistency with and lower latency than the system used to generate the CDR[3].

1.5 Overview of this document

Chapter 2 contains background. Chapter 3 contains QC results and validation. Chapter 4 relates Metop-C data to product requirements. Chapter 5 summarizes open issues. Chapter 6 contains conclusions.

[2] (i) GCOS 2016 Implementation Plan; (ii) `http://climatemonitoring.info/home/terminology`

[3] `http://climatemonitoring.info/home/terminology` (the ICDR definition was endorsed at the 9th session of the joint CEOS/CGMS Working Group Climate Meeting on 29 March 2018).

2 Background

2.1 Refractivity profiles

The input data 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, GRM-40 and GRM-60 (Level 2B). The validation in this report is based on EUMETSAT PPF 4.6 data from the Metop-A, Metop-B and Metop-C satellites, retrieved in the time period November 16 to 25, 2018 [RD.12]. 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 [RD.15]. 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 45r1, 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.

2.2.1 Description of algorithm and Level 2B configuration

The atmospheric refractivity 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.6, 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.13].

2.2.2 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 2.3)

2.2.3 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 smooth and there is practically 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

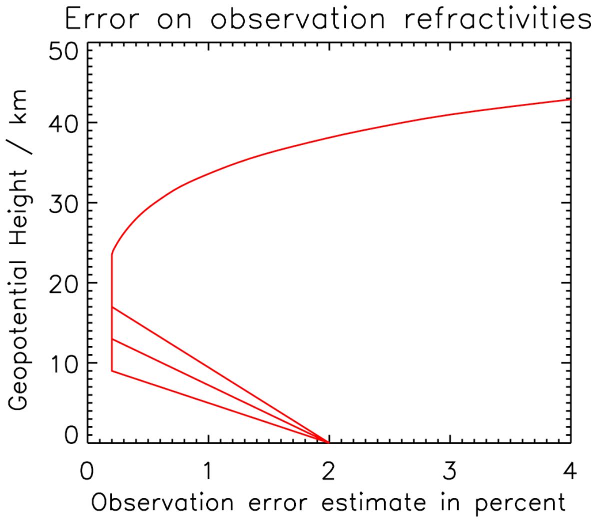

Figure 2.1: *Fractional refractivity error estimates for 3 different tropopause heights (9km, 13km, 17km).*

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.8]. 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).

2.2.4 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).

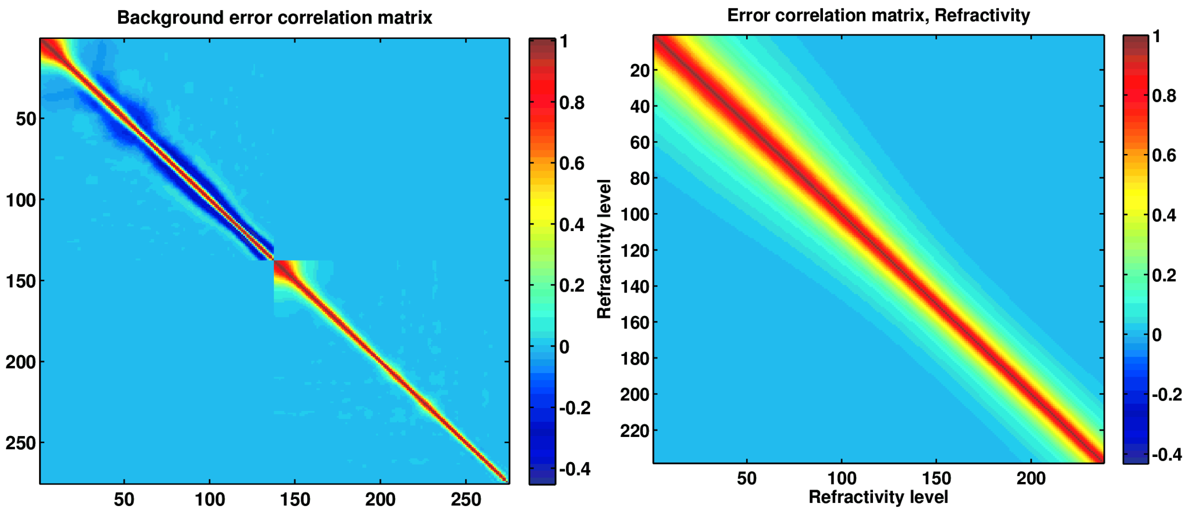

Figure 2.2: *Left: Error correlation matrix between 275 state-vector entries. Index 1-137; temperature error correlations. Index 138-274; specific humidity error correlations. Last row and column (index 275) shows surface pressure error correlations (zeros except for the diagonal). Right: Refractivity 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.13]. 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.

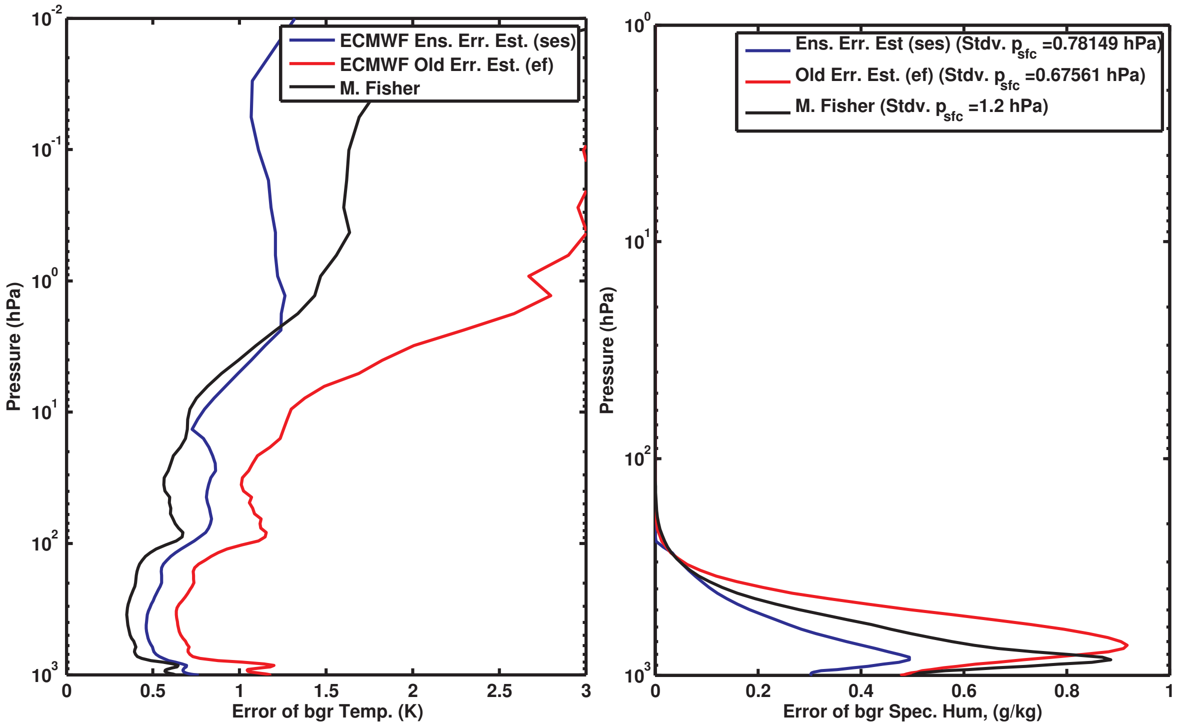

Figure 2.3: *Temperature background error profile (left) and specific humidity background error profile (right). (See caption for surface pressure background error). The figure also shows some previous background error assumptions based on the socalled "ef" (error of first guess) fields and an old error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

2.3 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 from 16 November 2018 to 31 January 2019, i.e. a data set which has assimilated Metop-A and Metop-B RO data. We show equivalent validation figures based on profiles produced from Metop-A, Metop-B and Metop-C from the same dates. Figures in this section are all based on Data version 1.3, Wave Optics, with background and analysis profiles from ECMWF IFS Cycle 45r1, processed width DMI ROM SAF 1DVar v3.1. 47,743 Metop-C profiles are included in this validation.

The validation results presented in this document are based on version 1.5 of the NRT refractivity profiles (GRM-01, GRM-40 and GRM 60). 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.

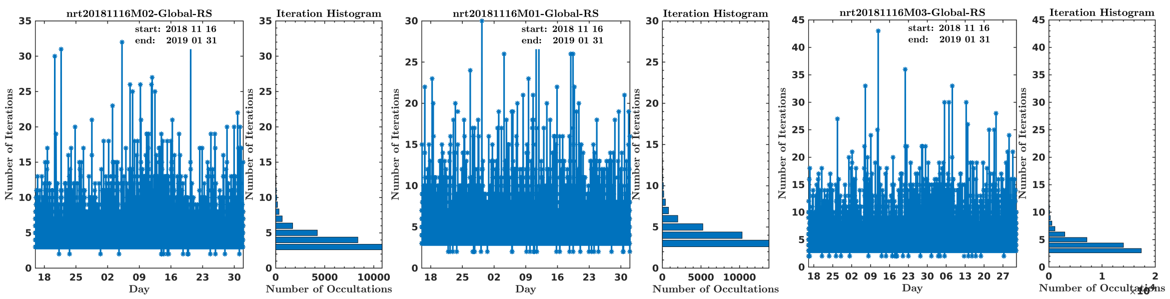

Figure 3.1: *Number of iterations of the minimiser needed to find a solution. Time series and histogram. Left: Metop-A, middle Metop-B, right: Metop-C.*

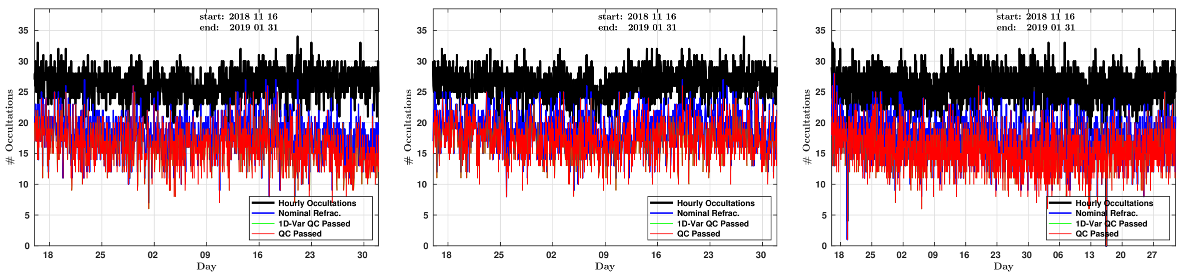

Figure 3.2: *QC performance time series plotted as hourly occultations. Total number of occultations (black), occultations with nominal refractivity (blue), occultations with nominal 1D-Var result (green) and the final number of successful profiles (red)). Left: Metop-A, middle Metop-B, right: Metop-C.*

Figure 3.2 shows the 4 key numbers (total number of occultations, occultations with nominal refractivity, occultations with nominal meteorology and the final number of completely successful profiles) illustrating the performance of 1D-Var as function of time through the 77 days period wich is the focus of the analysis. The dataset is subject to QC version 1.3. for which the threshold of the cost function $2J/m$ was set to 13.0. The QC results at different levels of processing are kept such that 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.

The QC performance is summarized in table 3.1. We note that the instruments on the three satellites perform equally well. A part of the profiles pass the refractivity QC but fails to be processed through 1D-Var. Only few of these, (1.1 - 1.3 %), are actually caught by he 1D-Var QC, the rest fails before an output is produced. The main reason for this is that 4.9% of the refractivity records are empty (these are counted as nominal, because that is the default). In a few cases the reason is that the 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; nrt20181116M02-Global-RS

Total # of profiles:	29036	100.0 %
Nominal refractivity:	19515	67.2%
$\frac{2J}{m} \geq 13$	320	1.1%
Passing QC, (incl. 1D-Var QC) :	17757	61.2%

QC performance; nrt20181116M01-Global-RS

Total # of profiles:	29266	100.0 %
Nominal refractivity:	20211	69.1%
$\frac{2J}{m} \geq 13$	357	1.2%
Passing QC, (incl. 1D-Var QC) :	18594	63.5%

QC performance; nrt20181116M03-Global-RS

Total # of profiles:	47743	100.0 %
Nominal refractivity:	31125	65.2%
$\frac{2J}{m} \geq 13$	522	1.1%
Passing QC, (incl. 1D-Var QC) :	28272	59.2%

Table 3.1: *QC summary for Metop-A (top), Metop-B (middle) and Metop-C (bottom).*

3.1.2 $2J/m$ quality measure

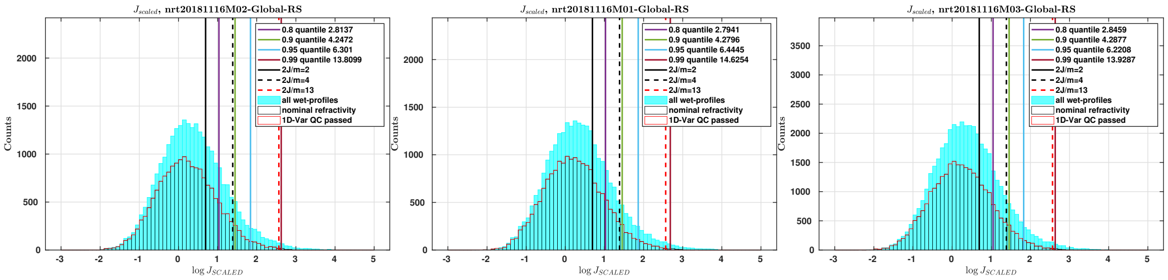

Figure 3.3: *$2J/m$ time series and histograms. Left: Metop-A, middle Metop-B and right: Metop-C.*

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.7]. 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 covaraínces $\boldsymbol{B}$ and $\boldsymbol{R}$ will be addressed in the future.

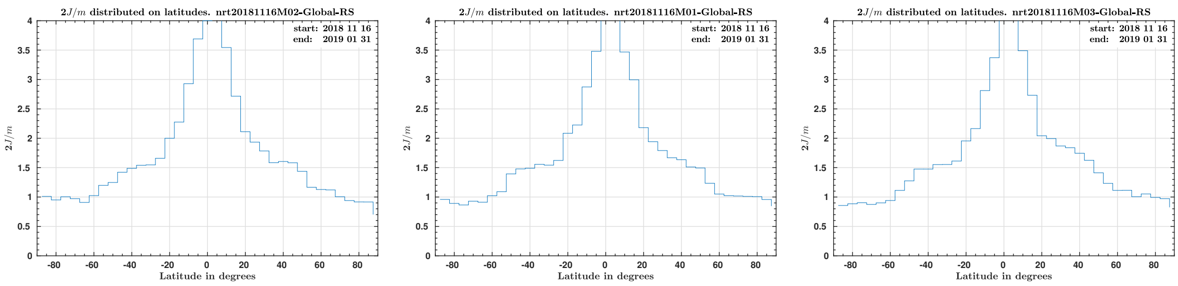

Figure 3.4: *Mean $2J/m$ as a function of latitude. Left: Metop-A, middle: Metop-B, right: Metop-C.*

The latitude dependence of $2J/m$ is also illustrated with histograms in figure 3.5. Even though the cost function distribution varies with latitude, it is reasonable to have a common $2J/m$ threshold (13.0) value for all latitudes. The increased values in the tropics reveals the 1D-Var solution is of less good quality than higher latitudes.

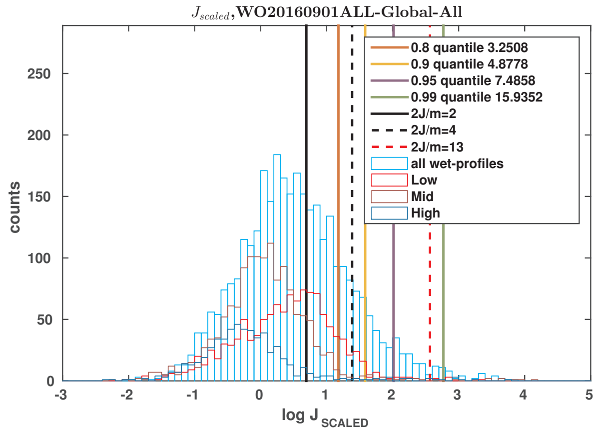

Figure 3.5: *$J_{scaled} = \frac{2J}{m}$ distribution for Metop-A and Metop-B (September 2016), partitioned on different latitude bands; Low < 30 deg ≤ Mid < 60 deg ≤ High.*

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 variables are 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 ythe 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. 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.

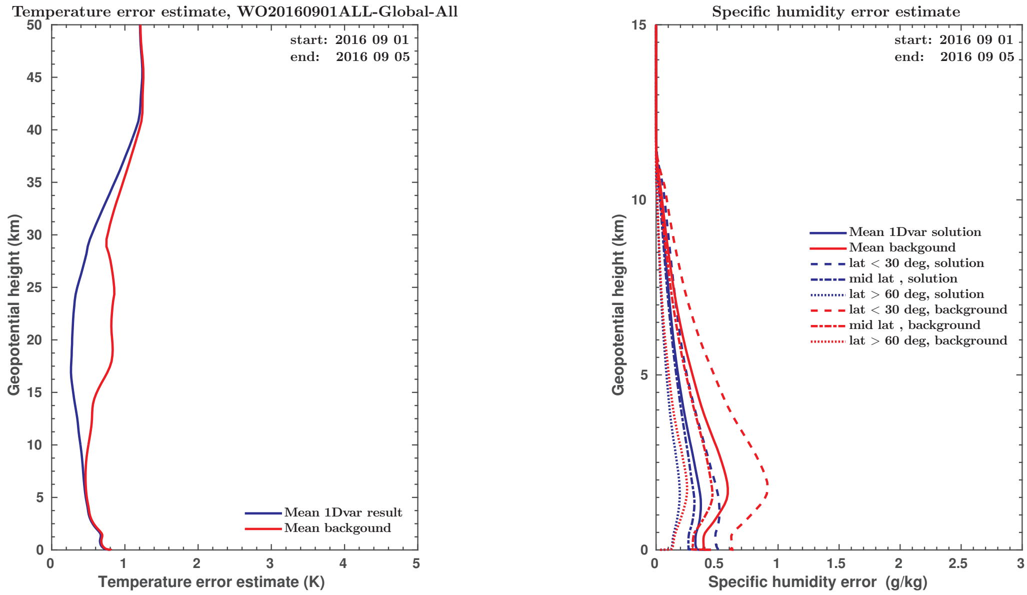

Figure 3.6: *Background (red) and solution (blue) error estimates for temperature (left) and specific humidity (right). Metop-A and Metop-B (September 2016).*

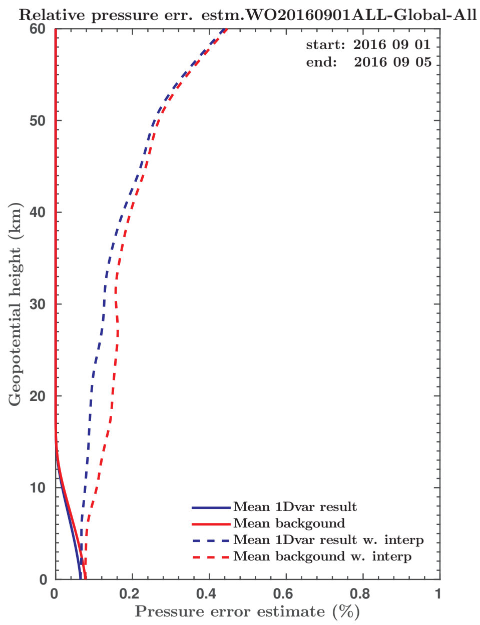

Figure 3.7: *Background (red) and solution (blue) error estimates for pressure. The solid branches represents the error of the pressure disseminated at model levels, and the dashed branches represents the effective error arising from interpolation to geopotential height levels. Metop-A and Metop-B (September 2016).*

Prior fractions

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.

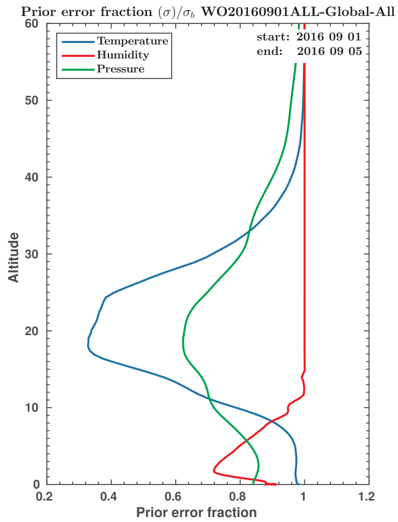

Figure 3.8: *Prior reduction vectors for temperature, specific humidity and pressure. All latitudes Metop-A and Metop-B.*

In Figure 3.8 it is shown that there is generally no observational information in the temperature in the troposphere. The observation broadly impacts the stratospheric temperature and the tropospheric specific humidity.

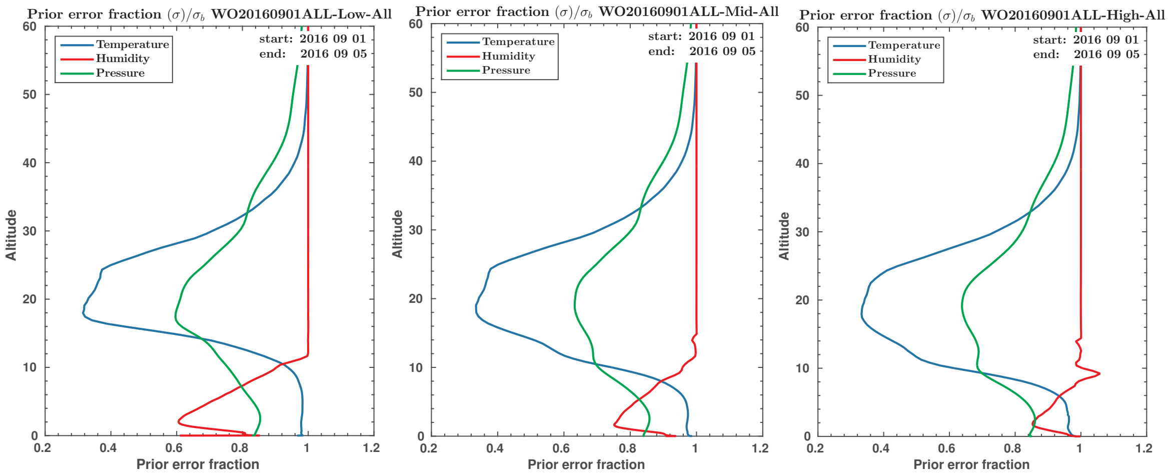

Figure 3.9: *Prior reduction vectors for temperature, specific humidity and pressure. Left: Low latitudes, middle: Mid latitudes and right: High latitudes. The positive prior fraction around 9 km altitude at high latitudes is understood. It is caused by the process of transforming the background specific humidity error covariance matrix to a logarithmic scale before 1D-Var is executed and then transforming the solution error back again, with a transform based on the solution, afterwards. The implementation of the transform is not reversible, and this is seen in particularly dry cases.*

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 around 10 km altitude 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 Cy45r1 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. The ECMWF analysis has in most cases assimilated the occultation which is being evaluated.

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.

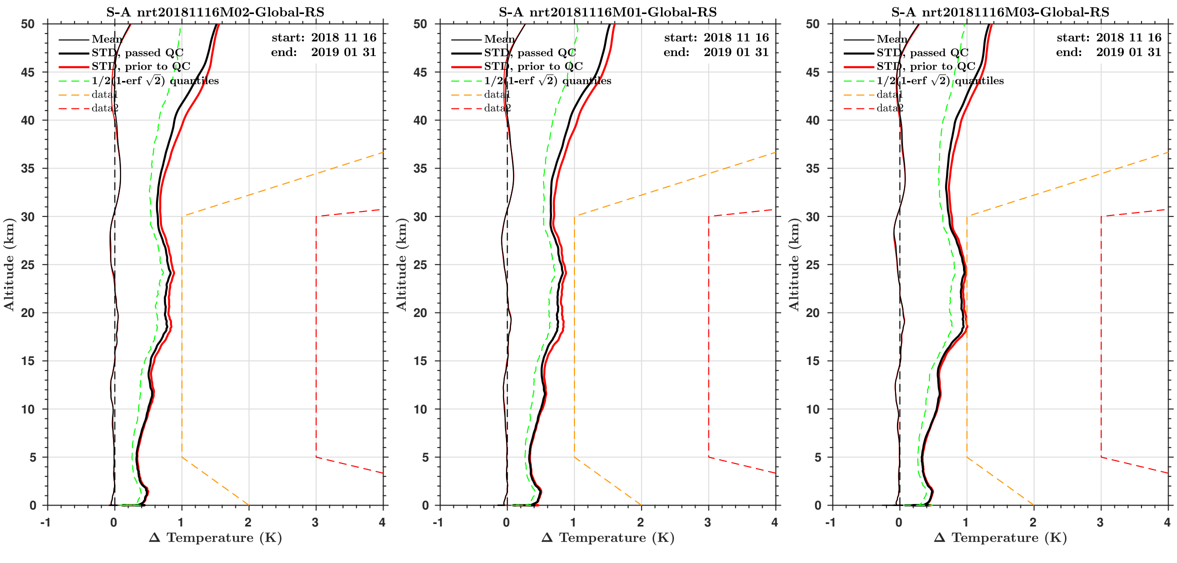

Figure 3.10: *Temperature; 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias ± STDV. Also shown; the formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]) and the quantile corresponding to 1 STDV in a Gaussian distribution (green). I.e, if the distribution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

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, and in figure 3.11 the differences between profiles in different latitude bands are 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 standard deviation 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 (S-A) standard deviation exceeds the target between 16 and 26 km at low latitudes for Metop-C. We assume that this is because Metop-C is not assimilated by ECMWF in the validation time interval, and therefore the ECMWF analysis deviates a bit more from Metop-C than from Metop-A and Metop-B. 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.
- Metop-C seems to have an apparent slightly higher standard deviation between 10 and 30 km than Metop-A and Metop-B (presumably because Metop-C is not assimilated in ECMWF). Metop-C is still within the target globally.
- The increased Metop-C standard deviation origins mostly from the tropics, peaking near the tropopause at 18 km (Figure 3.11).

1D-Var temperature in different latitude bands

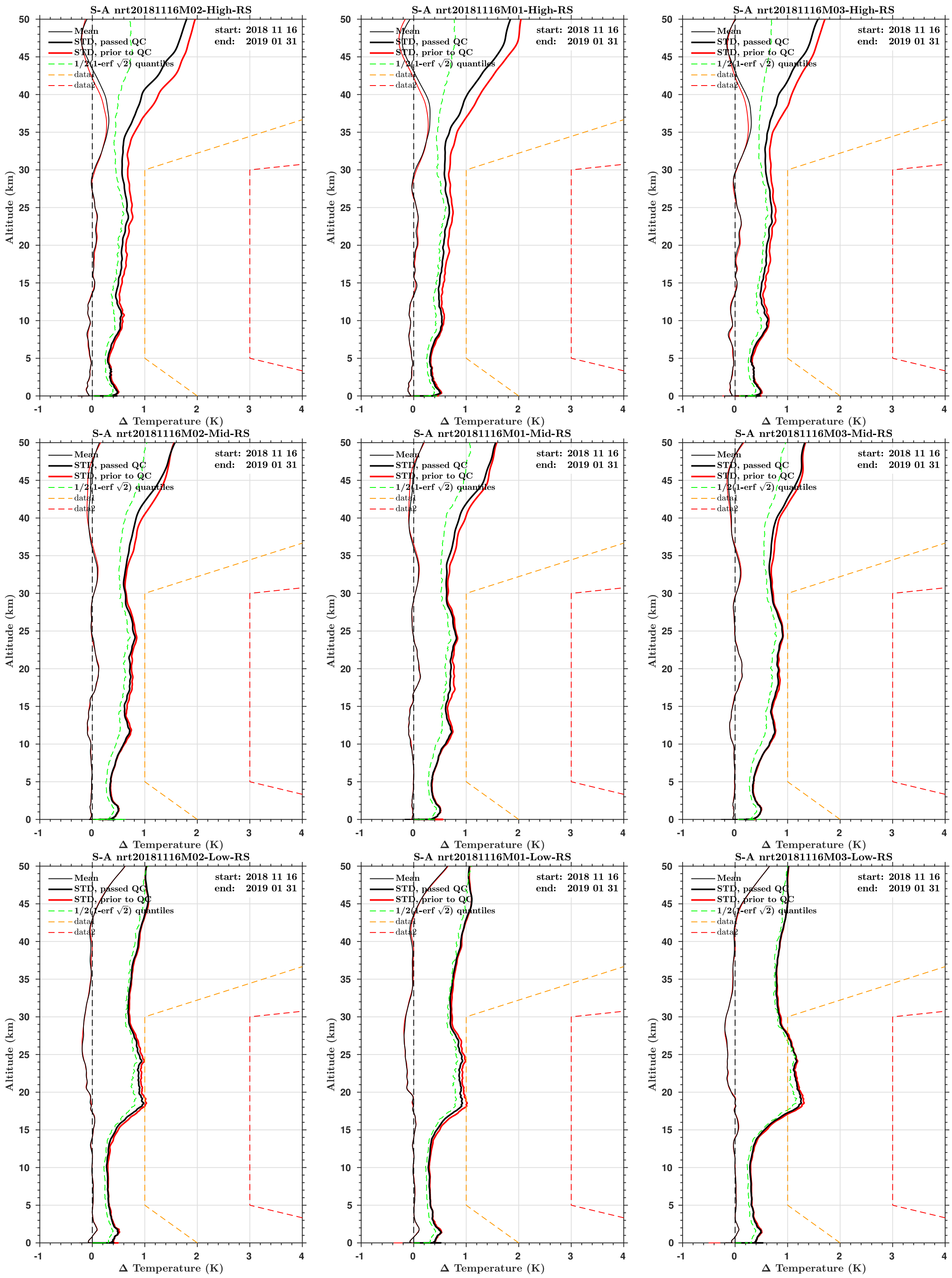

__Figure 3.11:__ Temperature; 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias ± STDV. As in figure 3.10. Top: 60 to 90 deg latitude; middle 30 to 60 deg latitude; bottom: 0 to 30 deg latitude. Left: Metop-A, middle: Metop-B, right: Metop-C.

3.3.2 Specific humidity

Figures 3.12 and 3.13 show comparisons of 1D-Var specific humidity solution profiles against ECMWF analyses. Figure 3.12 shows comparisons of the 1D-Var specific humidity solution profiles against ECMWF analysis (S-A statistics) together with the PRD specifications. Figure 3.14 show the specific humidity performance broken down on latitude bands. The following may be noted:

- The bias structures of the 3 instrumentations are different. Especially Metop-C is positively biased in the tropics. But we will not conclude anything about that on this early stage.
- Specific humidity S-A standard deviations complies with the PRD target value globally.
- Specific humidity S-A standard deviations exceeds the PRD target value in the tropics.
- 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. Especially in the middle troposphere.

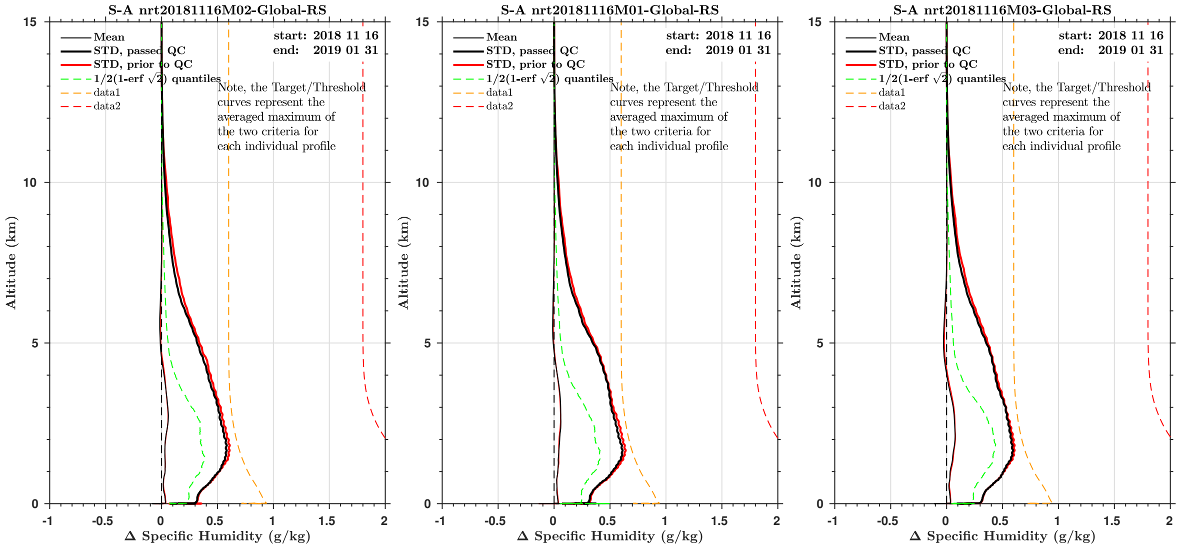

Figure 3.12: *Specific Humidity; 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias ± STDV. Also shown; the formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]) and the quantile corresponding to 1 STDV in a Gaussian distribution (green). I.e, if the distribution had been gaussian the green line would be on top of the black line. Left: Metop-A, middle: Metop-B, right: Metop-C*

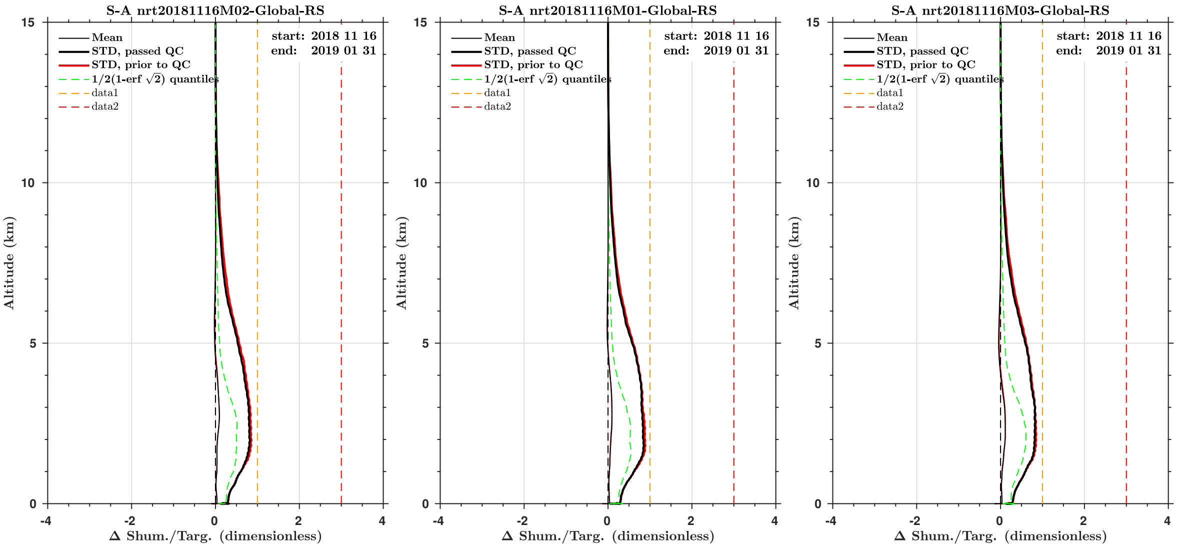

Figure 3.13: *Specific humidity; 1D-Var specific humidity minus ECMWF 4D-Var analysis relative to the target value. Also shown; the formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]) and the quantile corresponding to 1 STDV in a Gaussian distribution (green). I.e, if the distribution had been gaussian the green line would be on top of the black line. Left: Metop-A, middle: Metop-B, right: Metop-C*

1D-Var specific humidity in different latitude bands

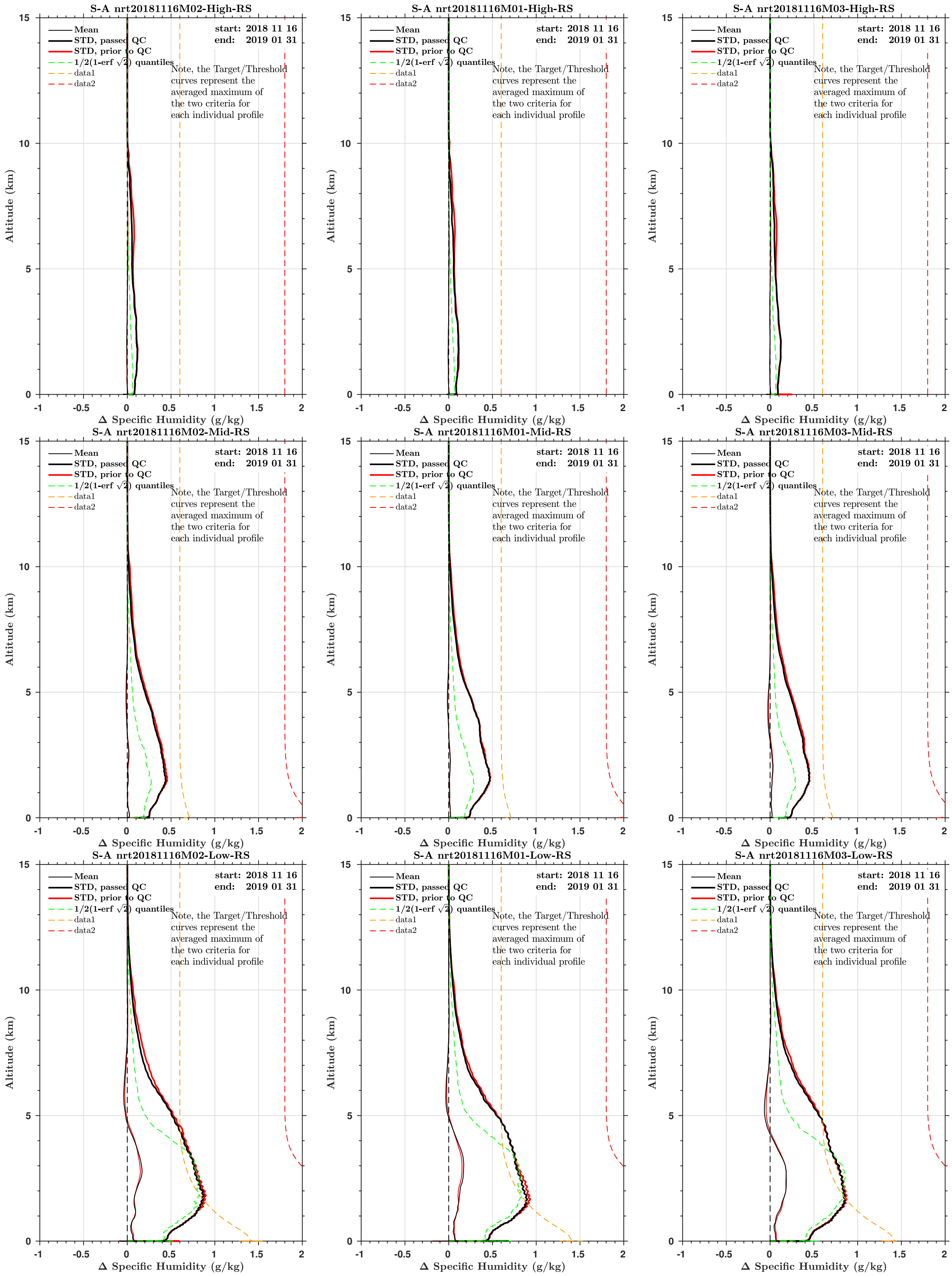

Figure 3.14: Specific humidity; 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias ± STDV. As in figure 3.12. Top: 60 to 90 deg latitude; middle 30 to 60 deg latitude; bottom:0 to 30 deg latitude. Left: Metop-A, middle: Metop-B, right: Metop-C.

3.3.3 Pressure profile and surface pressure

The absolute deviations of 1D-Var pressure from ECMWF analysis are shown in Figure 3.15, and the relative pressure deviations are shown in 3.16 and 3.17. Table 3.2 shows the bias and standard deviations of surface pressure. The following points are noticed:

- The surface pressure has a negative bias of 0.22 - 0.26 hPa at high and mid latitudes.
- The surface pressure has a positive bias of 0.11 - 0.15 hPa at low latitudes.
- The surface pressure standard deviation is generally between 0.62 and 0.70 hPa.
- Pressure standard deviations increase from less than 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 nearly touched around 35 km. See further discussion in4.1.

The positive pressure bias in all profiles above 30 has been fully understood during the ROM SAF reprocessing. It is as a consequence of a false vertical interpolation scheme in ERA-Interim. The solution to this problem is described in [RD.14]. The 1D-Var results presented here are based on positively biased linear pressure interpolation between model half levels, while the analysis profiles are produced with the more accurate scheme described in [RD.14], hence the pressure difference above 30 km.

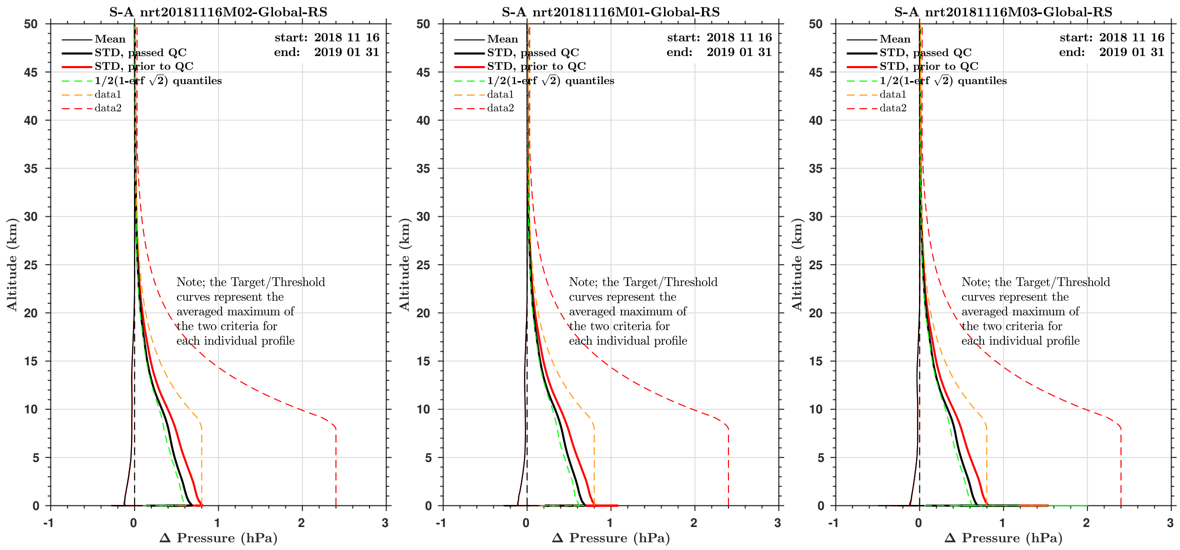

Figure 3.15: *1D-Var pressure minus ECMWF 4D-Var analysis pressure. Also shown: The formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a gaussian distribution (green). Left: Metop-A, middle: Metop-B, right: Metop-C*

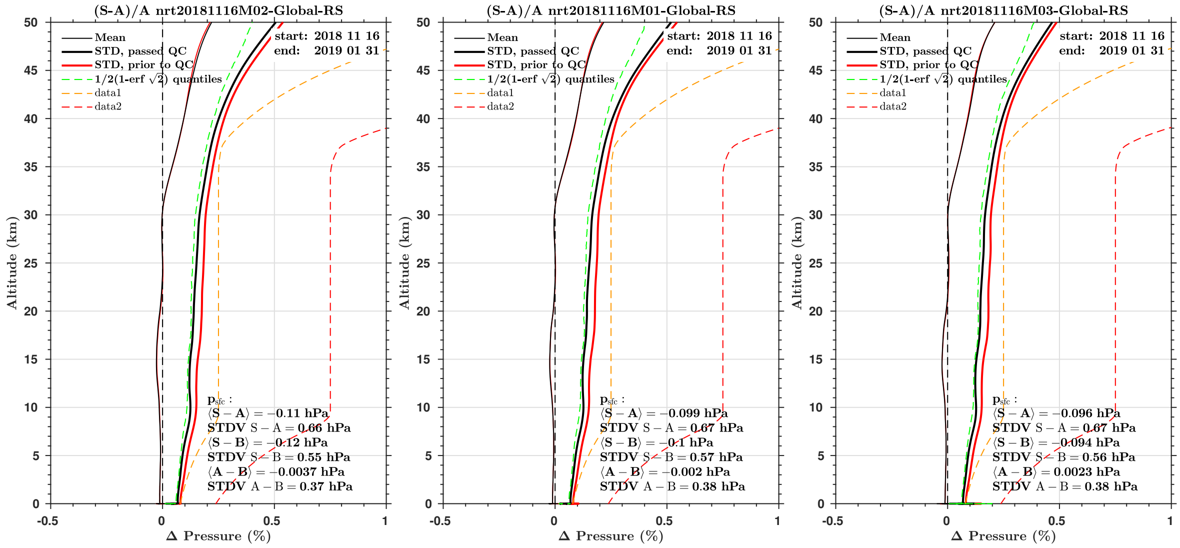

Figure 3.16: *Relative pressure deviations (S-A)/A . Also shown: The formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a gaussian distribution (green). Left: Metop-A, middle: Metop-B, right: Metop-C*

1D-Var pressure in different latitude bands

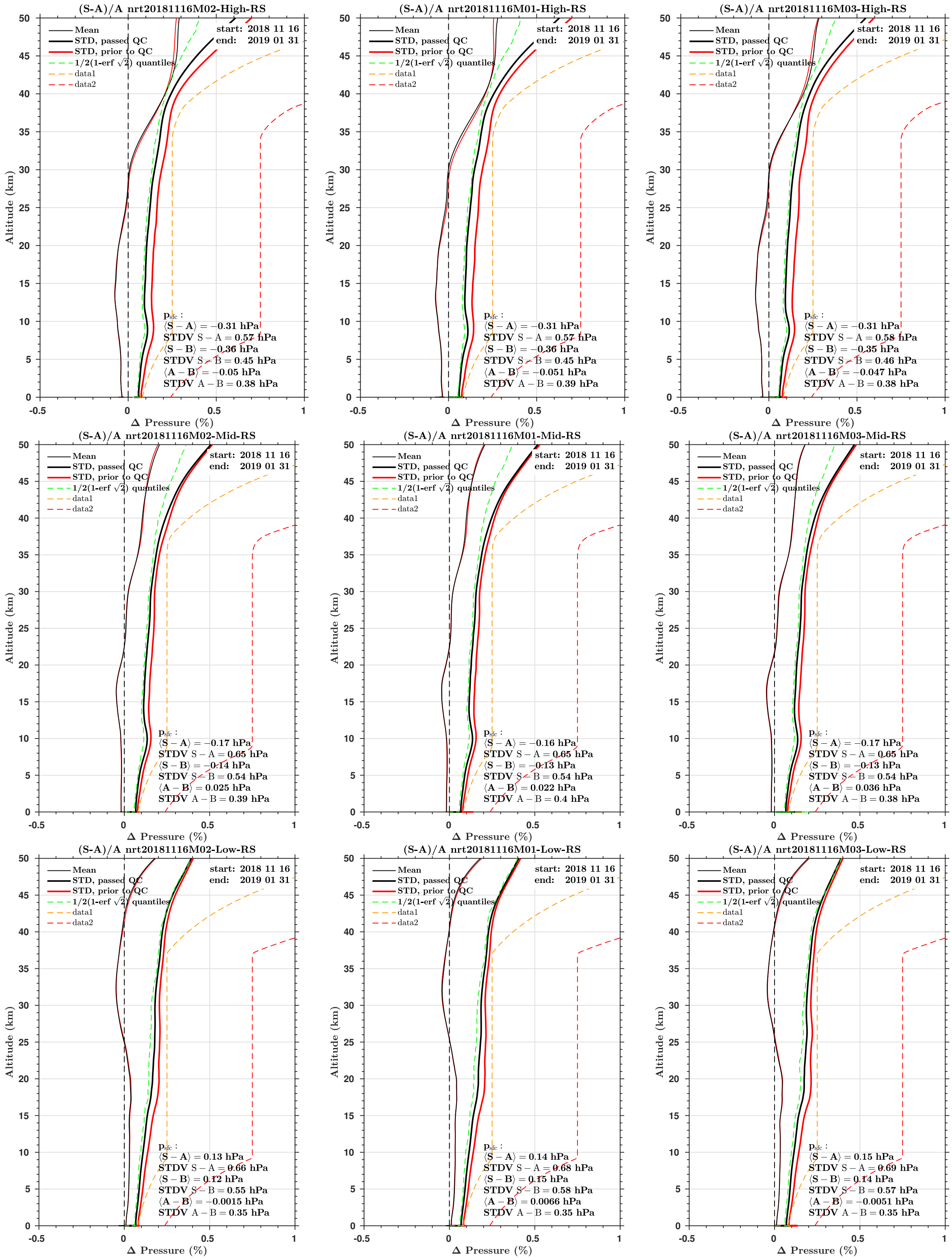

Figure 3.17: *1D-Var pressure relative to ECMWF 4D-Var analysis. Also shown are: The formal 'Threshold' (red) and 'Target' (orange) data quality requirements (see [AD.3]), and the quantile corresponding to 1 STDV in a Gaussian distribution (green). Statistics for surface pressure are inserted in lower right corners. Top: 60 to 90 deg latitude; middle 30 to 60 deg latitude; bottom:0 to 30 deg latitude. Left: Metop-A, middle: Metop-B, right: Metop-C.*

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

		Bias (hPa)	STDV (hPa)
Metop-A global	S-A	-0.12	0.67
Metop-A high	S-A	-0.27	0.62
Metop-A mid	S-A	-0.22	0.65
Metop-A tropics	S-A	0.11	0.67
Metop-B global	S-A	-0.11	0.70
Metop-B high	S-A	-0.26	0.64
Metop-B mid	S-A	-0.23	0.66
Metop-B tropics	S-A	0.15	0.70
Metop-C global	S-A	-0.11	0.67
Metop-C high	S-A	-0.22	0.62
Metop-C mid	S-A	-0.23	0.63
Metop-C tropics	S-A	0.12	0.70

1D-Var for setting and rising occultation.

In figure 3.18 we show a comparison between the Metop-C 1D-Var results and ECMWF analysis for rising and setting occultations for all latitudes. Globally there is no noticeable difference between standard deviations or biases from setting and rising occultations. In the previous validation [RD.11] of Metop-A and Metop-B wave optics data, we observed that the standard deviation of rising occultations was enhanced with more than 50%. We attribute this significant change to the instrument upgrade 1st of August 2018. This is in fact an improvement for Metop-A and Metop-B which failed to meet the target in the tropics in the previous validation [RD.11].

In figure 3.19 the pressure biases and standard deviations are broken down in rising/setting occultations for three latitude bands. We observe a very small negative bias difference for rising occultations of the order of 0.05 hPa which is mostly present at mid and high latitudes. There is also a decreased pressure STDV at low latitudes for rising occultations. Metop-C has a slightly different signature with increased standard deviation at high latitudes for rising occultations.

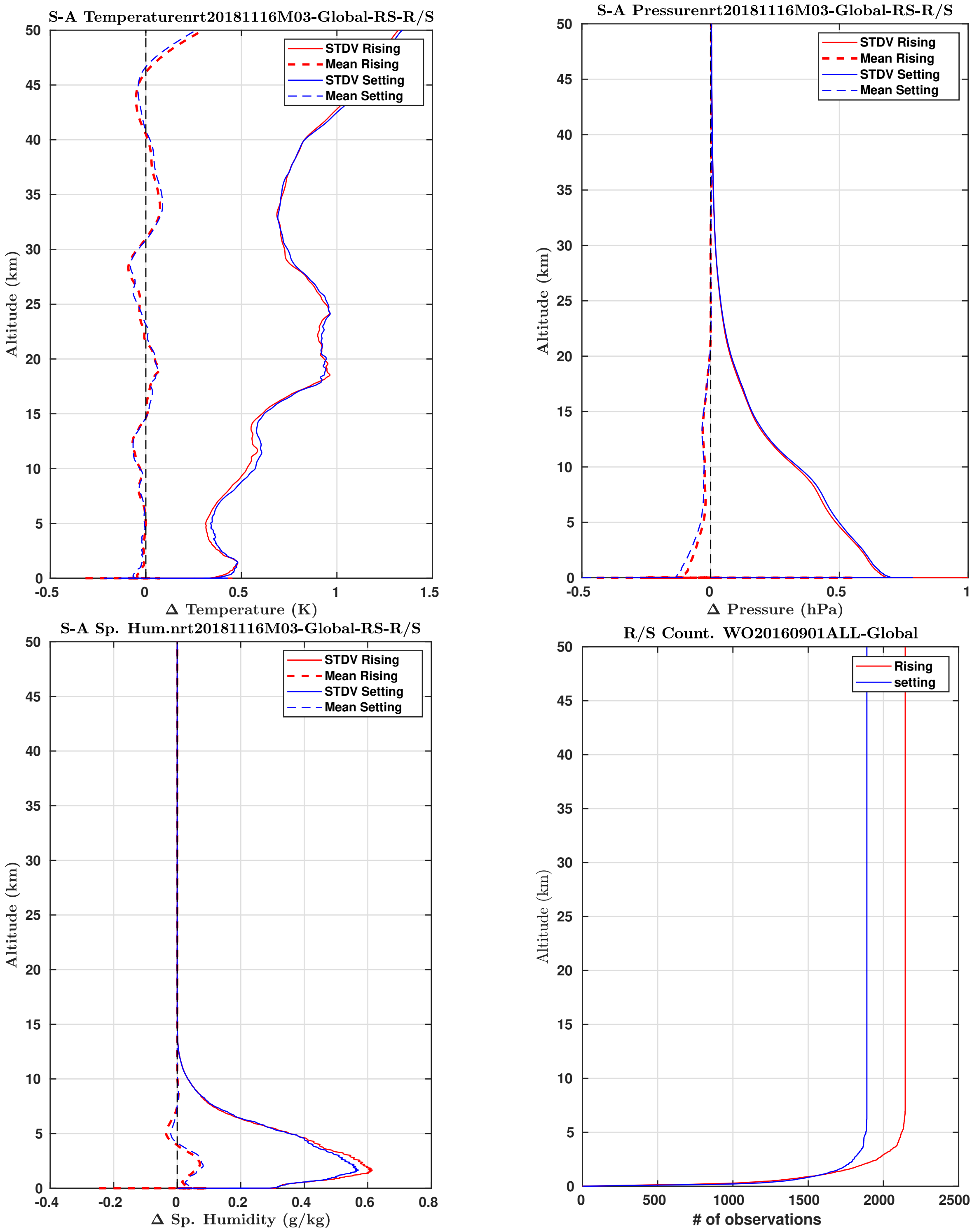

Figure 3.18: *Metop-C, (16th to 25th November 2018) rising (red) and setting (blue). Temperature, Sp. Humidity and Pressure; 1D-Var solution minus ECMWF 4D-Var analysis (S-A) bias and bias STDV.*

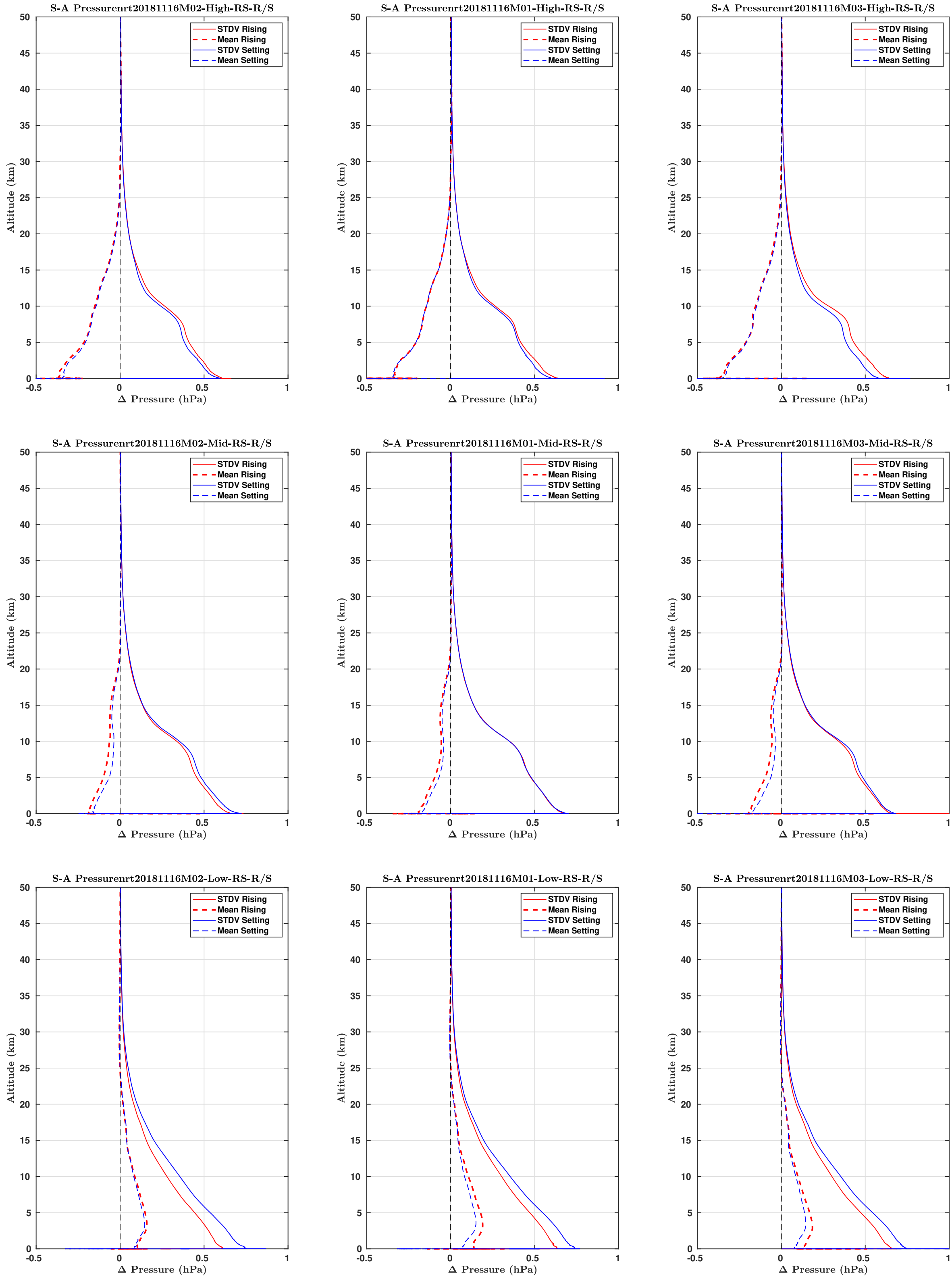

Figure 3.19: *(Metop-A (left), Metop-B (middle) and Metop-C (right), 16th to 25th November 2018). Rising (red) setting (blue) pressure (S-A) statistics for low (bottom), mid (middle) and high (top) latitudes*

4 Product Requirements

4.1 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, 3.15 and 3.17 as dashed red and orange curves. I.e. the QC requirements are interpreted as standard deviations of the S-A values. Table 4.1 is summarizing the QC requirements for the 1D-var products.

Table 4.1: *Threshold, Target, and Optimal accuracies for Metop-C according to the PRD [AD.3]*

Threshold	Target	Optimal
GRM-61		
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-62		
0-12 km: Max of 1.8 g/kg or 30%	0-12 km: Max of 0.6 g/kg or 10%	0-12 km: Max of 0.3 g/kg or 10%
GRM-63		
0-50 km: Max of 0.03 hPa or 0.75% but less than 2.4 hPa	0-50 km Max of 0.01 hPa or 0.25% but less than 2.4 hPa	0-50 km Max of 0.005 hPa or 0.1% but less than 2.4 hPa
GRM-64		
2.4 hPa	0.8 hPa	0.7 hPa

Standard deviations of observed temperature deviations from the ECMWF analysis (figure 3.10) are within target specifications globally, except for Metop-C which fails meet the target value in the tropical tropopause.

Specific humidities also meet target values globally, as well as on high and mid latitudes, but all instruments fails to meet the target in the tropics (figures 3.12 and 3.13).

Pressure profiles and surface pressure standard deviations (S-A) are within target values globally as well as in individual latitude bands.

4.2 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 are monitored regularly and documented as a part of normal operations. In the case of 1D-Var the service specifications (table 4.2) are identical to the target values of product requirements. The target values of table 4.2 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 4.2: *Service specifications for NRT Metop-C 1D-Var products*

Mean of S-A standard deviation
GRM-61
0-5 km: 2-1 K 5-30 km: 1 K 30-50 km: 1-10 K
GRM-62
0-12 km: Max of 0.6 g/kg or 10 %
GRM-63
0-50 km: Max of 0.01 hPa or 0.25 % but less than 0.8 hPa
GRM-64
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; see [RD.12]

5 Open Issues

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 a user might wish to look at the trend of a certain derived parameter, and our validation method does not ensure that possible un-physical 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 data records that are processed with the same configuration throughout the whole GNSS RO era, and re-analysis data are used for such products [RD.9]. 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 on which they are based.

Impact of error assumptions

There is 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 refractivity 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.

Reduced information content below 8-10 km

The current version (1.6) of the refractivity may have reduced information content below 8-10 km due to limitations in the input data. Despite the QC, there are suspicious cases left that are marked nominal. See [RD.12].

6 Conclusions

About 630 Metop-C refractivity profiles will be processed in NRT every day via the 1D-Var procedure to produce profiles of temperature, pressure and specific humidity. About 1 % of the profiles will subsequently fail a quality check based on diagnostics of the 1D-Var algorithm. A little more than 360 Level 2B Metop-C profiles can be expected to be produced on daily basis.

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 addressed in the future.

1D-Var solution 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.

Validation against co-located ECMWF analyses of 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. Temperature, solution - analysis, standard deviation of Metop-C exceeds the target of 1 K in the tropical tropopause region. Most likely this is due to Metop-C not being assimilated by ECMWF in the validation time period.

Specific humidity S-A standard deviation stays within target values globally, but exceeds the target in the tropical troposphere.

The bias of surface pressure for Metop-C is -0.17 and - 0.31 hPa at mid and high latitudes, and 0.15 hPa in the tropics. The standard deviation of is between 0.58 and 0.69 for all altitudes.

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

Temperature, specific humidity and pressure statistics stays within target requirements globally, and as such the product requirements are fulfilled.

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.