Validation Report:
Offline Level 2B and 2C 1D-Var products

Version 1.0

16 March 2020

ROM SAF Consortium
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European Centre for Medium-Range Weather Forecasts (ECMWF)
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1.0draft	16 March 2020	JKN	Version for internal review by S. Syndergaard
1.0	16 March 2020	JKN	Version prepared for the ORR12 review, with the following corrections from SSY: - p5 corrected Exec. sum. typos - p7 references to earler version sorted out - p9 changed ROM SAF acronym - p12 removed “best effort”. Agust 1-> August 31. Changed “refractivity” to “thinned input refractivity”. 2.4.0 -> 2.4.0.0 - sec 2.1 higher order ionos. mentionend. Metop C only from 1/8/19. - sec 2.3 reprocessed -> NRT. “missions”-> “satellites” (here and elsewhere) - sec 2.4.1 referenced shum figure - Chapter 3 updated re1 link to gpac_quality/ - sec 3.1 ERA-I -> ERA5 - Chapter 4 inserted footnote about using ERA5 instead of ECMWF(OPER) as reference. - Sec 1.5 inserted

ROM SAF

The Radio Occultation Meteorology Satellite Application Facility (ROM SAF) is a decentralised processing centre under EUMETSAT which is responsible for operational processing of radio occultation (RO) data from the Metop and Metop-SG 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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Executive Summary

The ROM SAF Offline v1.1 production is based on data from the Metop mission. These data are being processed from Level 1A (excess phase) to Level 2 (profiles of meteorological parameters) and Level 3 (latitudinal gridded monthly means).

The Level 1A data are provided by EUMETSAT. Here we validate the Level 2B (temperature, specific humidity and pressure) products against ERA5 and relate the results to an earlier validation of Offline v1.0 against ERA-I.

We conclude that the data set is sound and accurate within the product requirements, except for a few identified ranges where the reasons for slightly larger (solution - analysis) standard deviation has been accounted for. We also conclude that there is no noticable difference in (Level 2B) performance for Metop C when compared to Metop A and Metop B.

The report is concluded with an updated set of service specifications for the Offline v1.1 Level 2B products, which in general are more strict than the service specifications for Offline v1.0.

1 Introduction

1.1 Purpose of document

The purposes of this validation report is to formally evaluate the quality of the ROM SAF Offline v1.1 product with reference to the a priori defined product requirements listed in [RD.1], to assess the impact of the switch over on the ROM SAF Offline v1.0 to ROM SAF Offline v1.1, regarding change of background data from ERA-Interim to ERA5, and to validate Metop C data as part of ROM SAF Offline v1.1.

Table 1.1: *List of products covered by this Validation Report.*
**) The fifth column describes the original data source; satellite/instrument, data-level, institution. "Level 1A" refers to excess phase data. See also [RD.7]*

Product ID	Product name	Product acronym	Product type	Operational satellite input *	Dissemination means	Dissemination format
GRM-10	OFL Temperature Profile	OTPMEA	OFL	Metop-A/ GRAS	Web	BUFR netCDF
GRM-11	OFL Specific Humidity Profile	OHPMEA	OFL	Metop-A/ GRAS	Web	BUFR netCDF
GRM-12	OFL Pressure Profile	OPPMEA	OFL	Metop-A/ GRAS	Web	BUFR netCDF
GRM-13	OFL Surface Pressure	OSPMEA	OFL	Metop-A/ GRAS	Web	BUFR netCDF
GRM-48	OFL Temperature Profile	OTPMEB	OFL	Metop-B/ GRAS	Web	BUFR netCDF
GRM-49	OFL Specific Humidity Profile	OHPMEB	OFL	Metop-B/ GRAS	Web	BUFR netCDF
GRM-50	OFL Pressure Profile	OPPMEB	OFL	Metop-B/ GRAS	Web	BUFR netCDF
GRM-51	OFL Surface Pressure	OSPMEB	OFL	Metop-B/ GRAS	Web	BUFR netCDF
GRM-68	OFL Temperature profile	OTPMEC	OFL	Metop-C/ GRAS	Web	BUFR netCDF
GRM-69	OFL Specific humidity profile	OHPMEC	OFL	Metop-C/ GRAS	Web	BUFR netCDF
GRM-70	OFL Pressure Profile	OPPMEC	OFL	Metop-C/ GRAS	Web	BUFR netCDF

Continued on next page ...

Product ID	Product name	Product acronym	Product type	Operational satellite input *	Dissemination means	Dissemination format
GRM-71	OFL Surface Pressure	OSPMEC	OFL	Metop-C/ GRAS	Web	BUFR netCDF

1.2 Applicable and Reference documents

1.2.1 Applicable documents

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

[AD.1] CDOP-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] ROM SAF, Product Requirements Document (PRD), SAF/ROM/METO/MGT/PRD/001, -.

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

[RD.3] ROM SAF, Algorithm Theoretical Baseline Document: Level 2B and 2C 1D-Var products, SAF/ROM/DMI/ALG/1DV/002, .

[RD.4] ROM SAF, Validation Report: Reprocessed Level 1B bending angle, Level 2A refractivity, Level 2A dry temperature Offline v1.1 products, SAF/ROM/DMI/REP-/ATM/001, .

[RD.5] ROM SAF, Validation Report: Reprocessed Level 3 gridded Offline v1.1 products, SAF/ROM/DMI/REP/GRD/001, .

[RD.6] ROM SAF, Algorithm Theoretical Baseline Document: Level 2B and 2C 1D-Var products, SAF/ROM/DMI/ALG/1DV/002, Version 4.0, 2020.

[RD.7] ROM SAF, Algorithm Theoretical Baseline Document: Level 1B Bending angles., Ref. SAF/ROM/DMI/ALG/BA/001, Version 2.0, 2020.

[RD.8] ROM SAF, Algorithm Theoretical Baseline Document: Level 2A Refractivity profiles., Ref. SAF/ROM/DMI/ALG/REF/001, Version 2.0, 2020.

[RD.9] ROM SAF, website, http://www.romsaf.org/gpac_quality/, 2020.

1.3 Acronyms and abbreviations

1D-Var	1 Dimensional Variational Retrieval
1DV	Name of the 1D-Var implementation at DMI
ARSA	Analyzed Radio Soundings Archive
ATBD	Algorithm Baseline Document
BG	Background
CDR	Climate Data Record
CGS	Core Ground Segment
CHAMP	Challenging Mini–Satellite Payload
COSMIC	Constellation Observing System for Meteorology, Ionosphere & Climate
DMI	Danish Meteorological Institute
ECMWF	European Centre for Medium-Range Weather Forecasts
ECMWF(OPER)	ECMWF operational system
ERA-I	ERA-Interim (global atmospheric reanalysis)
ERA5	ECMWF Reanalysis 5th Generation
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FA	Federated Activity
GNSS	Global Navigation Satellite Systems
GPL	General Public Licence (GNU)
GRAS	GNSS Receiver for Atmospheric Sounding (onboard Metop)
IFS	Integrated Forecasting System
LEO	Low Earth Orbiter
Metop	Meteorological Operational polar satellites (EUMETSAT)
MSL	Mean Sea Level
N/A	Not Applicable or Not Available
NRT	Near Real Time
NWP	Numerical Weather Prediction
POD	Precise Orbit Determination
Q/C	Quality Control
RE1	First ROM SAF Reprocessing
RO	Radio Occultation
ROM SAF	Radio Occultation Meteorology SAF (former GRAS SAF)
ROPP	Radio Occultation Processing Package
SAF	Satellite Application Facility (EUMETSAT)
SAG	Scientific Advisory Group
SeSp	Service Specifications
SI	Système International (The MKS units system)
TBC	To Be Confirmed
TBD	To Be Determined
TP	Tangent Point
UKMO	United Kingdom Meteorological Office
VAR	Variational analysis; 1D, 2D, 3D or 4D versions (NWP data assimilation technique)
VT	Valid or Verification Time
WMO	World Meteorological Organization

1.4 Definitions

RO data products from the Metop and Metop-SG satellites 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:

NRT product: Data product delivered less than: (i) 3 hours after measurement (ROM SAF Level 2 for EPS); (ii) 150 min after measurement (ROM SAF Level 2 for EPS-SG Global Mission); (iii) 125 min after measurement (ROM 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

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

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

latency than the system used to generate the CDR[3].

1.5 Overview of this document

The document is organized as follows:

Chapter 1: Describes the purpose of the document and provides applicable and referenced documents, acronyms and definitions of product levels and types.

Chapter 2: Describes the processing context and the 1D-Var algorithm.

Chapter 3: Contains comparisons between retrieved products and ERA5.

Chapter 4: Summarizes performance with respect to product requirements.

Chapter 5:Briefly summarizes and concludes the validation.

Annex I: Repeats service specifications for the ROM SAF Offline-v1.1 1D-Var product.

[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

The ROM SAF Offline version 1.0 production was initiated in January 2018, with processing of Metop A and B beeing applied on data starting from January 1 2017. The retrieval configuration was basically inherited from the ROM SAF CDR v1.0. The algorithm is described in the ATBD [RD.6]. The ROM SAF Offline v1.0 was a reprocessing of Metop data which was meant to be subject to future algorithm updates.

By August 1 2019 the Offline v1.0 was terminated and a new processing chain, GPAC-v2.4.0.0, has been prepared for Offline v1.1 production. For Level 2B the main features of the Offline v1.1 upgrade includes use of ERA5 background profiles for 1D-Var and implementation of a new 1D-Var script version, 1DV 4.2 which is entirely based on ROPP routines. The upgrade has impact on the product format in the sense that the thinned input refractivity, which earlier was pruned from missing data, will contain levels with missing data values in 1DV v4.2 in accordance with ROPP style. The upgrade is expected to have marginal impact on the products themselves. The only real (minor) algorithm change is a slight change in procedure for refractivity uncertainty calculation: The tropopause climatology is no longer used as fallback option in cases where the tropopause cannot be determined from the background profile. Instead a constant tropopause height of 10 km is assumed in these cases. Details about the uncertainty assumptions are found in [RD.3].

A couple of bugs regarding treatment of missing values in GPAC-v2.4.0.0 was fixed in GPAC-v2.4.0.1 which was then applied on data starting from 1 June 2019 and ending by 31 October 2019. These data are the basis of the present validation report.

2.1 Brief description of ROM SAF Offline v1.1

The ROM SAF Offline v1.0 code was the same as the code used in ROM SAF CDR v1.0. The 1D-Var products in ROM SAF Offline v1.1 are expected to differ from the corresponding v1.0 products due to the following configuration features:

- A higher order ionospheric correction in has been applied, which may affect input refractivity. See [RD.4].
- Background profiles from ERA5 (137 Levels) forecast. ERA-I (60 Levels) was used in Offline v1.0.
- In some cases a slight change of input refractivity error when the tropopause is not well defined.

2.2 Mission and time coverage

The Metop satellites, and the covered periods are given in Table 2.1

Table 2.1: *Satellites, and time periods in the ROM SAF Offline products.*

Satellite	Period
Metop-A	1 January 2017–present
Metop-B	1 January 2017–present
Metop-C	1 August 2019–present

2.3 Input data

The input Level 1A data for ROM SAF Offline products are provided through the EUMETSAT Secretariat through the EUMETSAT NRT environment (PPF version 4.6). The ERA5 background analysis is provided by ECMWF through the MARS archive.

2.3.1 Description of algorithm and Level 2B configuration

The Offline v1.1 Level 2B retrieval is based on offline refractivity profiles from Metop these data are described in [RD.8] and [RD.4]. Background profiles are interpolated from the ERA5 forecast and the background error covariance is calculated in 5 deg latitude bands, ultimately obtained from ERA-I error of first guess fields. The refractivity uncertainty is modeled as a fractional error of 0.2 % above the tropopause, linearly increasing to 2 % at the surface.

1D-Var processing is performed with ROM SAF 1DV v 4.2 as a part of GPAC 2.4.0.1. The 1DV 4.2 implementation and configuration are described in detail in the 1D-Var ATBD, [RD.3].

Quality control is performed on each processing level. On Level 2B the QC is basically ensuring that the 1D-Var cost function is not exceeding a threshold ($2J/m < 5$) and that the number of iterations used by the 1D-Var minimizer stays below 25.

2.3.2 Description of 1D-Var products and their uncertainties.

The primary output variables of the ROM SAF 1DV in Offline v1.1 is a state vector containing temperature and specific humidity at 137 model levels and surface pressure. These parameters describe the atmospheric state. Pressure is calculated uniquely on all model levels from the surface pressure and geopotential heights are calculated from the hydrostatic equation. See the ATBD [RD.3] for details. Pressure and geopotential height are secondary variables, which can be calculated offline directly from the state vector, but they are implicitly calculated during the 1D-Var run because the forward model uses them.

The 1D-Var formalism provides an immediate profile to profile estimate of the expected uncertainty including error correlations of the primary solution variables. These uncertainties are then forward propagated into the secondary variables. Notice in Figure 2.1 that the pressure at high altitudes has practically no uncertainty because the IFS model levels are essentially defined as pressure levels at high altitudes [RD.3]. However, there is an uncertainty in the geopotential height of a given pressure level. Thus, when interpolated to a geopotential height grid the uncertainty in geopotential height is reflected in the pressure uncertainty. In Figure 2.1 examples of globally averaged uncertainty estimates of Metop A/B data for a few days of February 2016 are shown. For the pressure additional background and solution uncertainties, which takes into account interpolation to fixed heights, are plotted with dashed lines.

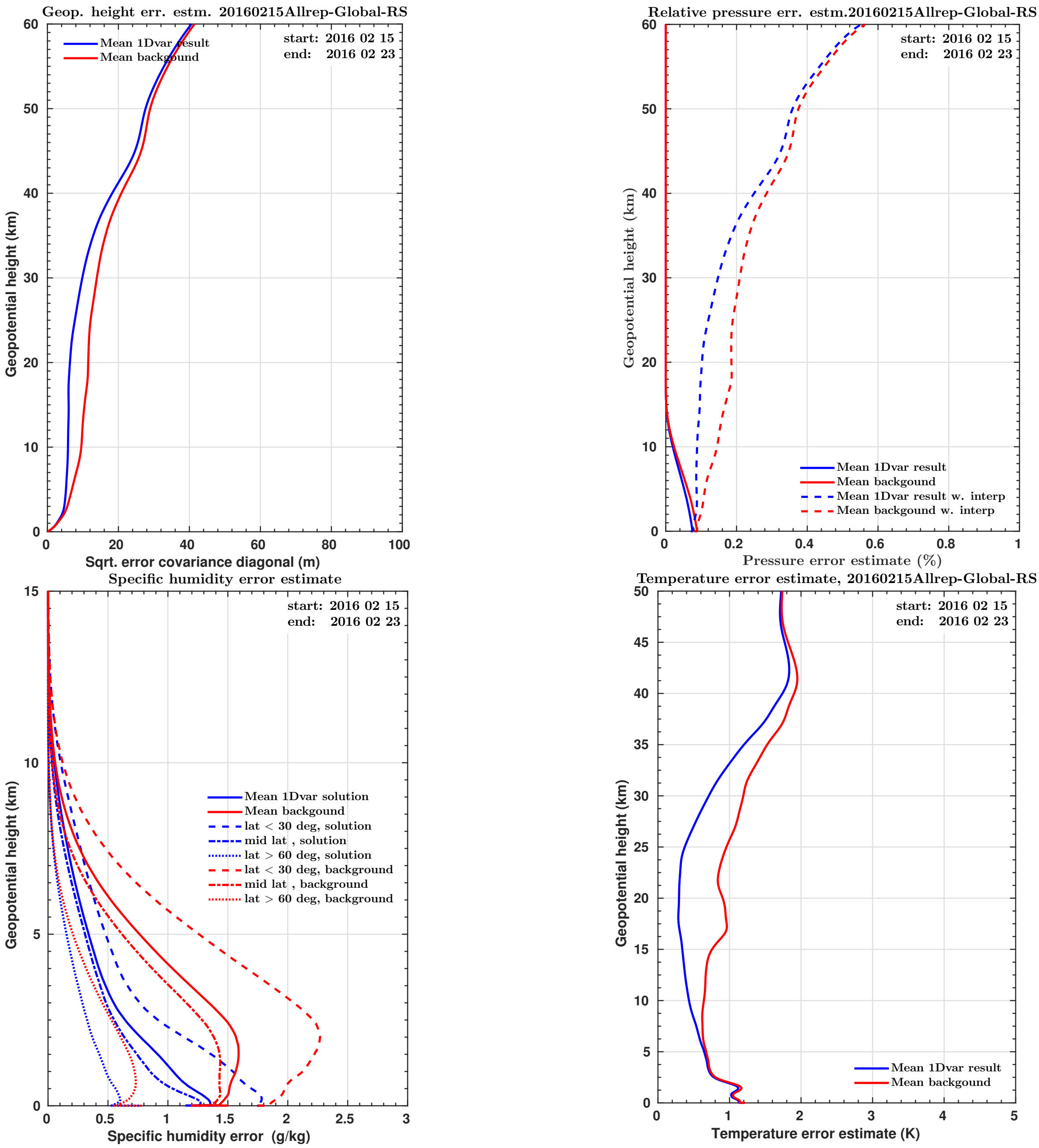


Figure 2.1: *Estimated errors of 1D-Var products (blue) and background variables (red). From upper left corner; geopotential height, pressure, specific humidity and temperature. In case of temperature the solid lines show the uncertainty, when pressure is evaluated at model levels, and the dashed lines show the uncertainty when pressure is evaluated at geopotential height levels. In case of specific humidity (lower left) the different line styles refer to different latitude bands - see figure legend for explanation. The error estimates are calculated for two weeks of date from ROM SAF CDR v1.0. Since the input uncertainty models of Offline v1.1 and CDR v1.0 are almost identical, it is safe to consider these plots as representative for Offline product uncertainty.*

In Figure 2.2 the ratios between expected solution uncertainty and background uncertainty are illustrated for different latitude bands. This property, sometimes referred to as the "prior fraction", shows how much 1D-Var reduces the error, and as such it is an indication of how much observation information is brought to the solution: The lower the prior fraction the more the observation has contributed to the solution. Note that there is practically no observation information in stratospheric humidity and tropospheric temperature.

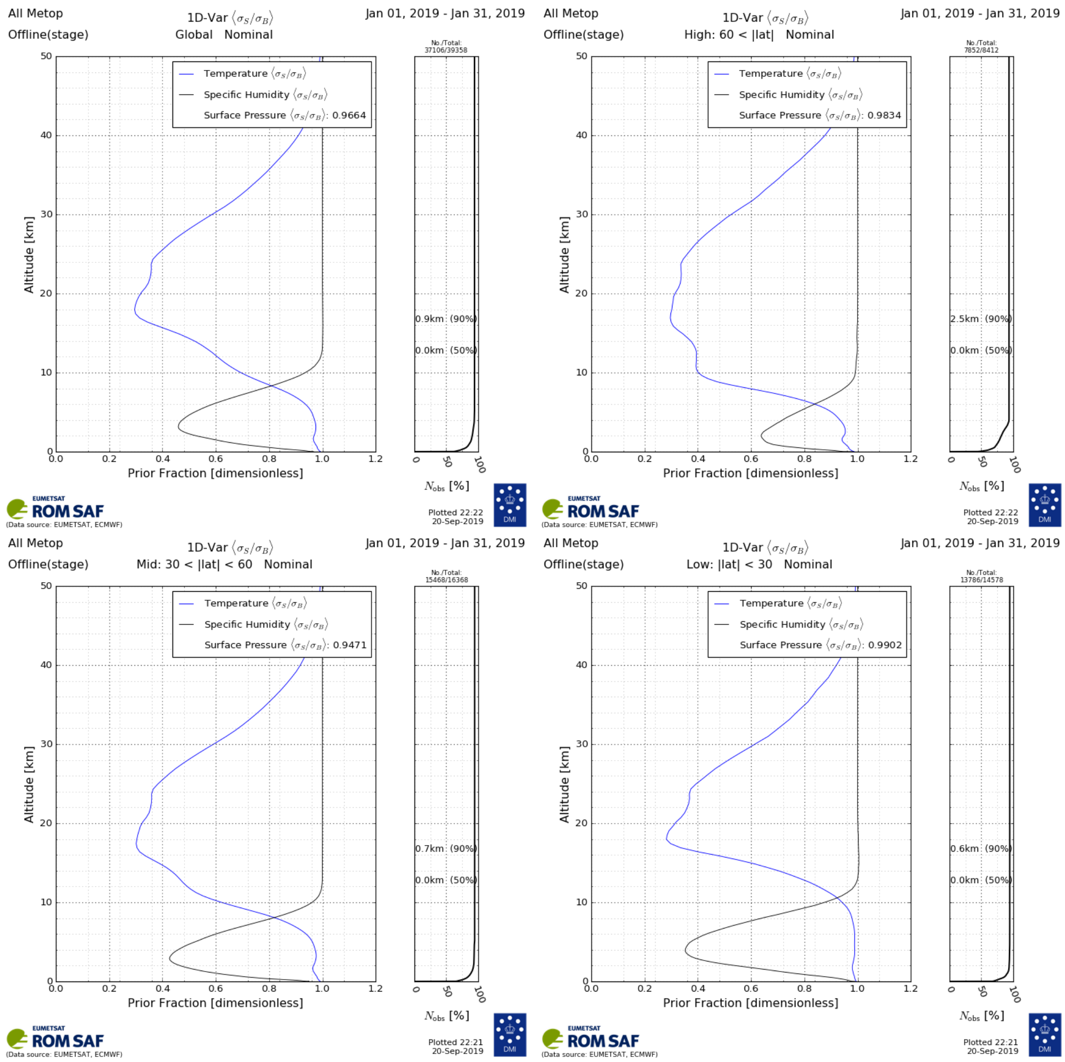


Figure 2.2: *Ratio between solution uncertainty and background uncertainty for temperature and specific humidity; globally, high, mid and low latitudes.*

2.4 Description of reference data used for comparison in this report

2.4.1 Time Series of operational ECMWF analysis versus ERA-I and ERA5 analysis

It is instructive to have a look at the ECMWF operational forecasting system ECMWF(OPER)[1] and ERA5 temperature difference (Figure 2.3). The data from the two models are sampled in the positions of the RO profiles from Metop. The ERA5 deviates quite a bit from ECMWF(OPER). Mostly these differences are caused by upgrades of ECMWF(OPER), but

[1] The ECMWF operational system will be referred to as ECMWF(OPER) through out the text.

since ERA5 assimilates, only to some extend, the same data as ECMWF(OPER), the comparison will contain some abrupt changes in some cases for instance when a new assimilation data set is introduced. In order to maximize the confusion we also plot the difference between ECMWF(OPER) and ERA-I. The abrupt changes in ERA5 mean values are also seen in the standard deviation, but to some extend smeared out (Figure 2.4). The validation has to be seen in light of these time dependent features of the ERA5 background data set. Strictly speaking it is only data after August 1 2019 and further on that is going to to be included in the Offline dataset, but the 34 month time series gives a feeling for the stability of the ERA5 which is used as validation reference.

Most noticeable is the drop in (ECMWF-ERA5) temperature bias mid 2017, which is attribued to ECMWF starting to assimilate Metop data to the surface in June 2017. But curiously there are also bias jumps spring and early summer 2019. ECMWF started to assimilate Metop C AMSU, MHS and GRAS on the 14th of March and ECMWF implemented an upgrade (IFS cycle 46R1) on 11th of June 2019, and that may account for some shifts. But probably more important the ERA5 analysis profiles was falsely interpolated from 6 hourly ERA5 fields, instead of 3-hourly, before June 2019, and that may very well explain a the specific humidity jump occurring around 1st of June 2019 in figure 2.5.

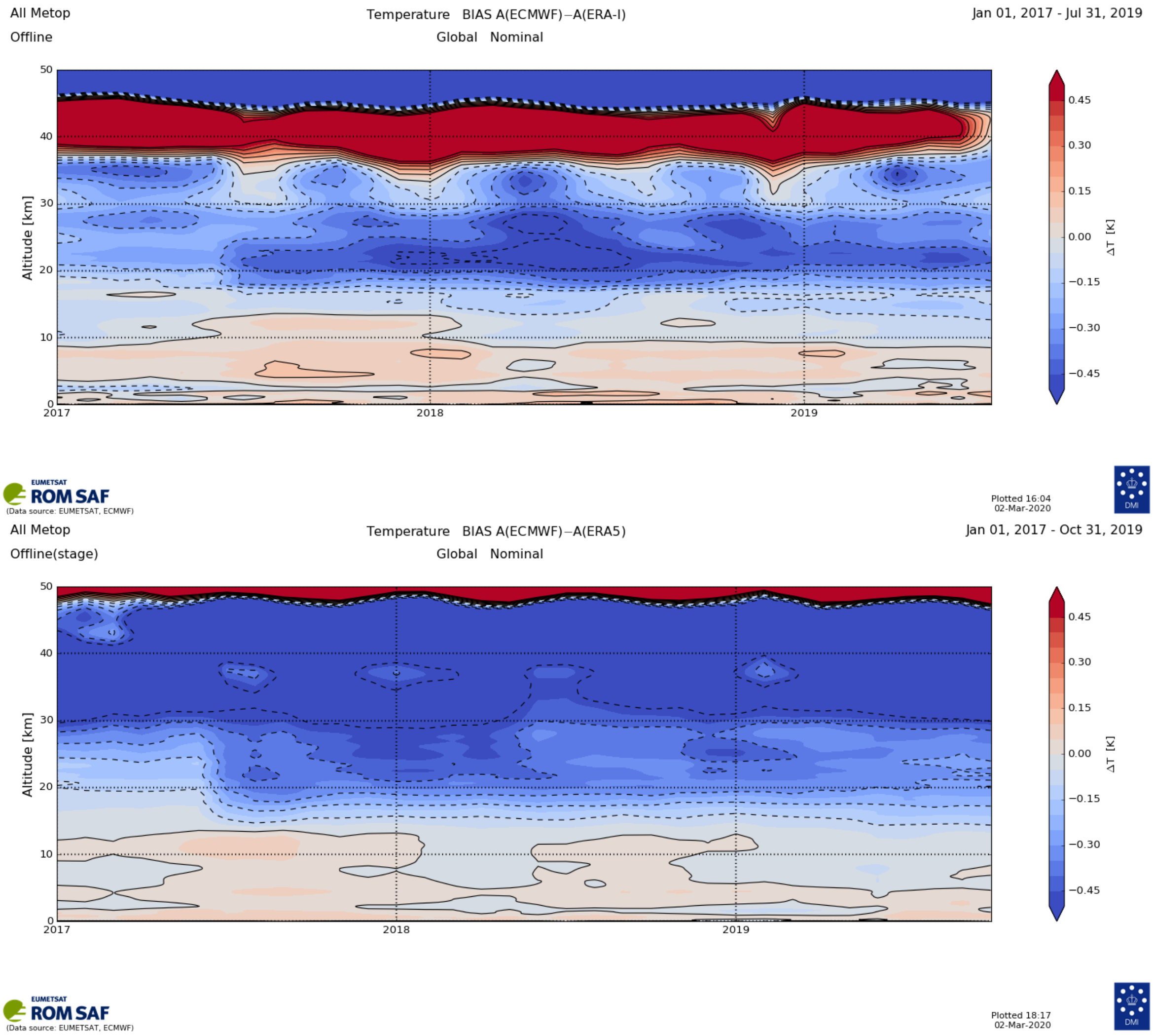
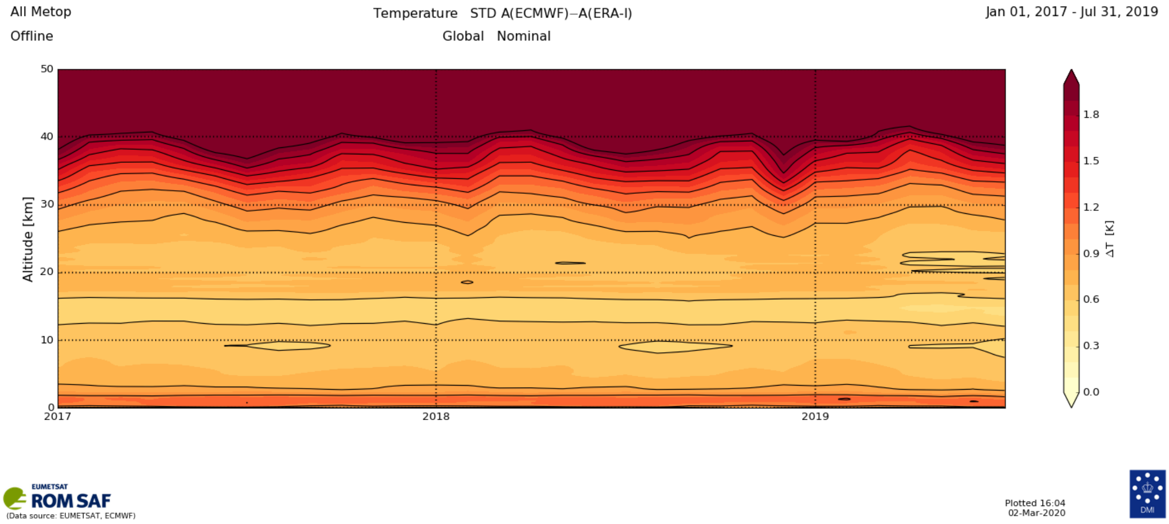


Figure 2.3: *All latitudes, temperature as function of time and altitude. Top; ECMWF OPER - ERA-I (analysis) and bottom; ECMWF OPER - ERA5 (analysis).*



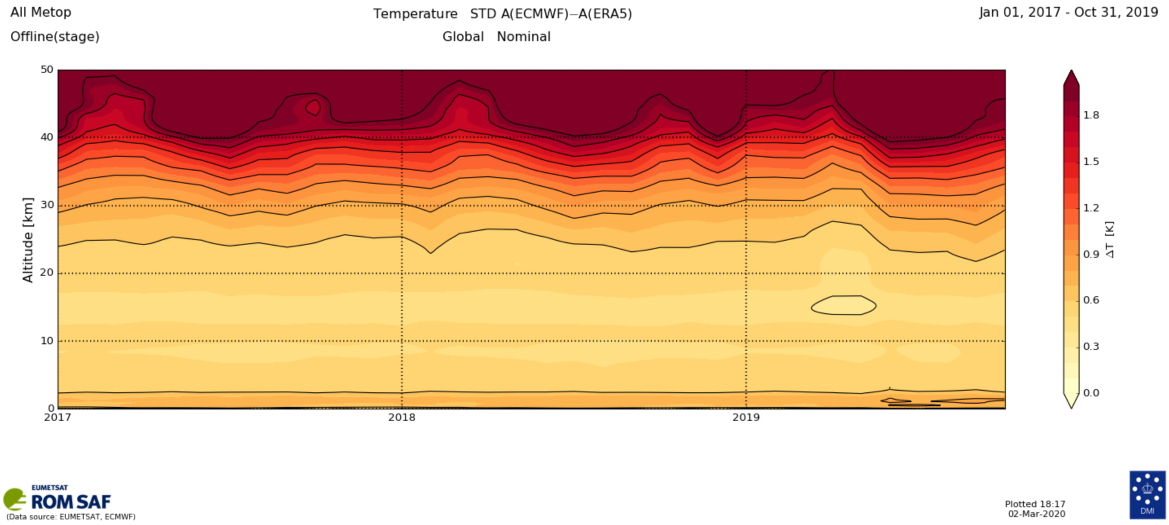


Figure 2.4: *All satellites, all latitudes. Standard deviation of ECMWF(OPER) - ERA-I (top) and ECMWF(OPER) - ERA5 (bottom) temperature as function of time and altitude.*

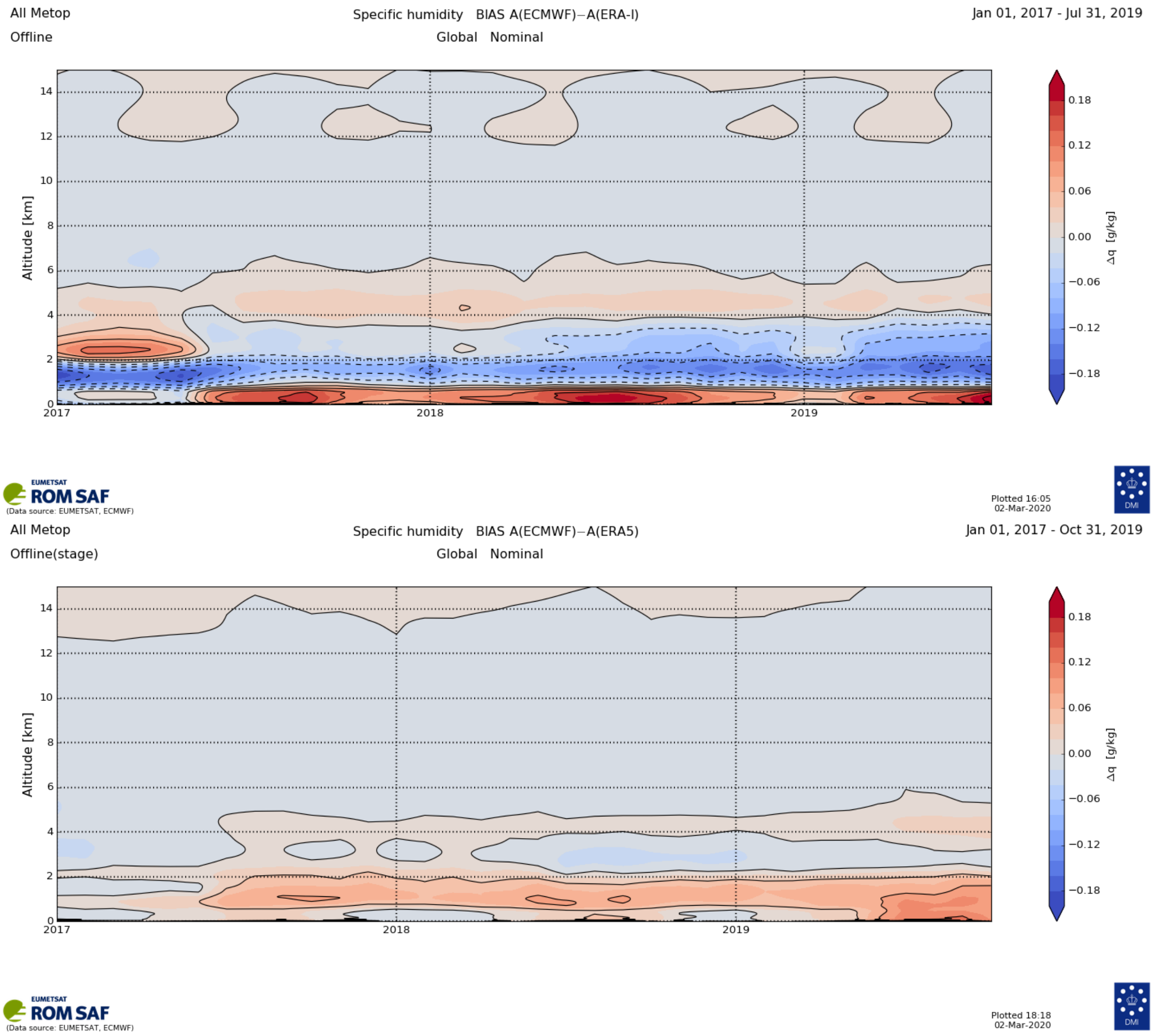


Figure 2.5: *Specific humidity bias ECMWF(OPER) - ERA-I (top) and ECMWF(OPER) - ERA5 (bottom), globally as function of time and altitude.*

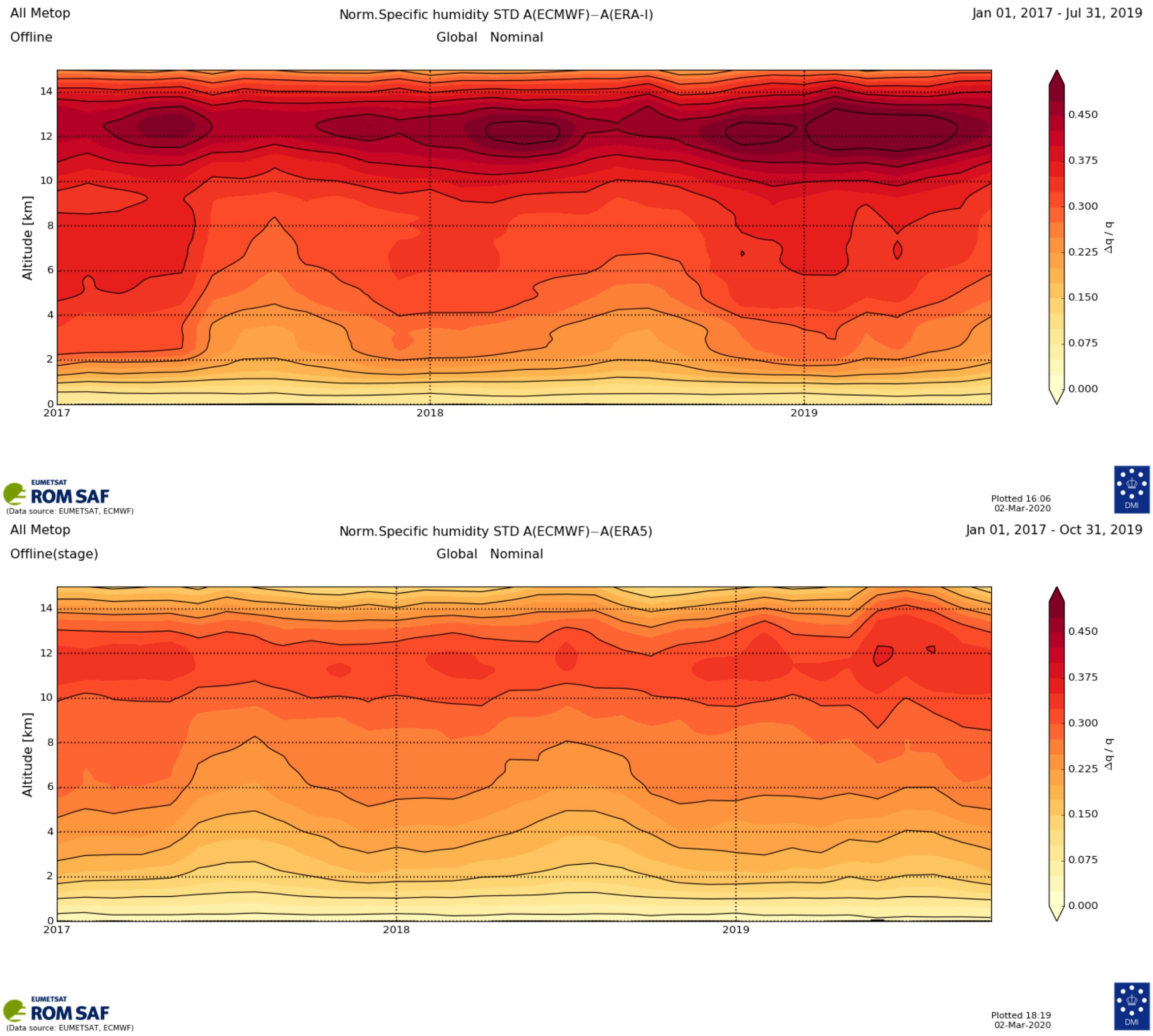
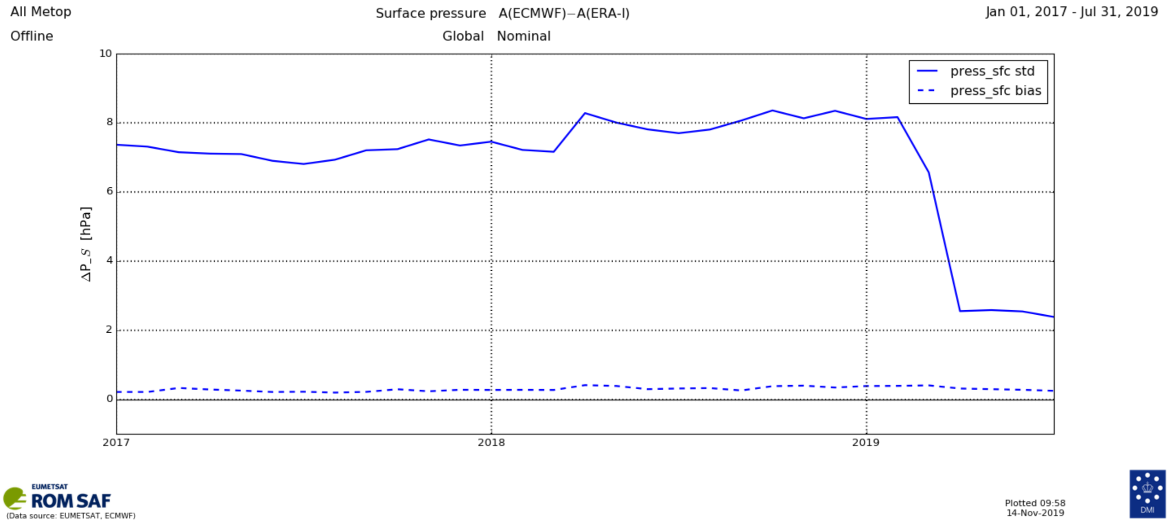


Figure 2.6: *All satellites, all latitudes. Standard deviation of ECMWF(OPER) - ERA-I (top) and ECMWF(OPER) - ERA5 (bottom) specific humidity as function of time and altitude.*



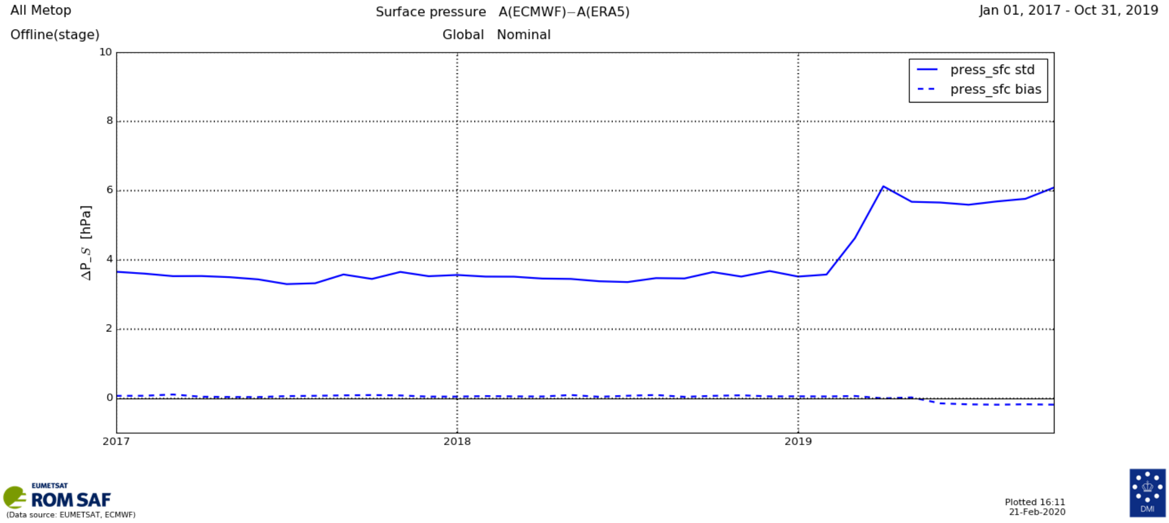


Figure 2.7: *All satellites, all latitudes, STDV of ECMWF(OPER) - ERA-I (top) and ECMWF(OPER) - ERA5 (bottom) and ERA5 surface pressure.*

Especially in the specific humidity ECMWF(OPER)-ERA-I and ECMWF(OPER)-ERA5 BIAS and STDV, shown in figures 2.5 and 2.6, it is seen that ECMWF(OPER) departs from ERA5 after start of assimilation of Metop data in the troposphere June 2017, and after the ECMWF upgrade in 11th of June 2019.

The signature of the identified jumps in ERA5 versus ECMWF(OPER) performance are also seen in surface pressure (Figure 2.7). Globally there is no impact on the surface pressure differences from the Metop onset of tropospheric Metop assimilation June 2017 in all three models, but it is clearly seen that ECMWF(OPER) starts to drift away from ERA5 after the ECMWF(OPER) starts to assimilate Metop C AMSU and GRAS 14 March 2019.

Overall there are quite large differences between different altitude bands in the ERA5 versus ECMWF(OPER) bias structure, especially for the specific humidity.

2.4.2 Comparison against ERA5

The formal validation of ROM-SAF Offline v1.1 Level 2B and Level 2C is done against ERA5, as described in the Product Requirements Document [AD.3]. The full set of validation plots is collected on the ROM SAF web page https://www.romsaf.org/gpac_quality. It is recommended to visit this page which contains the monthly statistics of specific instruments and parameters broken down on latitude and rising/setting occultations. In this chapter we only include a few of the available figures to emphasize selected features and perform the formal validation.

3 Profile comparisons

This chapter contains the comparisons Offline v1.1 Level 2B data to ERA5. The emphasis is put on the precision and accuracy of the 1D-Var products at the height levels where the accuracy is expected to be relatively high. For temperature this is the upper troposphere and lower stratosphere for specific humidity this is the free troposphere. Latitude bands are evaluated independently. The intention with the comparisons is to assess new service specifications for the Level 2B variables. The performance with respect to requirement/specification can be monitored at [RD.9].

The chapter is organized such that each variable type is dealt with in a separate section, which is concluded with a service specification recommendation. Throughout the comparisons terms Tropics ($|lat| < 30$deg), Mid Latitudes (30 deg $< |lat| <$ 60 deg) and High latitudes (60 deg $< |lat|$) are used. All ERA5 comparisons are averaged within these latitude bands. The service specifications are then summarized in chapter 5.1. Since differences between satellites are to some extent smeared out by 1D-Var, these are only briefly touched. The inter-satellite comparisons are briefly touched upon in [RD.4] and [RD.5].

3.1 Temperature (GRM-10/48/68)

The temperature is a primary state variable, and it is a high accuracy 1D-Var product in the lower stratosphere and upper troposphere. Formally the temperature product requirements [AD.3] only concerns the STDV. However, we do also compare the products mean value to reference data here.

3.1.1 1D-Var temperature compared to ERA5

In figure 3.1 the global comparison of 1D-Var temperature profiles against profiles extracted from ERA5 is presented. No remarkable abrupt bias jumps are observed in the global temperature between January 2017 and october 2019.

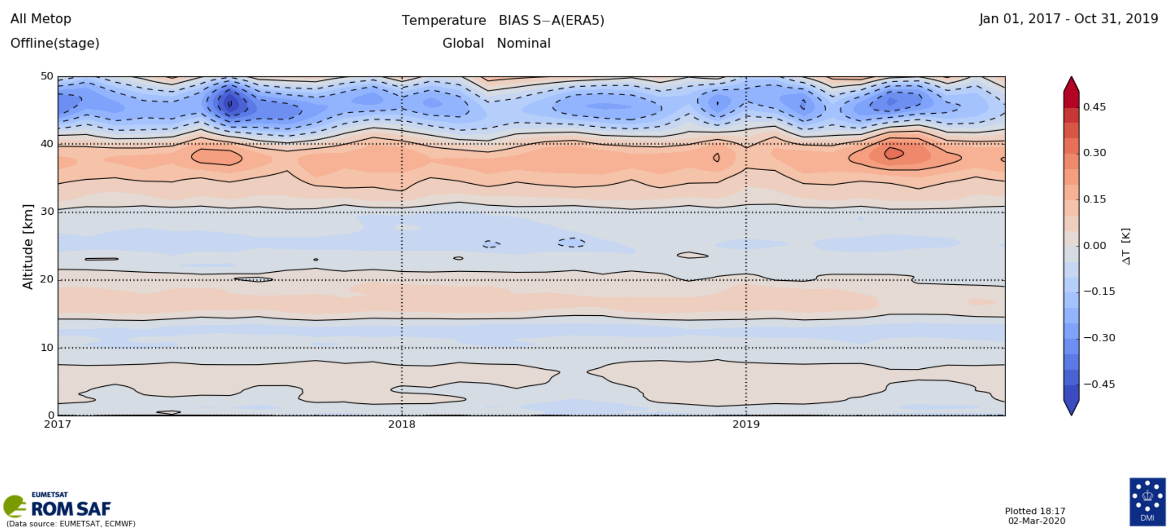


Figure 3.1: *All satellites, all latitudes. 1D-Var- ERA5 temperature as function of time and altitude.*

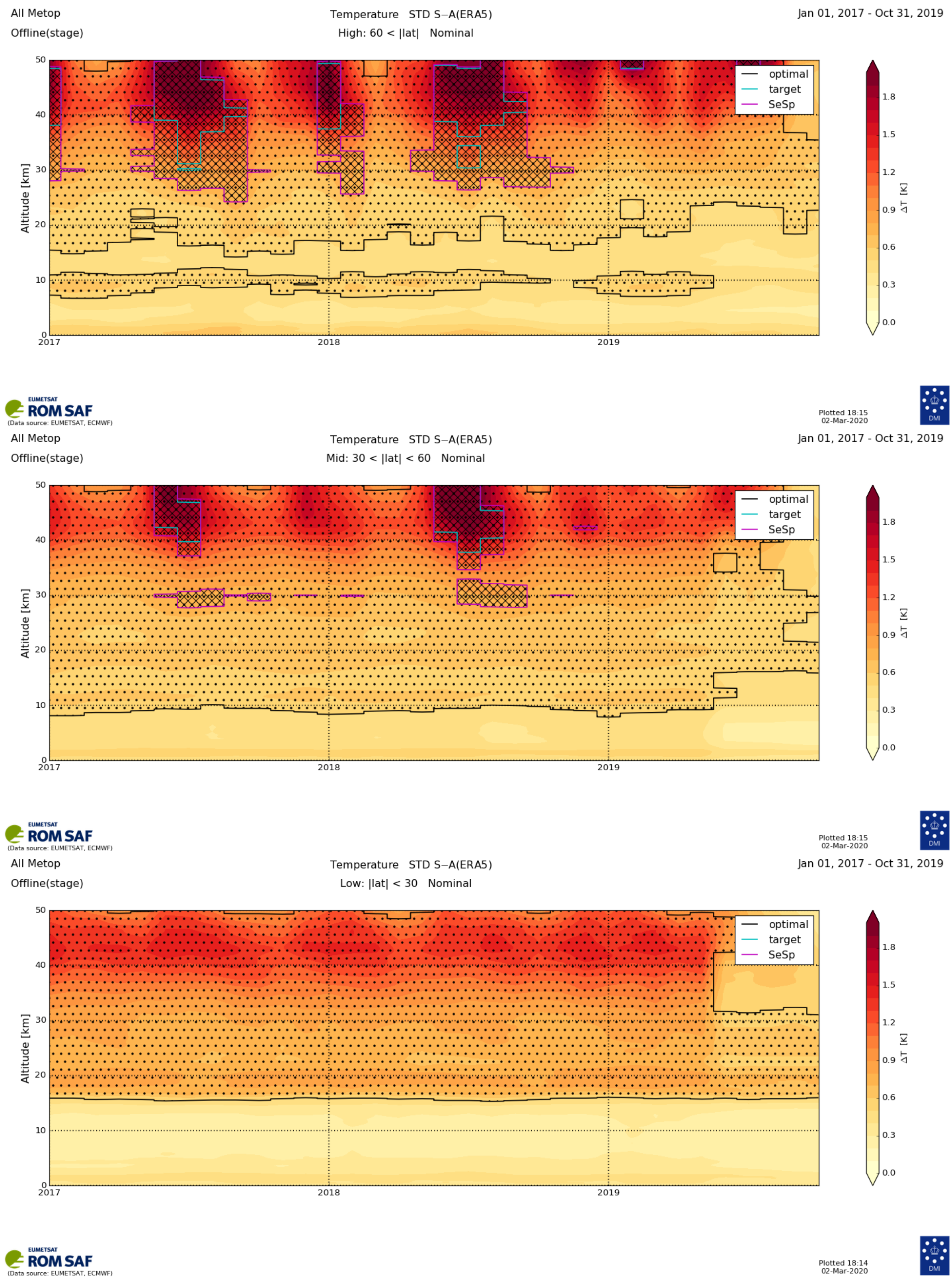


Figure 3.2: *All satellites, high, mid and low latitudes. STDV 1D-Var - ERA5 temperature as function of time and altitude.*

Turning to the temperature standard deviation, it appears that the Offline-v1.1 - ERA5 difference inherits some of the features in ECMWF(OPER)-ERA5, listed in section 2.4.1. There is a drop in beginning of June 2019. This drop is due to a shift from 6-hourly to 3-hourly ERA5 analysis fields, so it is not due to any changes in the 1D-Var data product quality.

In Figure3.2 3 latitude bands (high, mid and low) are shown. The STDV plots are also broken down on northern versus southern hemisphere in figures 3.3, 3.4, 3.5 and 3.5 to illustrate the annual cycle in the error statistics, implying systematic violation of PRD target value at high altitude in polar winter. The main point here is that the PRD target is mostly violated in the extra tropics, between 10 and 35 km, and that that these "violations" has to be taken into account in the service specifications.

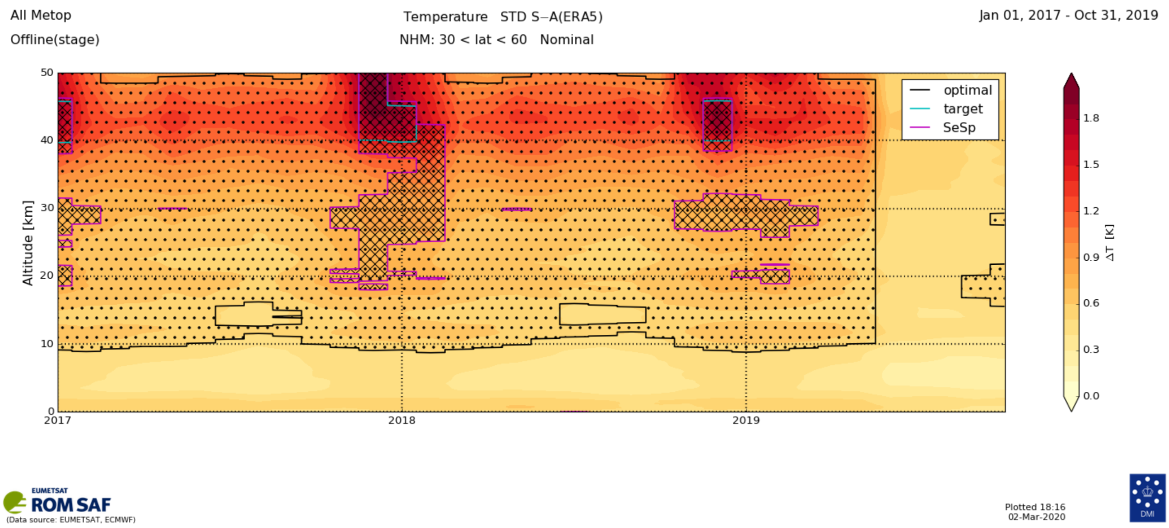


Figure 3.3: *All satellites, northern hemisphere mid latitudes. STDV 1D-Var - ERA5 temperature as function of time and altitude.*

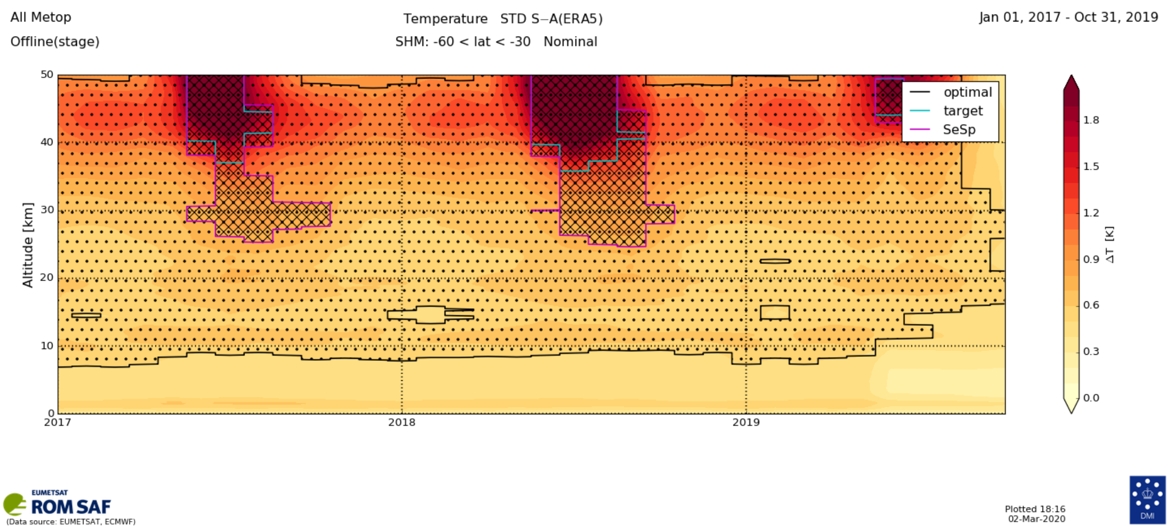


Figure 3.4: *All satellites, southern hemisphere mid latitudes. STDV 1D-Var - ERA5 temperature as function of time and altitude.*

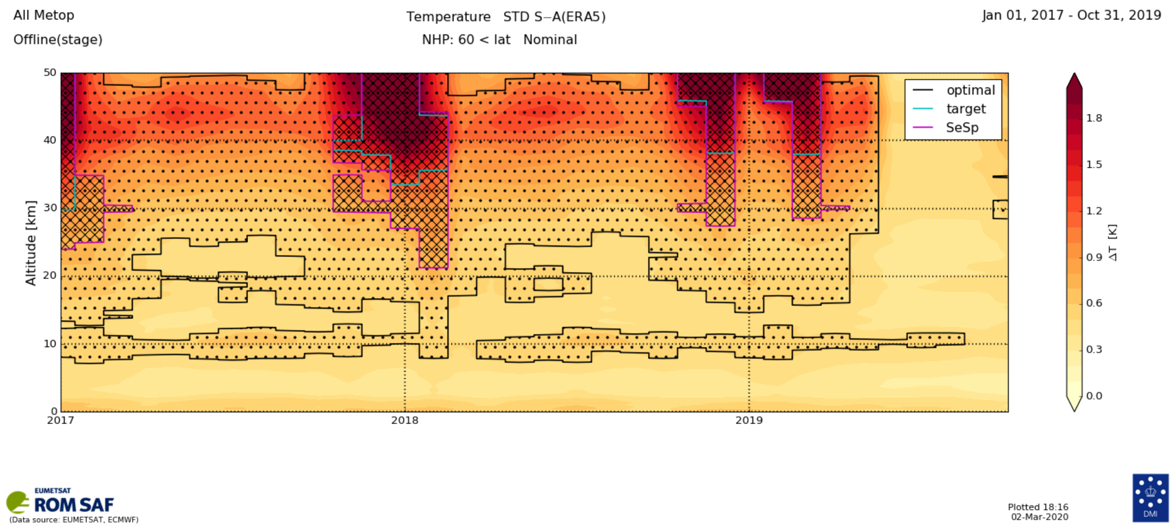


Figure 3.5: *All satellites, northern hemisphere polar latitudes. STDV 1D-Var - ERA5 temperature as function of time and altitude.*

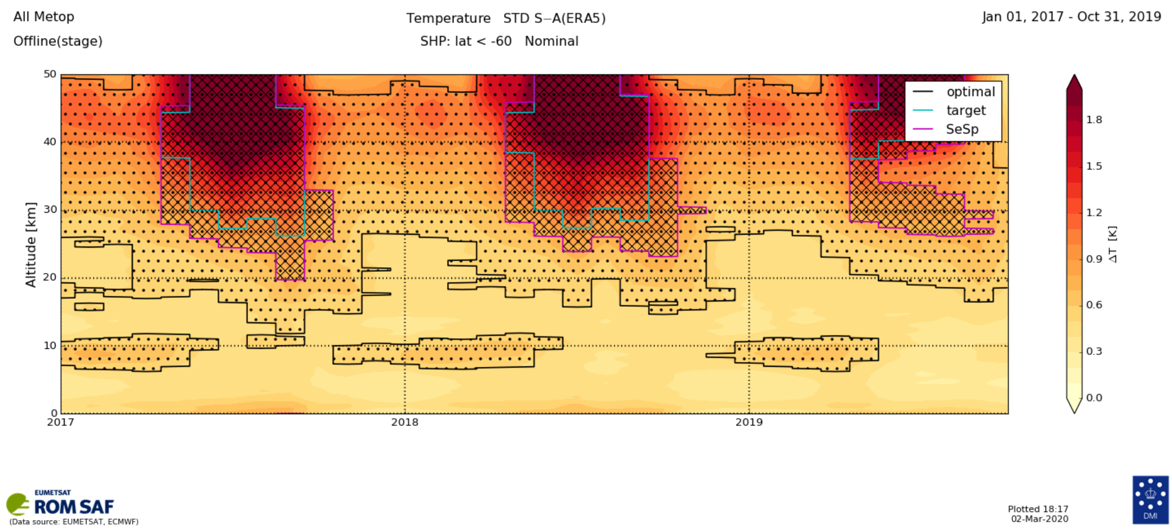


Figure 3.6: *All satellites, southern hemisphere polar. STDV 1D-Var - ERA5 temperature as function of time and altitude.*

Figure 3.7 shows that in general there is no noticeable temperature STDV difference between the satellites. Generally 1D-Var smears out mission and satellite diffrences.

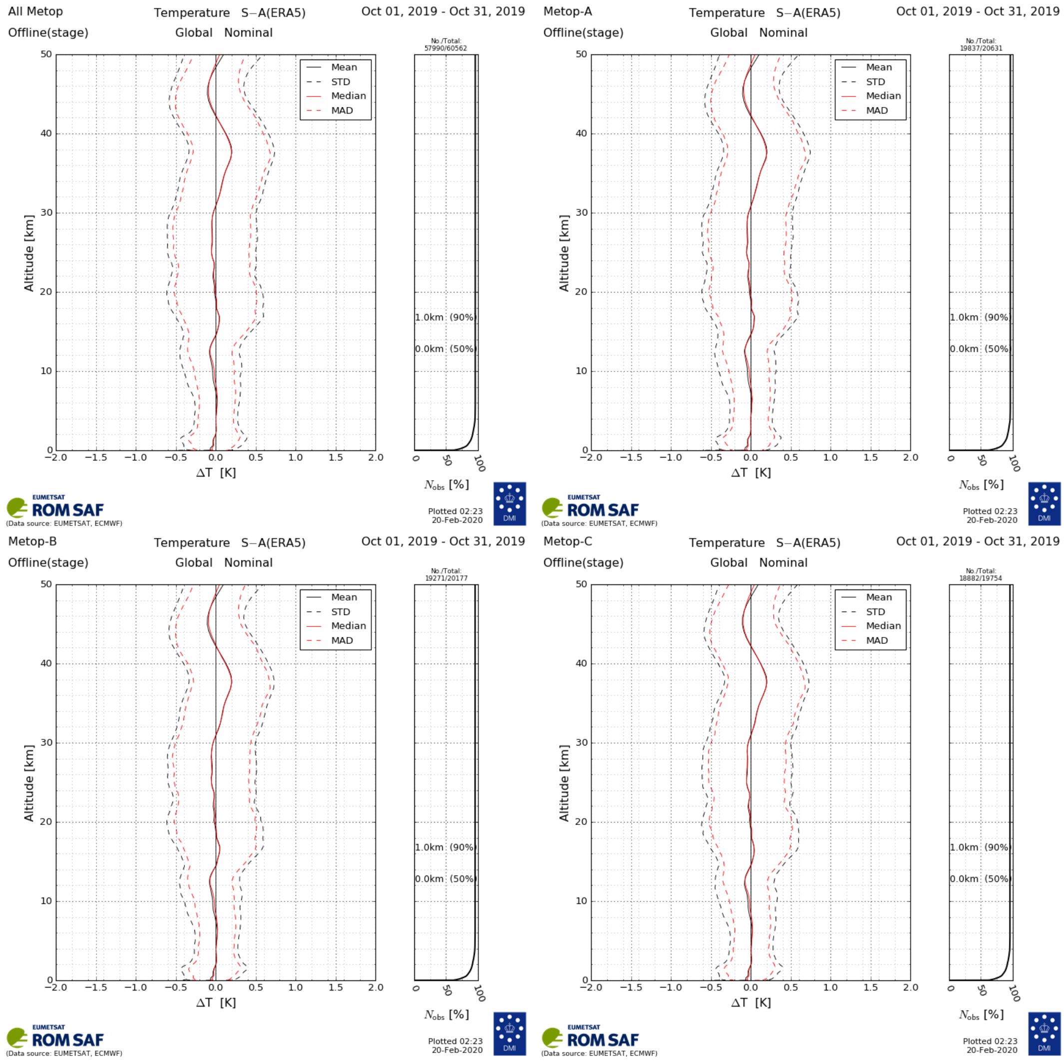


Figure 3.7: *Temperature statistics for October 2019. All Metop, Metop A, Metop B and Metop C.*

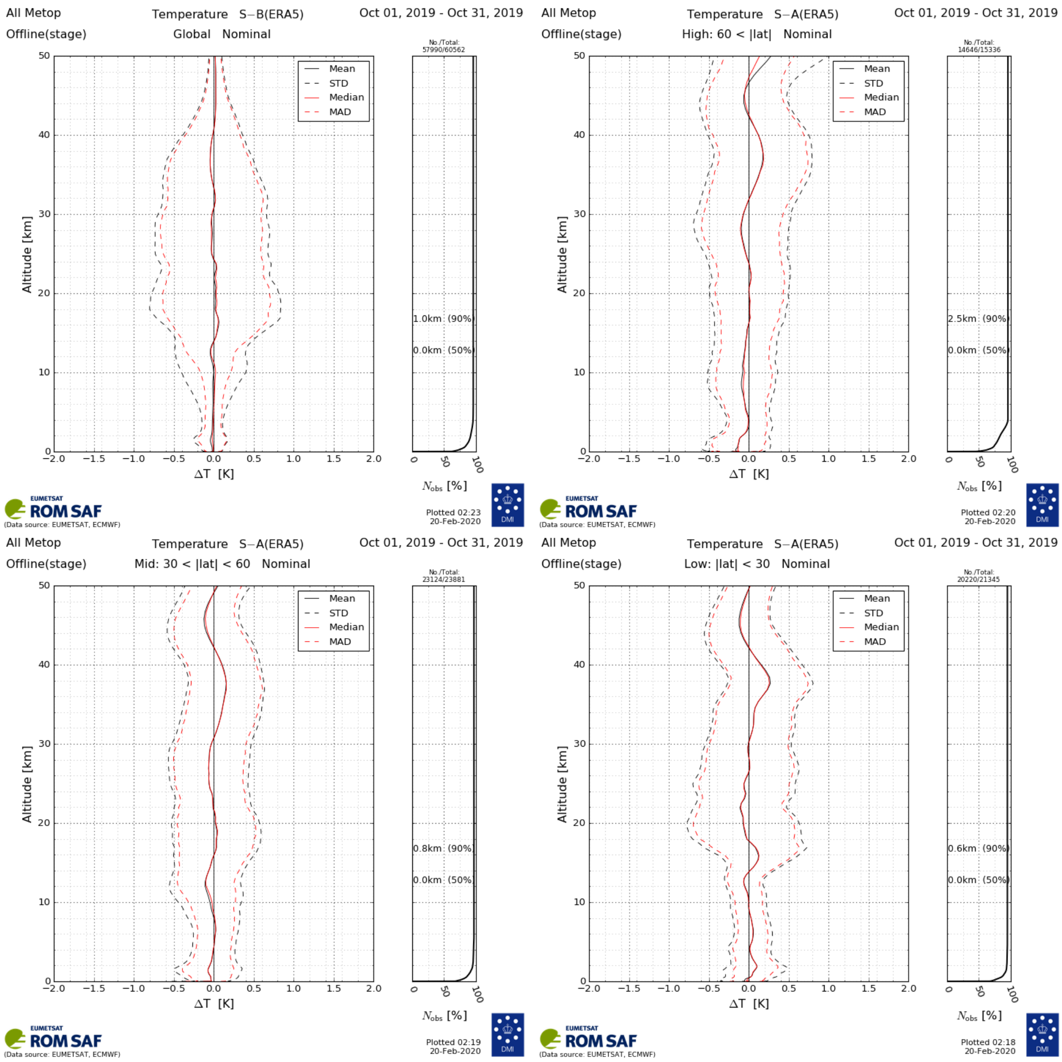


Figure 3.8: *Temperature statistics for October 2019. From upper left: Solution - background global, solution -analysis polar, solution -analysis mid latitudes, solution - analysis tropical.*

3.1.2 Intermediate summary regarding temperature service specifications

Figure 3.8 suggest that the temperature service specifications could be tightened a little in all latitude bands. Since there is not much annual variability in the tropical temperature standard deviation (deduced from figure 3.2, recalling that the drop in June 2019 is an artifact), we decide to reduce the tropical SeSp below 30 km from 1.0 K to 0.75 K. For mid and polar latitudes we keep the criterions, still allowing standard deviation up to 2.0 K at 50 km because there are some seasonal departures in the time series which are not fully covered by the validation dataset. These departures are not present in the tropics so we can choose to differentiate tropical from extra tropical latitudes. The suggested service specifications are then set at trop/mid/high latitudes to 0.75 K/ 0.75 K /0.75 K between 0/0/0 km and 30/30/30 km, and 0.75 K/ 0.75-2.0 K /0.75-2.0 K between 30/30/30 km and 50/50/50 km (An interval means a linearly changing quantity between the two values over the given vertical coordinate). All service specifications will be summarized in Annex I.

3.2 Specific Humidity (GRM-11/49/69)

The specific humidity is a primary state variable, and it is a moderately accurate 1D-Var product in the free troposphere. Formally the specific humidity product requirements [AD.3] only concerns the STDV. However, we do also compare the products mean value to reference data here.

3.2.1 1D-Var Specific Humidity compared to ERA5

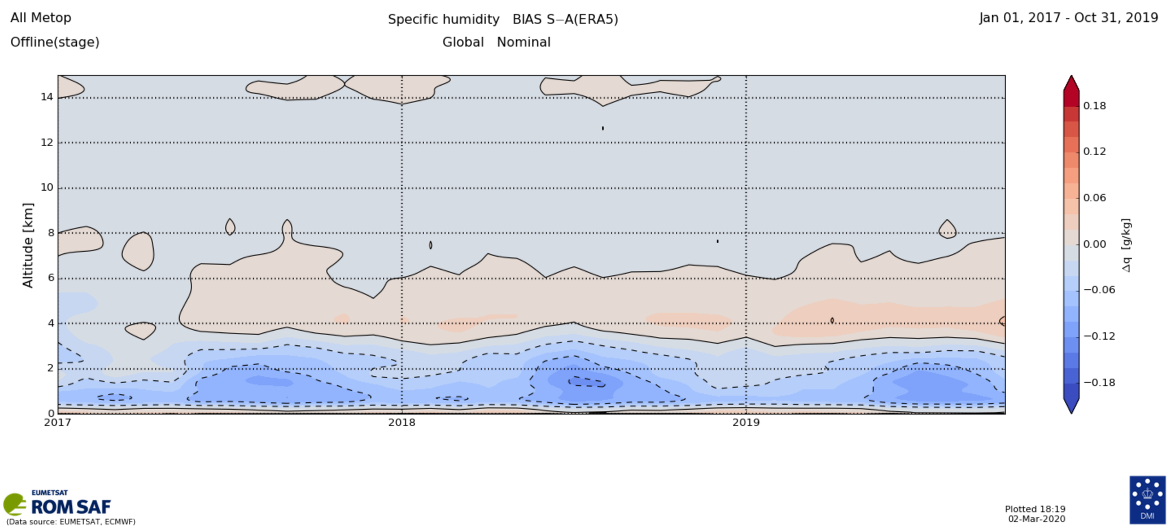


Figure 3.9: *All satellites, all latitudes. 1D-Var- ERA5 specific humidity as function of time and altitude.*

The specific humidity Offline v1.1 versus ERA5 bias contains an imprint of the onset of assimilation of Metop (GRAS) in the troposphere in ERA5, in June 2017. This effect is not going to affect the released Offline v1.1 data, because it is located outside the official time scope, but it shows the sensitivity of ERA5 to RO data and consequently it points out a potential limitation of the Offline v1.1 specific humidity. A similar effect, with slightly different signature, was seen in Offline v1.0 versus ERA-I (see https://www.romsaf.org/quality/time_series.php).

A remarkable feature of Offline v1.1 is absence of the seasonal, upper troposphere, positive bias and increased STDV of the specific humidity at mid latitudes, which was inherent in Offline v1.0. This improvement is exposed in Figure 3.10, where northern hemisphere mid latitude specific humidity bias (normalized) is shown for both Offline v1.0 and Offline v1.1.

The reason for this malfunction was earlier identified (see [RD.2]) as a consequence of the relatively low temperature background uncertainty and relatively high humidity background uncertainty near the mid latitude tropopause, combined with a systematic positively biased tropopause near the tropopause in ERA-Interim. The problem was in fact expected to go away with adoptation of ERA5.

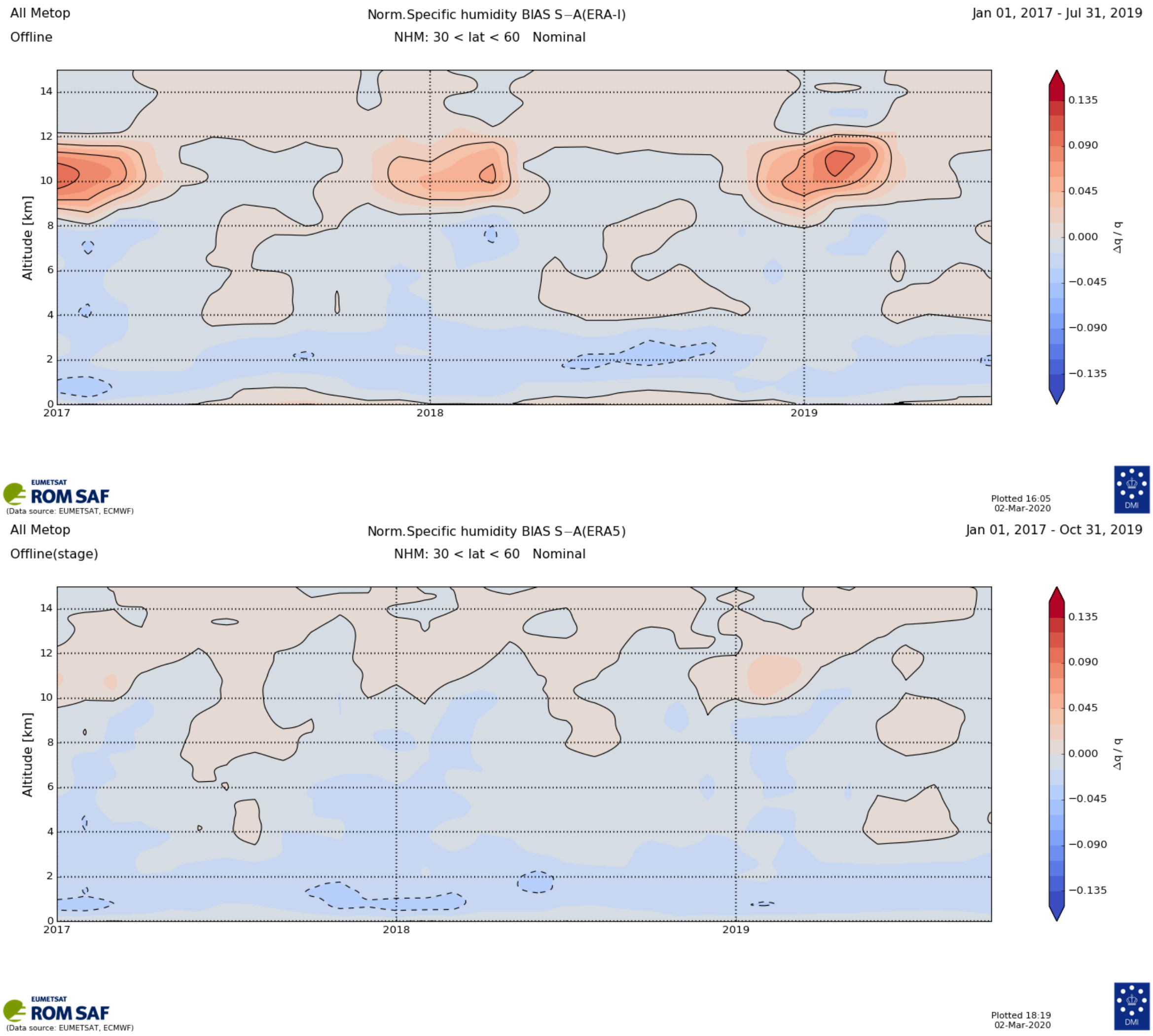


Figure 3.10: *All satellites, mid latitudes. STDV of 1D-Var-ERA5 specific humidity (normalized) as function altitude, top: Offline v1.0, bottom Offlne v1.1.*

The main issue with the specific humidity STDV in Figure 3.11 is the violation of the current product requirement target around 2 km throughout the whole RO era. The issue arises from tropics and to some extent mid latitudes. However, the error is not unreasonably large. In Figure 2.1 (lower left) representative specific humidity uncertainty for background and solution is shown for the three latitude bands. The tropical background specific humidity uncertainty is very large - more than 2 g/kg at 2 km, and the 1D-Var reduces the error considerably.

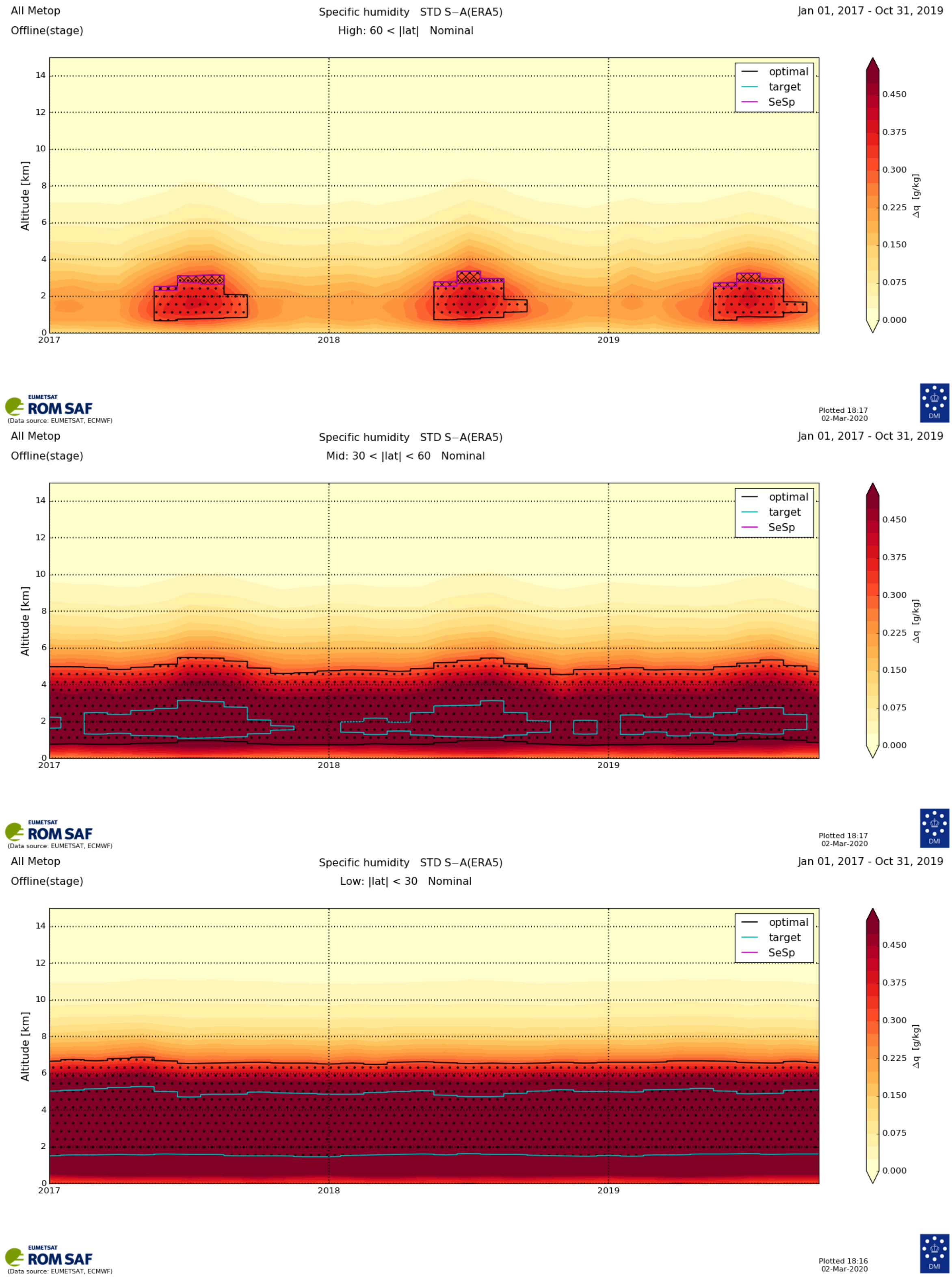


Figure 3.11: *All satellites, high, mid and low latitudes, STDV of 1D-Var- ERA5 specific humidity as function of time and altitude.*

Seasonal and latitudinal quality differences

Figures 3.12 and 3.13 are included to show that there are differences in performance on northern and southern hemispheres, especially at the poles. Never the less the north and south latitude bands are pooled together in the service specifications.

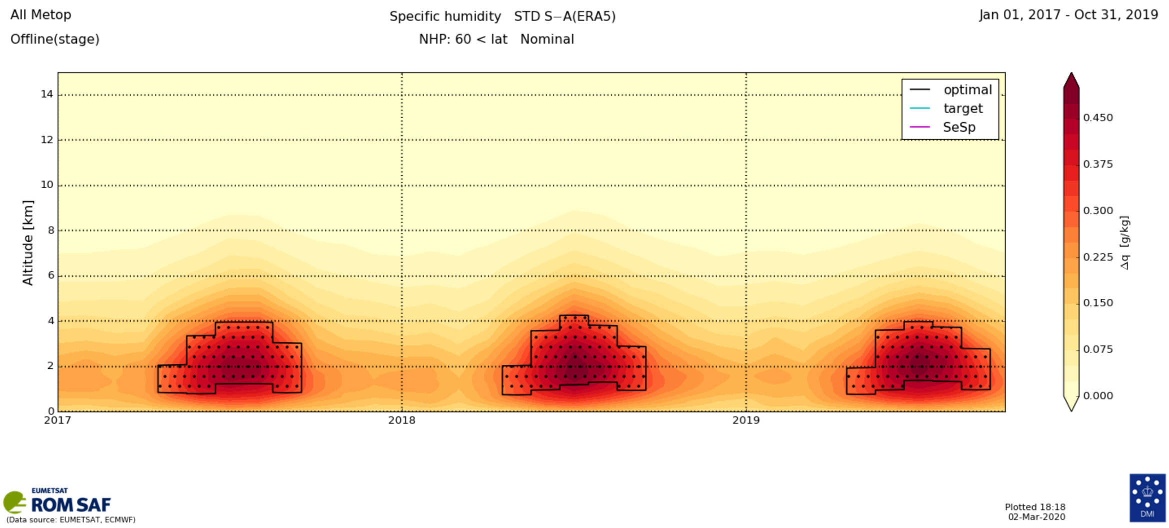


Figure 3.12: *All satellites, northern hemisphere polar, STDV of 1D-Var- ERA5 specific humidity as function of time and altitude.*

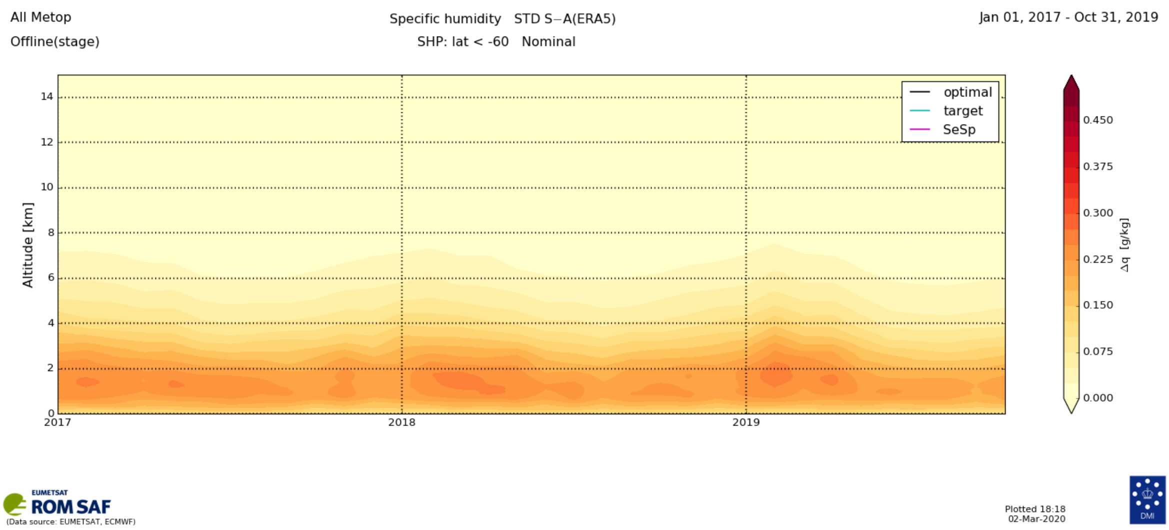


Figure 3.13: *All satellites, southern hemisphere polar, STDV of 1D-Var- ERA5 specific humidity as function of time and altitude.*

Regarding differences between Metop A, Metop B and Metop C: There is generally not much to see in the 1D-Var products regarding satellite differences, and that is also the case with Offline 1.1 specific humidity, as seen in Figures 3.14 and 3.15.

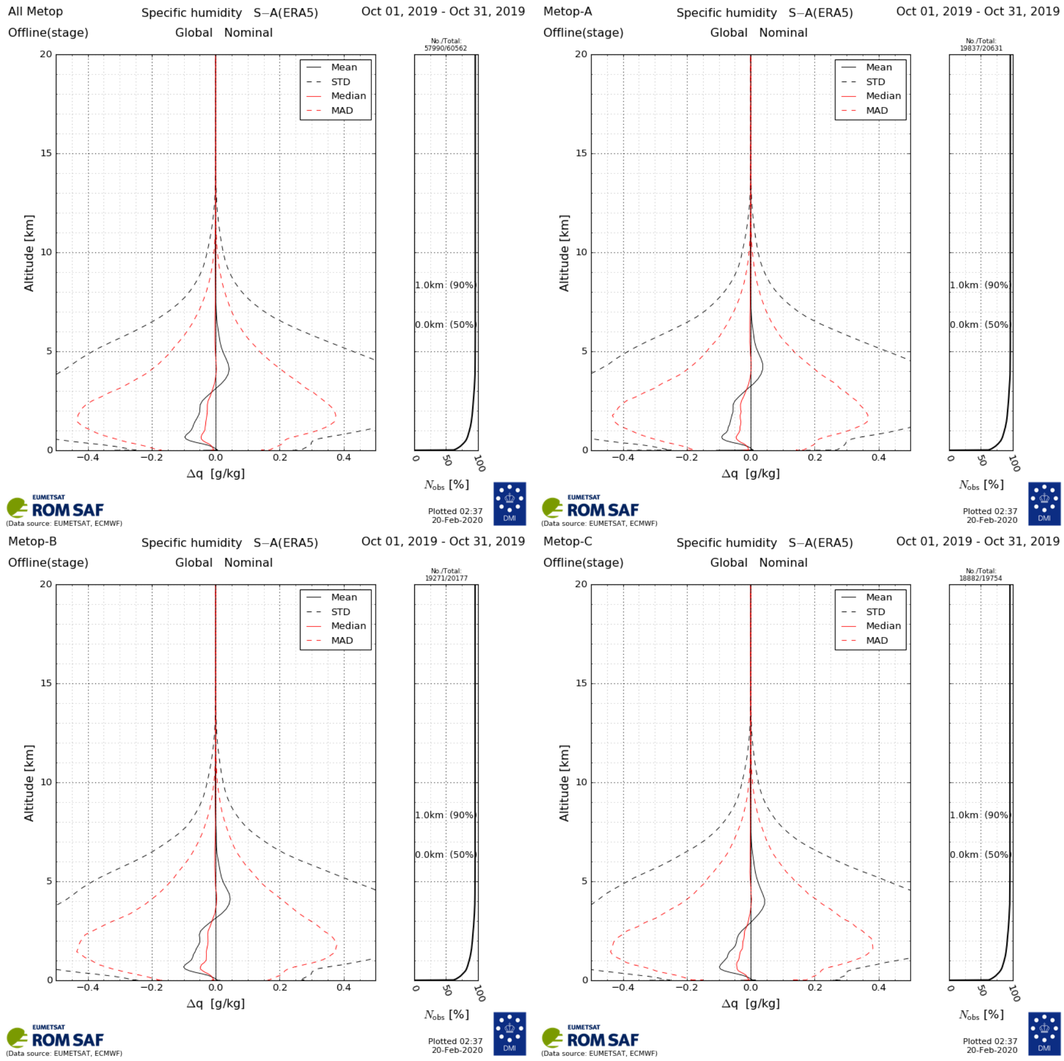


Figure 3.14: *Specific humidity statistics for October 2019. All Metop, Metop A, Metop B and Metop C.*

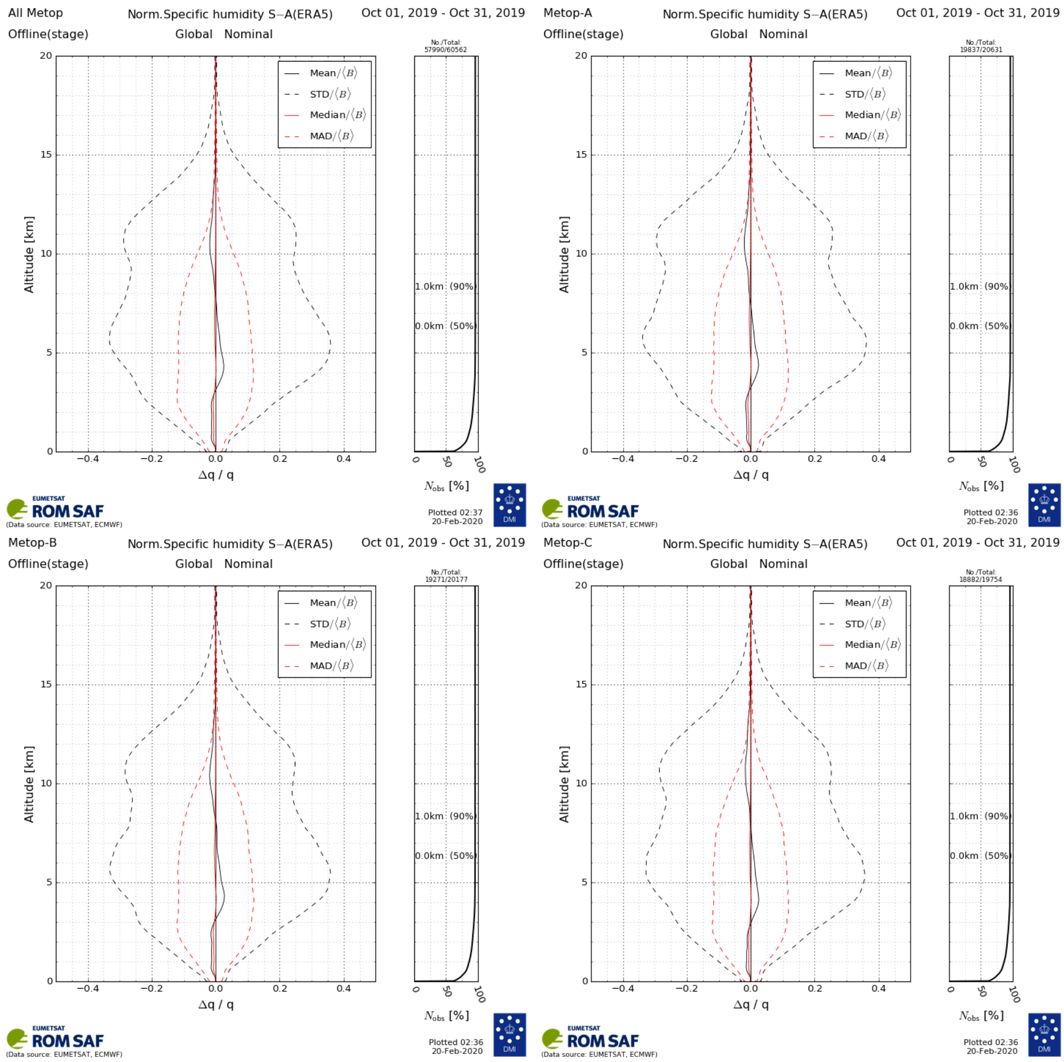


Figure 3.15: *Normalized specific humidity statistics for October 2019. All Metop, Metop A, Metop B and Metop C. The STDVs are divided with the monthly mean analysis (A) specific humidity.*

3.2.2 Intermediate summary regarding specific humidity service specifications

We can justify a deflation of the service specifications to match the actual S-A statistics of the data record. The modified service specs have to be dependent on latitude and they will be summarized in section 3.2.2. As seen in Figures 3.7 and 3.15 the standard deviation is behaving more stable in the normalized plots than in the absolute plots. This gives an opportunity to redefine the service specifications.

The previous specific humidity service specifications were defined as maximum of an absolute and a relative criterion, where the relative threshold is evaluated per profile with respect to the ERA5 background. The issue with that is that in the tropics both absolute and relative errors can occasionally grow very large when evaluated on single (nominal) profiles. Especially rare cases, where the background for whatever reason has a extreme low absolute value, are weighted unreasonably high in the evaluation of monthly means. If the normalized error (Figure 3.15) is applied these singular cases cannot have so much weight. Originally the combined absolute and relative criterion was applied to combine high altitude (high relative error) with low altitude hig absolute error. But that is an unnecessary complication, because the normalized error remains in the same range throughout the troposphere.

Therefore it is proposed to simplify the service specifications as follows. The normalized standard deviation (1D-Var solution minus ERA analysis)/mean(background) has to be within; Tropics: 30 %, Mid latitudes: 35 % and High latitudes: 25 %. The numbers are chosen such that there will be occational violations of service specifications when evaluated on monthly basis. The proposed service specifications are listed in Annex I.

3.3 Surface pressure (GRM-13/51/71)

The surface pressure is a primary output variable from the ROM SAF 1D-Var implementation as described in section 2.3.2. The surface pressure is a scalar which is used along with temperature and specific humidity in the calculation of pressure and geopotential height profiles.

3.3.1 1D-Var surface pressure compared to ERA5

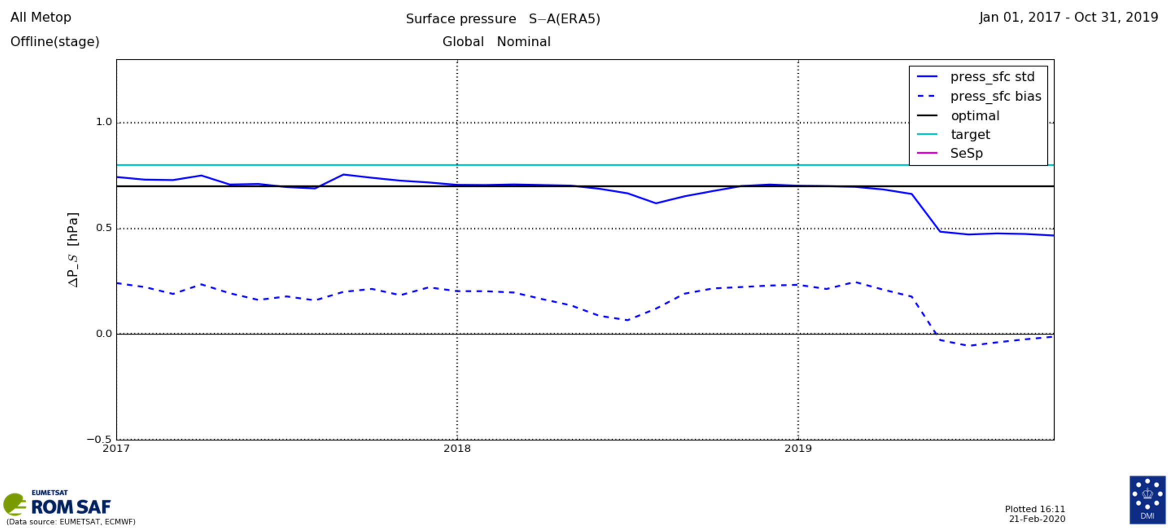


Figure 3.16: *All satellites, all latitudes, STDV of 1D-Var - ERA5 surface pressure.*

The most striking feature is the bias (and standard deviation) drop in June 2019, which is not synchronized with the standard deviation change in March in pure model data (Figure 2.7). This feature is related to the shift in interpolation time intervals from 6 hours to 3 hours in the analysis data. We shall therefore consider only the last part (June to October) of the time series.

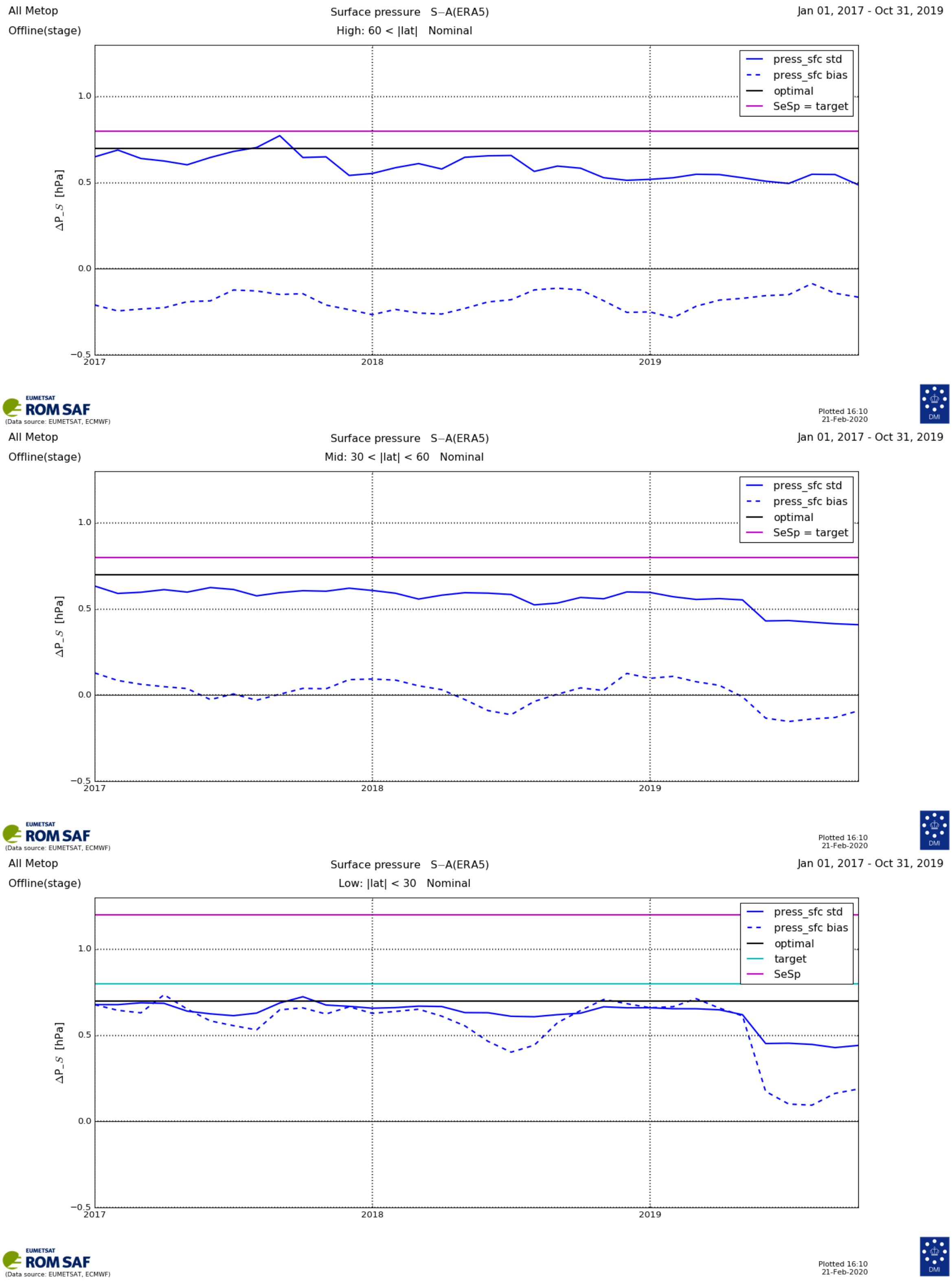


Figure 3.17: *All satellites, high, mid and low latitudes, STDV of 1D-Var- ERA5 surface pressure.*

3.3.2 Intermediate summary regarding surface pressure service specifications

From figure 3.17, the following service specifications are inferred High latitude bands: S-A STDV < 0.6 hPa, Mid latitude bands: S-A STDV < 0.5 hPa and Tropics: S-A STDV < 0.5 hPa.

3.4 Pressure (GRM-12/50/70)

The pressure profile is a secondary variable, as described in section 2.3.2. Pressure profiles as function of geopotential height are formal ROM SAF products. Their quality reflects the quality of the geopotential height profile which is also a secondary product ultimately derived from the temperature, specific humidity and surface pressure state vector. As such the pressure profile is not really an interesting property for any known applications. We monitor the pressure profiles for the sake of sanity.

3.4.1 1D-Var pressure compared to ERA5

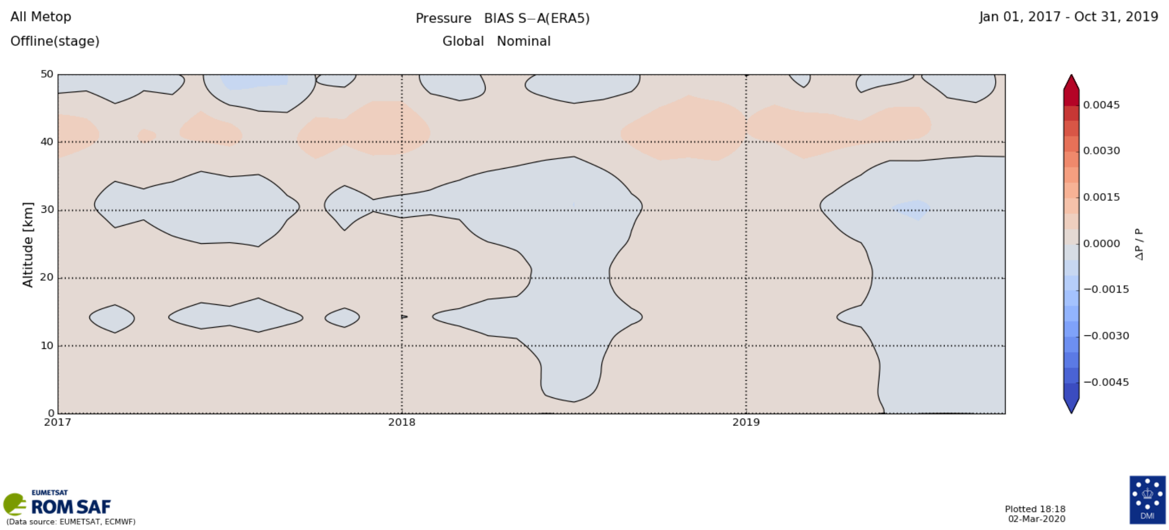


Figure 3.18: All satellites, low latitudes, bias of 1D-Var- ERA5 pressure.

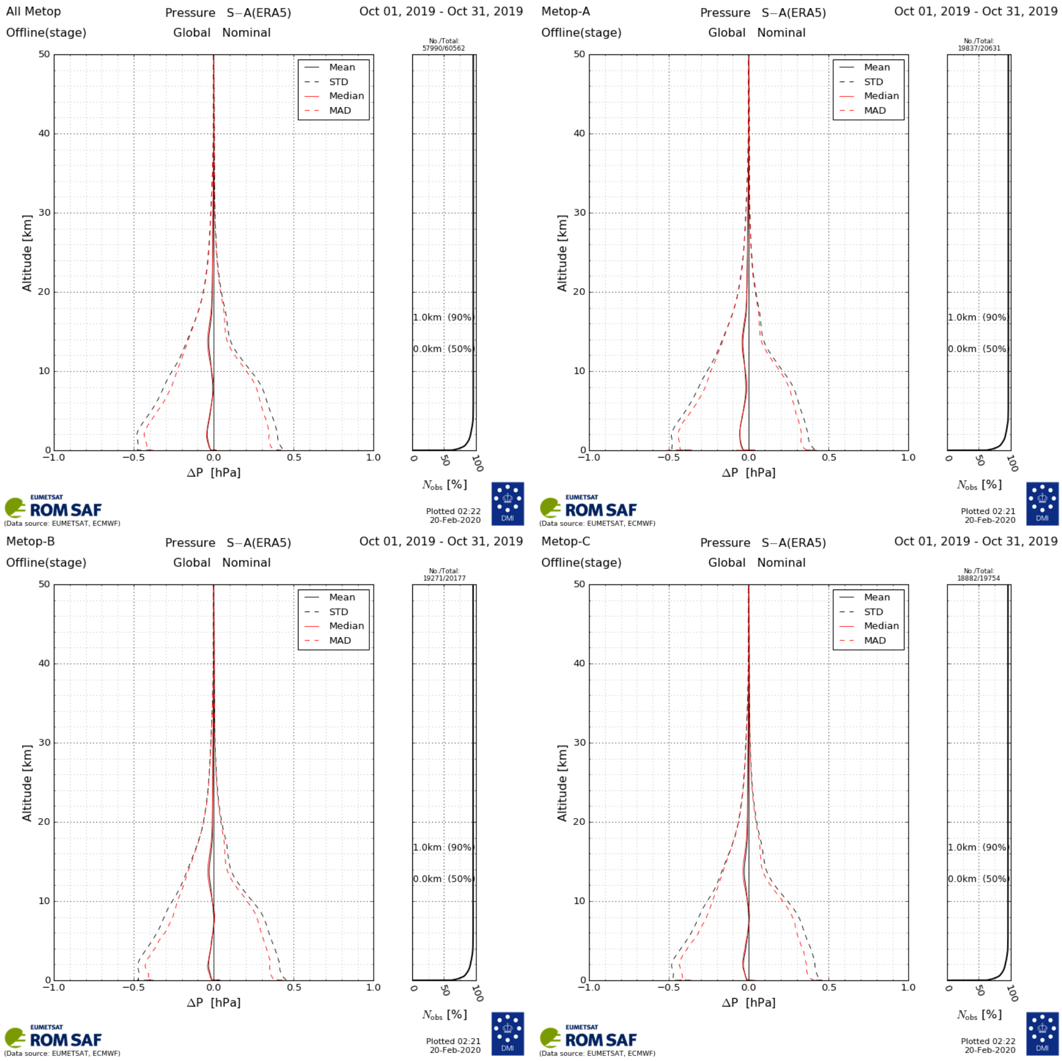


Figure 3.19: *Pressure statistics for October 2019. All Metop, Metop A, Metop B and Metop C.*

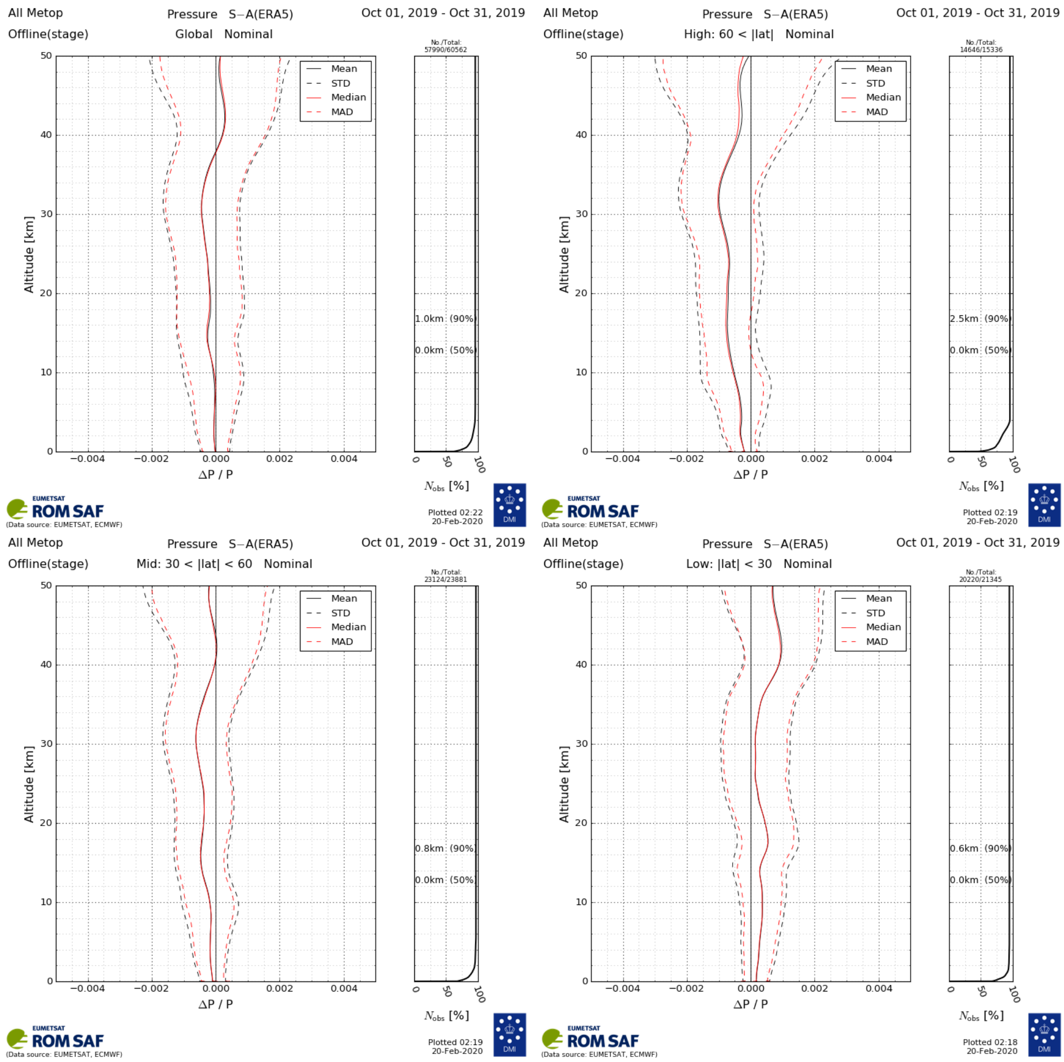


Figure 3.20: *All Metop satellites (from left top; global, polar, mid latitudes and tropical) pressure statistics for October 2019. The standar deviations are divided with the monthly mean background (B) pressure.*

3.4.2 Intermediate summary regarding pressure service specifications

From Figure 3.20 the following service specifications are inferred for the pressure in the altitude range 0 to 50 km; High latitude bands: max of 0.01 hPa or 0.2 % but less than 0.6 hPa, Mid latitude bands: max of 0.01 hPa or 0.2 % but less than 0.5 hPa and Tropics: max of 0.01 hPa or 0.2 % but less than 0.5 hPa.

4 Product 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 ERA5. The formal requirements for the ROM SAF data products are given in the Products Requirements Document [AD.3][1]. Table 4.1 is summarizing the product requirements for offline 1D-var products. The standard deviations, and consequently the service specifications extracted in Chapter 3, does not match the product requirements target values very well. Especially the specific humidity has a much larger uncertainty (and consequently larger error standard deviation) than was anticipated during design phase. This is ultimately due to the choice off B-matrix that has been changed during the developing phase.

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

Threshold	Target	Optimal
GRM-10/48/68		
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-11/49/69		
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-12/50/60		
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-13/51/71		
2.4 hPa	0.8 hPa	0.7 hPa

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

[1] In the PRD [AD.3] the Offline product requirements are defined with reference to "ECMWF analysis", at the time when the PRD was written the intention was that offline Level 2B and 2C data was to be produced with ECMWF(OPER) as input. In the present report we use ERA5 analysis as reference.

5 Conclusions

ROM SAF Offline v1.1 Level 2B and 2C product conmbines the RO data from all Metop satellites. The observed biases and standard deviations in comparisons with ERA5 are consistent with the theoretical uncertainty estimates of involved data sets. Generally the Offline v1.1 Level 2B and Level 2C data are of better quality than corresponding Offline v1.0 products, and this has allowed for a strengthening and simplification of service specifications for all parameters.

5.1 Constraints and limitations

Then ROM SAF 1D-Var products only contain observational information in ranges where prior fractions are low. Outside these ranges the products reflects the ERA5 background model.

In particular the Offline v1.1 specific humidity is not expected to contain valuable information above 10 km.

The ROM SAF offline data records are subject to upgrades and changes, and therefore not suitable as climate data records and must in particular not be used for trend studies.

Annex I. Service specifications for Offline v1.1 Level 2B and 2C

The Service Specifications 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 product. Note that adherence to SeSp cannot be taken as an indicator of absolute quality of the 1D-Var products. ERA5 analysis cannot be used as an absolute standard in this context, since ERA5 analysis may contain some of the same issues as ERA5 forecast which is used as background in 1D-Var. This could for instance include limitation in representation due to vertical gridding. In table 5.1 we summarize the 1D-Var service specifications that have been emphasized by the end of each section in chapter 3.

Table 5.1: *Service specifications for Ofline-v1.1 1D-Var products. For profile products (temperature, specific humidity and pressure), the SeSp are compared to the monthly STDV of the 1D-Var solution minus ERA5 (S-A) on fixed altitude levels.*

Service Specifications Offline v1.1 1D-Var products			
Applications and Users	Climate and atmosphere researchers		
Characteristics and Methods	1D-Var algorithm, ERA5 forecast as background		
Operational Satellite Input Data	Reprocessed level 1A Metop from EUMETSAT Secretariat		
Other Operational Input Data	ECMWF ERA5 fields		
SeSp Metrics:	Monthly mean of S-A standard deviation. An interval means a linearly changing quantity between the two values over the given vertical coordinate. If the SeSp are violated at one level, the product is violating the SeSp for the given month, latitude range and altitude range.		
Dissemination			
	Format netCDF	Means Web	Timeliness n/a
Latitude bands			
	0-30 degrees North / South	30-60 degrees North / South	60-90 degrees North / South
Offline temperature profile (GRM-10/48/68)			
Altitude STDV(S-A) <	0 - 30 km 0.75 K	0 - 30 km 0.75 K	0 - 30 km 0.75 K
Altitude STDV(S-A) <	30 - 50 km 0.75 K	30 - 50 km 0.75-2.0 K	30 - 50 km 0.75-2.0 K
Offline specific humidity profile (GRM-11/49/69)			
Altitude STDV(S-A) < 30 %	0 - 12 km 35 %	0 - 12 km 25 %	0 - 12 km
Offline pressure profiles (GRM-12/50/70)			
Altitude STDV(S-A) < max of - not larger than	0 - 50 km 0.01 hPa or 0.20 % 0.5 hPa	0 - 50 km 0.01 hPa or 0.2 % 0.5 hPa	0 - 50 km 0.01 hPa or 0.2 % 0.6 hPa
Offline surface pressure (GRM-13/51/71)			
STDV(S-A) <	0.5 hPa	0.5 hPa	0.6 hPa
Coverage and Resolution			
Spatial Coverage	Spatial Resolution	Vertical Resolution	Temporal resolution
global	RO resolution	model levels	RO resolution