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EUMETSAT
NWC SAF
SUPPORT TO NOWCASTING AND VERY SHORT RANGE FORECASTING

Algorithm Theoretical Basis Document for iSHAI Product Processors of the NWC/GEO

NWC/CDOP2/GEO/AEMET/SCI/ATBD/iSHAI, Issue 2, Rev.1

21 January 2019

Applicable to GEO-iSHAI v4.0 (NWC-032)

Prepared by   Agencia Estatal de Meteorología (AEMET)

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DOCUMENT CHANGE RECORD

Version	Date	Pages	Changes
2.1	*21 January 2019*	50	Updated version after NWC/GEO v2018 DRR.
2.1d	*31 October 2018*	57	Updated for version 2018 DRR
			Updated for GOES-R processing
2.0d	*27 February 2017*	47	Updated from GEO-iSHAI v2016 ATBD for version 2018 and the support of Himawari.
			The specific use of RTTOV-11.2 has been changed for a generic RTTOV version.
			The specific phrasing of SEVIRI instruments has been changed for a generic satellite phrasing with specific use of SEVIRI and Himwari.

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1. INTRODUCTION

The Eumetsat "Satellite Application Facilities" (SAF) are dedicated centres of excellence for processing satellite data, and form an integral part of the distributed EUMETSAT Application Ground Segment (http://www.eumetsat.int).

This documentation is provided by the SAF on Support to Nowcasting and Very Short Range Forecasting, hereafter NWC SAF. The main objective of NWC SAF is to provide, further develop and maintain software packages to be used for Nowcasting applications of operational meteorological satellite data by National Meteorological Services. More information can be found at the NWC SAF webpage, http://nwc-saf.eumetsat.int. This document is applicable to the NWC SAF processing package for geostationary meteorological satellites, NWC/GEO.

1.1 PURPOSE AND SCOPE OF THE DOCUMENT

The purpose of this document is to present the Algorithm Theoretical Basis Document (ATBD) for the GEO-iSHAI Product Processor of the NWC/GEO software package release 2018. iSHAI (**i**maging **S**atellite **H**umidity **A**nd **I**nstability) is the clear air product of the NWC/GEO software package release 2018.

GEO-iSHAI product is a heritage of former PGE13 SEVIRI Physical Retrieval (SPhR) product. The name of the product was changed to avoid the word SEVIRI because NWC/GEO software package since release 2018 can be used with other GEO imager instruments different from MSG (like AHI on board Himawari satellites and ABI on board GOES-R class satellites). The name iSHAI was chosen to be coherent with names of NWC SAF products from MTG-FCI and MTG-IRS in CDOP-3 and future CDOP-4.

In this document a description of the algorithm is provided. The algorithm is composed of a statistical retrieval followed by a physical retrieval of temperature and moisture profiles using infrared (IR) brightness temperatures (BTs) measured by GEO imager satellites and a background NWP forecast as main inputs.

In this version IR brightness temperatures measured by the supported GEO imager instruments on board meteorological satellites can be used as input. In version 2018 the supported GEO imager instruments are SEVIRI on board METEOSAT Second Generation satellites and AHI on board Himawari satellites. The iSHAI code version 2018 for AHI is being adapted to ABI instrument on board GOES-R satellites (it requires minor changes in the code and generation of a set of GOES-R iSHAI coefficients) and it will be distributed as a patch to the version 2018. Thus, GEO-iSHAI is updated to the state of art satellites and the GEO-iSHAI products could be compared with the products using the JMA and NOAA legacy algorithms. The main objective is to improve GEO-iSHAI algorithm and to be ready for the MTG-FCI era.

The algorithm retrieves temperature and moisture profiles that are used to derive total precipitable water (TPW), layer precipitable water (LPW), Lifted Index (LI), Showalter Index (SHW), K-Index (KI), total ozone (TOZ) and the skin temperature (SKT) parameters from clear sky brightness temperatures within individual pixels or in a Field of Regard (FOR); a FOR is a region of M x M IR satellite pixels. Also the difference of these parameters with the calculated ones from the background NWP are output parameters.

This document describes the GEO-iSHAI product objectives, the scientific algorithm, the needed input data and the resulting output. It also provides basic information on the algorithm implementation.

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1.2 SOFTWARE VERSION IDENTIFICATION

This document describes the theoretical basis of the algorithm implemented in the GEO iSHAI version 4.0 product, to be included in the release 2018 of NWC/GEO software package.

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1.3 IMPROVEMENTS FROM PREVIOUS VERSION

GEO-iSHAI algorithm remains based in Jun Li's algorithm for GOES Sounder physical retrieval algorithm (physical retrieval approach with non-linear regression as first guess) but adapted for RTTOV and other GEO imager instruments. Jun Li (CIMSS-Wisconsin) algorithm is also the one proposed as Day-1 algorithm for the GOES-R processing by NOAA (Li, 2010).

GEO-iSHAI release 2018 has some major updates due to the introduction of the support of other GEO satellites than MSG.

The use of RTTOV-11.2 in version 2018 implies that the number of RTTOV pressure levels remains in 54 RTTOV pressure levels. For this reason all the coefficients has been calculated using the GEO-iSHAI validation dataset for 2017 year with vertical dimensions adjusted to the used RTTOV pressure levels.

One of the main achievements in version 2018 has been the modifications of the tools for the generation of GEO-iSHAI coefficients for other satellites than MSG ones. It will be basic for future releases of GEO-iSHAI, the generalization also of the process to generate training and validation dataset to other GEO and LEO satellites (GOES-R, IASI and future MTG-FCI and MTG-IRS).

In previous versions there were separated EOFs coefficients files for temperature and humidity that after reading where combined to build the full EOF matrix. In version 2018, the full EOFs matrix is read from a single coefficient file.

The GEO-iSHAI code version 2018 is being adapted to ABI instrument on board GOES-R satellites with minor changes in the code and the generation of a set of iSHAI coefficients for GOES-R. The delivery of iSHAI for GOES-R will be made as a patch to the version 2018.

GEO-iSHAI Total Ozone (TOZ) output was introduced as a new output in release 2016. TOZ is calculated from the ozone profile after applying only the non-linear regression step. In version 2016 in the ozone non-linear regressions, the collocated real bias corrected satellite BTs and the temperature profile, the logarithm of ozone profile and the skin temperature from background NWP profile were used as inputs.

Thus, neither the physical retrieval step nor the iSHAI retrieved profile (result of FG or physical retrieval step depending on BT_RMS_THRESHOLD keyword) were not used in the ozone profile estimation.

In version 2018; this has been changed and in the ozone non-linear regressions, the collocated real bias corrected satellite BTs and the temperature profile, the logarithm of specific humidity profile and the skin temperature from the iSHAI retrieved profile and the logarithm of ozone profile from the background NWP profile are used as inputs.

1.4 DEFINITIONS, ACRONYMS AND ABBREVIATIONS

Please refer to the "Nowcasting SAF Glossary" document in the NWC SAF web for a wider glossary and a complete list of acronyms for the NWC SAF project.

ABI	Advanced Baseline Imager
AEMET	Agencia Estatal de Meteorología Meteorology State Agency (Spain)
AHI	Advanced Himawari Imager
ASCII	American Standard Code for Information and Interchange

ATBD	Algorithm Theoretical Basis Document
BL	Precipitable water in low layer (P_{sfc} – 850 hPa)
BT	Brightness Temperature
CDOP (CDOP-1)	Continuous Development and Operations Phase (1)
CDOP-2	Continuous Development and Operations Phase 2
CDOP-3	Continuous Development and Operations Phase 3
CF	NetCDF Climate and Forecast (CF) Metadata Conventions
CIMSS	Cooperative Institute for Meteorological Satellite Studies (USA)
CMa	Cloud Mask
COTS	Commercial-Off-The-Shelf
CPU	Central Processor Unit
DEM	Digital Elevation Model
ECMWF	European Centre for Medium-range Weather Forecasts
EOF	Empirical Orthogonal Function
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FCI	Flexible Combined Imager (MTG)
FG	First Guess
FOV	Field Of View
FOR	Field Of Regard
GEO	Geostationary Satellites
GEO-CMa	GEO Cloud Mask and Cloud Amount
GEO-iSHAI	GEO imaging Satellite Humidity And Instability
GRIB	Gridded Information in Binary Form
HDF5	Hierarchical Data format version 5
HL	Precipitable water in High Layer (500 – 0 hPa)
hPa	Hecto Pascal
HRIT	High Rate Image Transmission
IDL	Interactive Data Language
IR	InfraRed
IREMIS	InfraRed Emissivity
IRS	Infrared Sounder (MTG)

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iSHAI	imaging Satellite Humidity And Instability
K	Kelvin
KI	K-Index
km	kilometre
LI	Lifted Index
LPW	Layer Precipitable Water
LST	Land Surface Temperature
MARS	ECMWF Meteorological Archive and Retrieval Facility
McIDAS	Man Computer Interactive Data Access System
ML	Precipitable water in Medium Layer (850 – 500 hPa)
MSG	Meteosat Second Generation
MTG	Meteosat Third Generation
MTG-FCI	Meteosat Third Generation Flexible Combined Imager
MTG-IRS	Meteosat Third Generation Infra Red Sounder
netCDF	Network Common Data Form
NRT	Near Real Time
NWC	Nowcasting
NWC/GEO	Geostationary part of the Nowcasting SAF
NWCLIB	Nowcasting Library
NWCSAF	Nowcasting SAF
NWP	Numerical Weather Prediction
NWP SAF	SAF for Numerical Weather Prediction
LPW	Layer Precipitable Water
PGE	Product Generation Element PGE01 Cloud Mask (GEO-CMa) Product Generator PGE13 SEVIRI Physical Retrieval (SPhR) Product Generator
PW	Precipitable Water
RTM	Radiative Transfer Model
RTTOV	Radiative Transfer for TOVs
SAF	Satellite Application Facility
SEVIRI	Spinning Enhanced Visible InfraRed Imager

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SG	Steering Group
SHAI	Satellite Humidity And Instability
SHW	Showalter Index
SKT	Skin Temperature
SST	Sea Surface Temperature
SW	Software
TOZ	Total ozone
TPW	Total Precipitable Water
TM	Task Manager
UM	User Manual
VR	Validation Report
VSA	Visiting Scientist Activities
WV	Water Vapour Channel

1.5 REFERENCES

1.5.1 NWC SAF Applicable Documents

The following documents, of the exact issue shown, form part of this document to the extent specified herein. Applicable documents are those referenced in the Contract or approved by the Approval Authority. They are referenced in this document in the form [AD.X]

For versioned references, subsequent amendments to, or revisions of, any of these publications do not apply. For unversioned references, the current edition of the document referred applies.

Current documentation can be found at the NWC SAF Helpdesk web: http://nwc-saf.eumetsat.int.

Ref.	Title	Code	Vers
[AD.1]	Proposal for the Third Continuous Development and Operations Phase (CDOP-3) March 2017-February 2022	NWC SAF: CDOP-3 proposal	1.0
[AD.2]	Project Plan for the NWCSAF CDOP3 phase	NWC/CDOP3/SAF/AEMET/MGT/PP	1.0
[AD.3]	Configuration Management Plan for the NWC SAF	NWC/CDOP3/SAF/AEMET/MGT/CMP	1.0
[AD.4]	NWC SAF Product Requirements Document	NWC/CDOP3/SAF/AEMET/MGT/PRD	1.0
[AD.5]	Interface Control Document for Internal and External Interfaces of the NWC/GEO	NWC/CDOP3/GEO/AEMET/SW/ICD/1	1.0
[AD.6]	Data Output Format	NWC/CDOP3/GEO/AEMET/SW/DOF	1.0
[AD.7]	System and Components Requirements Document for the NWC/GEO	NWC/CDOP2/GEO/AEMET/SW/SCRD	2.1
[AD.8]	NWC SAF CDOP-3 Project Plan Master Schedule	NWC/CDOP3/SAF/AEMET/MGT/PP/MasterSchedule	1.1
[AD.9]	Component Design Document for the NWCLIB of the NWC/GEO	NWC/CDOP2/GEO/AEMET/SW/ACDD/NWCLIB	2.0
[AD.10]	Interface Control Document for the NWCLIB of the NWC/GEO	NWC/CDOP3/GEO/AEMET/SW/ICD/2	1.0
[AD.11]	User Manual for the Tools of the NWC/GEO	NWC/CDOP3/GEO/AEMET/SCI/UM/Tools	1.0

Table 1: List of Applicable Documents

1.5.2 Reference Documents

The reference documents contain useful information related to the subject of the project. These reference documents complement the applicable ones, and can be looked up to enhance the information included in this document if it is desired. They are referenced in this document in the form [RD.X]

For dated references, subsequent amendments to, or revisions of, any of these publications do not apply. For undated references, the current edition of the document referred applies.

Ref.	Title	Code	Vers	Date
[RD.1]	Scientific and Validation Report for the iSHAI Processors of the NWC/GEO	NWC/CDOP3/GEO/AEMET/SCI/VR/iSHAI	1.0	21/01/19
[RD.2]	User Manual for iSHAI Product Processors of the NWC/GEO: Science Part	NWC/CDOP3/GEO/AEMET/SCI/UM/iSHAI	1.0	21/01/19

Table 2: List of Referenced Documents

2. GEO-ISHAI PRODUCT ALGORITHM

This product has been developed within the NWC SAF context, aiming to support nowcasting applications. GEO-iSHAI algorithm version 4.0 is responsible for the retrieval of the atmospheric temperature and moisture profiles as well as surface skin temperature for one clear sky satellite pixel, or a Field-Of-Regard (FOR) which contains M x M pixels. Then, several parameters of interest for nowcasting applications are calculated from the retrieved profile.

Also TOZ can be optionally calculated using nonlinear regression estimation of ozone profile.

The main outputs of GEO-iSHAI product are:

1. Total Precipitable Water (TPW)

2. Layer Precipitable Water (LPW). Corresponding to the precipitable water in three layers:

    a. BL: Precipitable water in low layer [surface pressure - 850 hPa]

    b. ML: Precipitable water in middle layer [850 - 500 hPa]

    c. HL: Precipitable water in high layer [500 – 0 hPa]

3. Stability indices: they are calculated from the retrieved profiles of temperature and humidity. The calculated indices are:

    a. Lifted Index (LI)

    b. Showalter Index (SHW)

    c. K-index (KI)

4. Skin Temperature (SKT)

5. Total Ozone (TOZ). This parameter is optional, must be activated by the users and the background NWP GRIB files must contains ozone fields.

6. Besides the main outputs, the differences between the above parameters calculated from the retrieved profiles of temperature and humidity (and ozone profile if activated) with the parameters calculated from the spatial, temporal and vertical interpolated profiles from background NWP are written as other outputs (following 2007 Madrid Workshop recommendation). Thus the parameters diffTPW, diffBL, diffML, diffHL, diffLI, diffSHW, diffKI, diffSKT and diffTOZ are also written in the netCDF output file.

7. BT_Residual: root mean square of differences between the real bias corrected satellite and RTTOV calculated brightness temperatures on absorption channels.

In future versions and if any users requirement is set, other stability indices could be calculated from the retrieved temperature and humidity profiles and they could be added. In the meantime, the users can activate the writing as binary files of structures with T/q/ozone profiles together with some surface and ancillary parameters, read the written structures and calculate their own stability indices or parameters.

The main inputs of the product are real satellite IR brightness temperatures (BTs) and forecast NWP model GRIB files. Geostationary satellites provides full resolution images with high spatial resolution (3x3 km in SEVIRI case and 2x2 km in AHI or ABI case) and with high temporal resolution (every 15 minutes or 10 minutes in operation mode and 5 or 2 or 1 minute from rapid scan mode) at the satellite nadir for every IR channel. Thus, these products are useful in the prediction of severe weather due to their ability to measure with high temporal and spatial resolution variations of atmospheric stability and moisture. A time sequence of the images is the best way to monitor drying and moistening tendencies and stability tendencies; as example, NWC SAF GEO-iSHAI animations are available at

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the NWC SAF MSG web page (http://nwc-saf.eumetsat.int/) generated with NWC/GEO reference system at AEMET.

GEO-iSHAI is only generated in clear sky pixels. For this reason a cloud mask is also a mandatory input to GEO-iSHAI; GEO-CMA must be executed before GEO-iSHAI. In NRT operation this is made by the NWC SAF Task Manager who synchronises the execution of the products and the first product that is generated upon the arrival of a new image is the cloud mask (GEO-CMA).

Once the outbreak of convection occurs, TPW, LPWs, LI, SHW, KI, SKT and TOZ values provided by GEO-iSHAI in clear air pixels surrounding the convective system may help the forecasters to foresee the evolution of convection. GEO-iSHAI outputs cannot predict by themselves whether storms will occur. They provide forecasters a localization and evolution of some of the key ingredients and the convective forcing before thunderstorms develop. Regions with unstable values on the stability indices combined with high precipitable water values indicate that the troposphere is near saturation and convection could be triggered. Convection can be produced with stable values in stability indices due to other ingredients, not correlated with the stability indices, which can also be responsible of the convection (elevated convection, dynamic forcing without thermodynamic forcing and isentropic lifting). Therefore, these NWC SAF products must be used in conjunction with other data sources (NWP profiles, radio-sounding, satellite data, Radar data, lightning strokes detectors, etc.) in order to alert the forecasters about the possibility of occurrence of mesoscale events.

Products can be generated at every single time step, on pixel by pixel or on a Field-of-Regard (FOR) basis. A FOR consists of M x M real satellite pixels of infrared channels. The default FOR size for iSHAI processing is 3 x 3 pixels which is equivalent to near 4 (AHI or ABI) to 9 (SEVIRI) km^2 spatial resolution at nadir. However, following the users' requirements, the FOR size is configurable. The size of the FOR width is a parameter on the ASCII GEO-iSHAI configuration file. Only clear IR brightness temperatures within each FOR are averaged for sounding product. Temperature and moisture from NWP forecast information is used together with real satellite IR BTs on clear air pixels for generation of nowcasting products. Two steps are used in the algorithm: non-linear regression and the iterative physical retrieval. The cloud mask processing sometimes identifies cloud contaminated pixels as clear, and therefore another option is to process the warmest clear pixel at the cleanest channel in the IR window (IR10.8 channel in case SEVIRI, IR10.4 in case AHI or IR10.3 in case ABI) inside the FOR (it has less probability to be contaminated by clouds). This option can be activated editing the configuration file.

Since the physical basis of temperature and humidity retrieval is based in the minimization of the error between the real and the synthetic satellite BTs calculated from the profiles and taking into account the limited number of channels and the spectral information of the GEO imager instruments, GEO-iSHAI improves mainly the humidity profiles of the background NWP. This improvements is mainly made in middle to high levels. The main advantage of GEO-iSHAI is the high spatial and temporal resolution of the retrieved fields. Thus, GEO-iSHAI provides a good spatial and temporal monitoring of the variations of precipitable water and stability indices fields. This fact must be taken into account by the users when the GEO-iSHAI outputs are used in nowcasting.

In the section 2.1 the outline of the GEO-iSHAI algorithm is described. In the Section 2.2 it is made a description step by step in the order described in the outline; while the mathematical basis of the physical retrieval module are described in sections 2.2.5 and 2.2.6. Section 2.3 has been written to describe briefly the multiple files used in the algorithm as well as to provide references and theoretical basis of how the files have been obtained. In Section 2.4 the GEO-iSHAI outputs are described briefly.

2.1 GEO-iSHAI PROCESSING OUTLINE

As a whole, GEO-iSHAI code is designed in a modular way, so that it can be easily handled and modified.

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For the selected region, the initialization gives access to real satellite BTs, Cloud Mask (CMA), satellite zenith angle and ancillary data (topographic data, land-sea mask, longitude, latitude). Only if the pixel or the FOR (in case of MxM pixels processing) is labelled as clear air and the satellite zenith angle of this pixel or FOR is below the configurable maximum zenith threshold, GEO-iSHAI algorithm is applied and the parameters are calculated for this pixel or FOR.

The main input values are the real satellite BTs from the selected infrared channels and forecasted NWP fields which are used as background information. GEO-iSHAI also uses elevation dataset as static input information to determine the pixels where the land emissivity maps, pre-computed for each IR channel and for every month of the year, are used.

If the user activates it, also TOZ is calculated from the estimated ozone profile using only non-linear regressions. In this case IR BTs of the nearest IR channel to the ozone absorption region at 9.7 μm are used also as input to the First-Guess non-linear regressions together with the background NWP ozone profile.

Cloud Mask (CMA) computed by GEO-CMA is used as mandatory input to GEO-iSHAI and the process is only performed for pixels, or FOR (in case of MxM pixels processing), labelled as clear air.
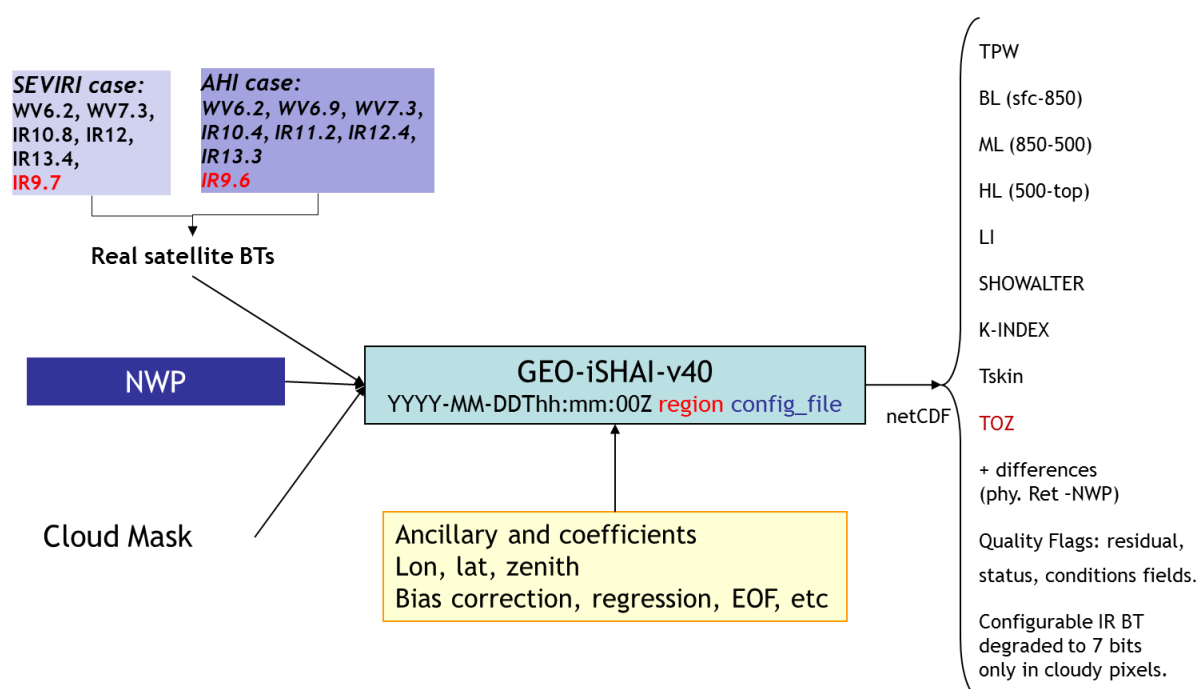
Figure 1: GEO-iSHAI inputs and outputs scheme.

Below, the main steps in the algorithm are described; in the User Manual [RD.2] there is a similar description where the GEO-iSHAI configurable parameters of the algorithm at each step can be found. The whole process includes the following main steps:

1. Pre-processing:

   - Initialisation: reading of processing options from the configuration file, reading of all coefficient file names, initialisation of RTTOV, getting calibrated real satellite BTs, associated geographical ancillary data, IR emissivity maps and CMA for the region to process.

   - Optional thinning of real satellite BTs to process on FOR of M x N pixels (M and N are configurable parameters in the configuration file). Two methods are allowed to

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calculate BTs of the FOR: 1) mean value of clear pixels BTs on FOR or 2) BTs of the warmest clear pixel at the cleanest channel in the IR window (See section 2.2.1)

- Get collocated background NWP forecast temperature and moisture profiles. Background NWP fields of temperature and humidity (*t+00* to *t+24* hours range forecast) must be spatially, temporally and vertically interpolated to get collocated (T, q) profiles and skin temperature. Also, it is obtained collocated ozone profile from the background NWP ozone fields if TOZ calculation is activated.

  In the case of P mode: The spatial (horizontal) and temporal interpolation is made outside of GEO-iSHAI. It is made by reading the NWP files generated by the pre-processing tool *AllMappingNWP* with common functions of the NWC/GEO NWCLIB library. The vertical interpolation to the RTTOV pressure levels is made from the user profile at fixed levels (see section 2.2.2).

  In the case of HYB mode: all the NWP process is made inside the GEO-iSHAI code. GEO-iSHAI opens directly the previous and next (relative to the time of the MSG image) ECMWF GRIB files on hybrid levels, makes the vertical interpolation on ECMWF position to the RTTOV pressure levels, makes the temporal interpolation to the date of the image and finally makes the spatial interpolation just over the clear air processed FOR.

- Bias adjustment of real satellite BTs. The bias correction regression coefficients are read from the common NWC/GEO datasets and bias BT correction is made (see section 2.2.3).

- Execution of nonlinear regressions to calculate the first guess profiles of temperature and specific humidity and the skin temperature using as main inputs: a) real satellite bias corrected BTs and b) the background NWP temperature and specific humidity profiles and the skin temperature spatially, temporally and vertically interpolated (see section 2.2.4) at FOR.

- Calculation of synthetic RTTOV BTs from first guess profile.

2.   Processing:

- Iterative execution of Physical Retrieval Module up to the maximum number of times established. This step is only executed if the differences between synthetic calculated RTTOV BTs from first guess profile and real bias corrected satellite BTs are greater than a predefined threshold. (see sections 2.2.5 and 2.2.6)

- If activated by the user, calculation of ozone profile using only non-linear regression step. It is estimated the ozone profile using as main inputs: a) real bias BT corrected satellite BTs using also the IR ozone absorption channel and b) the background NWP ozone profile (logarithm of ozone profile) spatially, temporally and vertically interpolated to FOR and c) the retrieved temperature and humidity profile and the retrieved SKT. See figure 5.

- Perform direct calculation of TPW, LPWs, LI, SHW and KI parameters at FOR from the retrieved profiles of T and q.

- Calculation of TOZ, if activated, from the estimated ozone profile.

- Compute the differences between the products (TPW, LPWs, LI, SHW and KI) calculated from retrieved profiles of T and q and the ones calculated from the background NWP profiles of T and q. Calculate the difference between SKT and the background NWP SKT.

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- If activated, TOZ calculation, to compute the differences between TOZ calculated from retrieved profiles of ozone and the ones collocated from the background NWP profiles of ozone.

- Optional writing of the intermediate T, q and ozone profiles at the different algorithm steps. Also other parameters as surface pressure, skin temperature, real satellite BTs, ancillary data, etc are written.

3. Post-processing:

- Quality control: Several quality flags have been added to the output product (see section 2.2.7).

- Filling clear pixels inside the FOR: the default method is to copy the same FOR value to all clear pixels. Another configurable option is to write the output only at the clear FOR positions (see section 2.2.8.1).

- Over cloudy pixels, one IR BT channel degraded to 7 bits (range [0 – 127]) values is stored as another field. This will be later used to generate adequate images in which cloudy pixels are grey scaled and clear pixels are colour scaled (see section 2.2.8.2). The number of the IR BT channel is a configurable parameter in the configuration file; by default it is the cleanest channel in the IR window (the IR10.8 channel in the case of SEVIRI, the IR10.4 in the case of AHI and the IR10.3 in the case of ABI instruments).

- The outputs are written in a netCDF format file (see section 2.2.8.2).

2.2 GEO-iSHAI ALGORITHM DESCRIPTION

In this section, the theoretical basis and some implementation details of the algorithm are described. Although the core of the algorithm is the physical retrieval, they are presented in the order that they are used in the algorithm.

In cloud free skies, the radiation received at the top of the atmosphere in an IR channel is the sum of contributions from the Earth's surface (dependent on emissivity and surface temperature) and from all levels in the atmosphere (dependent on the atmospheric conditions). Therefore, IR long wave channels are sensitive to temperature and water vapour conditions and allow a retrieval of precipitable water parameters and the stability indices.

The problem to be solved here is to retrieve, with enough accuracy, profiles of temperature and humidity from a few infrared brightness temperature observations. Although many IR channels exhibit correlation with temperature and humidity in a non-linear way, some infrared brightness temperature observations are interdependent. Furthermore, small variations in the brightness temperature observations produce changes in the retrieved profiles.

Physical retrieval of atmospheric profiles is a process of adjusting the first guess profiles of temperature and humidity based on the brightness temperature residuals between real bias corrected satellite IR BTs and calculated synthetic RTTOV IR BTs with the first guess (see section 2.2.5). Real satellite spectral and spatial brightness temperature signatures are used in the retrieval process.

SEVIRI instrument has 7 IR channels in the range [6.2 – 13.4] microns. Two channels (WV6.2 and WV7.3 channels) contain strong water vapour absorption; they are located at the strong water vapour absorption band and the radiances contain both temperature and water vapour concentration information. One channel has strong ozone absorption (IR9.7 channels). The SEVIRI infrared channels IR10.8 and IR12.0 are window channels that provide information of the surface skin temperature,

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surface emissivity and low level moisture information. The IR 13.4 channel is located at the CO_2 absorption band and the radiances contain temperature information. [WV6.2, WV7.3, IR10.8, IR12.0, IR13.4] SEVIRI BTs are used in the version 2018 for T and q profiles retrieval; also SKT is retrieved in this process.

AHI and ABI instruments have 9 IR channels in the range [6.2 – 13.4] microns. Three channels (WV6.2, WV6.9 and WV7.3 channels) contain strong water vapour absorption; they are located at the strong water vapour absorption band and the radiances contain both temperature and water vapour concentration information. One channel has strong ozone absorption (IR9.6 channels). The AHI/ABI instruments have three channels in the split window region (IR10.4/IR10.3, IR11.2 and IR12.4/IR12.3) that provides information of the surface skin temperature, surface emissivity and low level moisture information. The IR 13.3 channel is located at the CO_2 absorption band and the radiances contain temperature information. [WV6.2, WV6.9, WV7.3, IR10.4, IR11.2, IR12.4, IR13.3] AHI and ABI BTs are used in the version 2018 for T and q profiles retrieval; also SKT is retrieved in this process.

The ozone channel (the channel in 9.7 µm region) is optionally used (user must activate it) to estimate the ozone profile using ozone non-linear regressions similar to the non-linear regressions used to calculate the T/q profiles at First-Guess step. The estimated ozone profile is used to calculate TOZ and the difference between GEO-iSHAI TOZ and background NWP TOZ.

The current version of the software does not use the channels in IR8.7/IR8.6 BTs. The decision to not use the IR channel in the 8.7 µm region in release 2018 is due to the uncertainties in the performance over the desert pixels (caused by the lower IR8.7 emissivity on desert pixels) and the low improvement of the performance when IR8.7 is used on sea pixels. This decision was based in tests made using the techniques described in the validation report of version 2016 with SEVIRI, but could be reconsidered after future validation activities.

The GEO-iSHAI algorithm tries to infer a real temperature and humidity profile from the satellite observed brightness temperatures in a given set of IR channels. The algorithm is an optimal estimation using an inversion technique, i.e. tries to find an atmospheric profile which best reproduces the observations. In general, this is a multi-solution problem, and a "background profile" is used as a constraint. This background profile is often from short range forecast model, as it is fed to the iteration scheme as an initial proposal for a solution. The original background is then slowly modified in a controlled manner until its radiative properties fit the satellite observations.

However, it was found that a First-Guess regression is usually better than the forecast since the regressions combine forecast and real satellite brightness temperatures as predictors. Afterwards, the regression will be used as the first guess in GEO-iSHAI (see section 2.2.4).

The air mass parameters are then derived from the retrieved profile. From clear sky brightness temperatures within the M x M real satellite pixels window (FOR) or over pixel by pixel, the algorithm retrieves temperature and moisture profiles that are used to derive total precipitable water (TPW), layer precipitable water (LPW), stability indices (Lifted Index (LI), Showalter Index (SHW) and K-Index (KI)) and skin temperature (SKT).

Major limitations of the optimal estimation are the high computational effort and the fact that the retrieved profiles tend to retain features of the background NWP due to the low spectral resolution and the use of a few IR channels.

In order to assure that the IR brightness temperatures are not contaminated by clouds, dust or snow/sea ice, the cloud mask GEO-CMA product must be previously run. Thus, the GEO-iSHAI will be processed and calculated only over clear pixels determined by CMA.

2.2.1 Use of Field of Regards (FOR)

The GEO-iSHAI execution on FOR (window of M x M pixels) basis was recommended, instead of pixel by pixel basis, in Jun Li's 2008 VSA. This has been considered in order to speed up the processing

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and because the processing in FOR could reduce noise. A window of 3x3 pixels has been considered as adequate as the default width of the FOR. The width of the FOR (M x N pixels) is an adjustable parameter in the configuration file. This allows adjusting M or N parameters depending on the size of the region to process and the computer resources of the user.
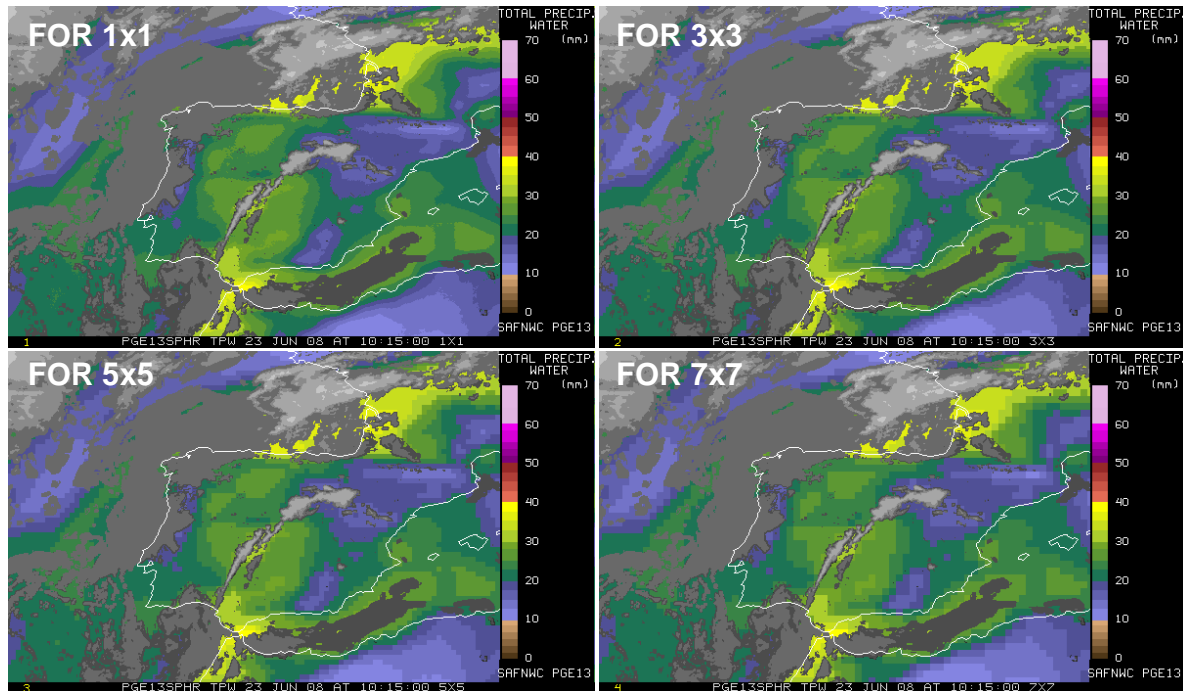
Figure 2: Examples of former PGE13 SPhR TPW at 10:15UTC on 23 June 2008 calculated with different size of FOR. FOR 1x1 (top left), FOR 3x3 (top right), FOR 5x5 (bottom left) FOR 7x7 (bottom right)

Figure 3 shows the differences on the spread between RTTOV simulated BT versus SEVIRI brightness temperature (BT) obtained with the mean of clear pixels and with the IR10.8 warmest clear pixel SEVIRI BT. ECMWF analysis 00 and 12 UTC have been used as input to RTTOV radiative transfer model (RTM). Due to the different behaviour, two methods for calculating the FOR BTs have been implemented and checked:

(1) Mean BTs of all clear pixels within the FOR.

(2) The BTs at warmest clear pixel in the cleanest channel in the IR window within the FOR.

The first option, "Mean BTs of all clear pixels within the FOR", is the default one. It has been selected because it is the most usual choice and because in this option the assigned geographical and ancillary data are the ones of FOR's centre.

Figure 4 shows an example of a comparison of the outputs generated with the two methods for calculating the FOR. As it can be seen in the figure, the largest differences are found in cloudy FOR. The method selected by default is the mean BTs of all clear pixels within the FOR.

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Figure 3: Scatter plots of IR13.4 SEVIRI BT versus ECMWF+RTTOV synthetic BT. On the left, mean of SEVIRI BT clear pixels in 0.5º x 0.5º box. On the right, SEVIRI BT at IR10.8 warmest clear pixel in 0.5º x 0.5º box for MSG-N region.

Figure 4: Top:K-Index processed with options FOR 5x5 and BTs from IR10.8 warmest clear pixel Bottom: K-Index processed with options FOR 5x5 and BTs mean of BTs clear pixel.

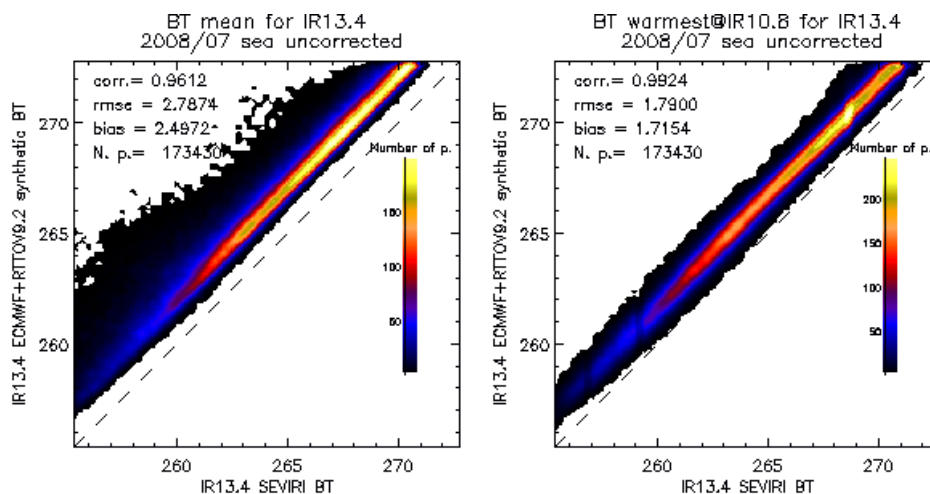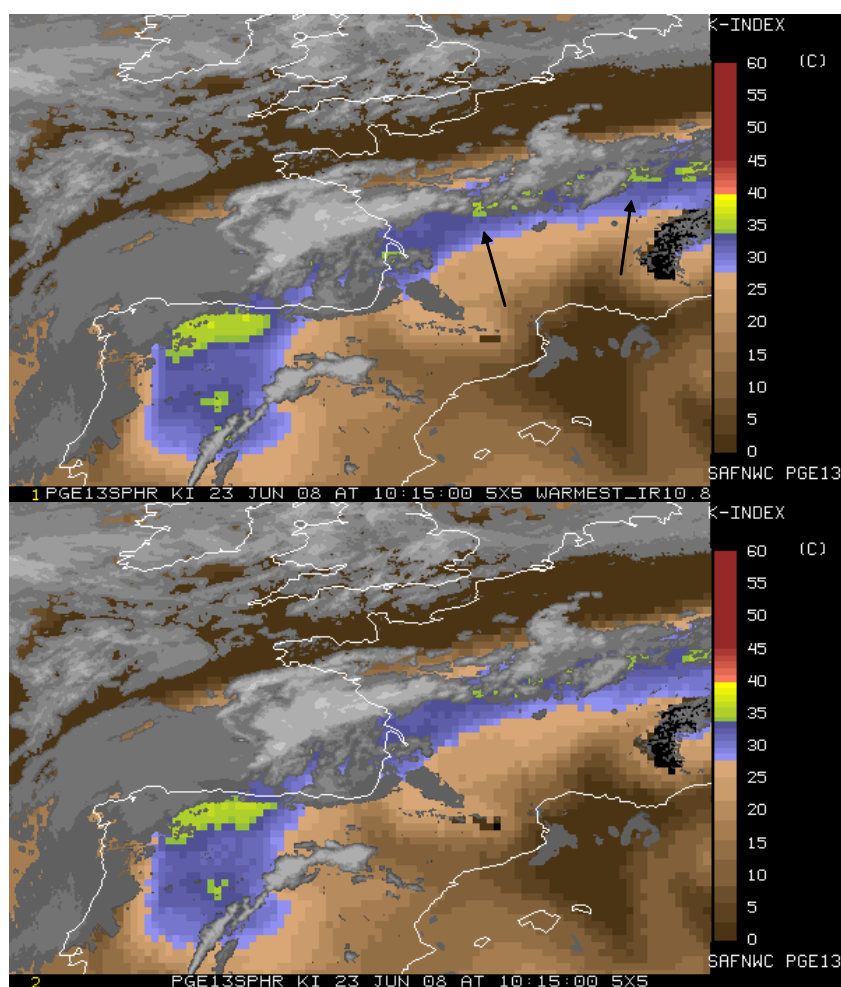|		**Code:** NWC/CDOP2/GEO/AEMET/SCI/ATBD/iSHAI
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2.2.2 Background NWP data Interpolation to RTTOV pressure levels of NWP profiles.

As explained before, it is convenient to use as background profile a NWP forecast in the [*t+00, t+24*] hours range. The NWC/GEO library provides software which should be able to work with any NWP model and it should accept the set of fixed pressure levels available on the NWP files provided by the users to the NWC/GEO package. The same fixed pressure levels NWP GRIB files that are actually used with NWC/GEO release 2018 to generate other products can be used. Hence, any user that is running NWC/GEO 2018 package should be able to run GEO-iSHAI.

In the case of GEO-iSHAI release 2018, ECMWF GRIB files on hybrid levels could be also used as inputs. As an improvement, for future use with any NWP model, it is also possible to use GRIB files on hybrid levels on a regular representation (equidistant lon-lat) as input. It is done by configuring in the GEO-iSHAI configuration file the codes of section 1 of GRIB header to identify T, q, O_3, SKT and P_{sfc} fields (see details in User Manual [RD.2]). But, always GRIB files on fixed pressure levels are also needed in order to execute CMA before execution of GEO-iSHAI code.

Since it is not adequate to provide specific error matrices, EOFs, regression coefficients, etc for the great number of combinations in user pressure levels, the interpolation of different NWP model levels to RTTOV pressure levels is performed.

The selection of P mode or HYB mode is a GEO-iSHAI configurable parameter; see the User Manual [RD.2] for details.

In the case of executing GEO-iSHAI in P mode: the spatial and temporal interpolation, at one level, is made outside the GEO-iSHAI code with the tools existing in the NWCLIB of NWC/GEO package. In real time, the NWC SAF's Task Manager makes the spatial interpolation upon the arrival of new NWP GRIB file as a predefined task. Temporal interpolation is made at user supplied NWP pressure levels between previous and following available NWP data close to the time of the image. It is made using functions of the NWCLIB library.

Vertical interpolations are made inside GEO-iSHAI. For vertical interpolation, an "ad hoc" function has been added to GEO-iSHAI. The solution adopted has been the development of a function that interpolates the temperature and humidity profiles from any set of pressure levels to the RTTOV pressure levels calling the RTTOV function "*rttov_intavg_prof*". This RTTOV function interpolates linearly, in the logarithm of the pressure, the background NWP forecast temperature and humidity fields available on user-defined vertical pressure levels to the RTTOV pressure levels.

This RTTOV function copies the value of the lowest user pressure level profile to all RTTOV pressure levels with value greater than the lowest user pressure level. Since the lowest RTTOV pressure levels have values greater than normal lowest fixed pressure levels, it has been implemented in GEO-iSHAI one extrapolation process based in the one made by ECMWF and described in section 1.3 of IFS DOCUMENTATION – Cy40r1 Operational implementation 22 November 2013. First, the extrapolation of T profile using the process described is made, and then the extrapolation of the q profile maintaining the relative humidity value at the lowest fixed pressure level is made.

As the fixed pressure levels GRIB files contain relative humidity profiles and not specific humidity, the conversion from relative humidity to specific humidity is done within *AllMappingNWP* tool using code of the NWCLIB of NWC/GEO package.

In the case of executing GEO-iSHAI in HYB mode: the whole NWP management is made inside the GEO-iSHAI code. GEO-iSHAI opens directly the previous and next ECMWF GRIB files on hybrid levels, compared to the time of the satellite image, from *$SAFNWC/import/NWP_data*; makes the vertical interpolation from ECMWF levels to the RTTOV pressure levels; makes the temporal interpolation to the date of the image and finally makes the spatial interpolation just at clear air processed FOR.

Another difference is that the specific humidity profile is read from the ECMWF GRIB files on hybrid levels and the conversion from relative humidity to specific humidity is not needed.

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Since the lowest RTTOV pressure levels have values greater than the lowest hybrid level at P_{sfc} (especially on mountains pixels) it has been implemented, in GEO-iSHAI, one extrapolation process based in the one made by ECMWF. The extrapolation process is the same as that explained above, but starting at P_{sfc} instead of at the lowest user fixed pressure level.

As a result of this process, time and spatial collocated, with the real satellite image, background NWP (T, q) profiles interpolated at the RTOV pressure levels are obtained from the background NWP GRIB files with (T, q) profiles.

If the TOZ calculation is activated, also the ozone profile is interpolated to the RTTOV pressure levels.

This processing allows NWC/GEO users to run GEO-iSHAI without modifying their background NWP GRIB files supply in P mode. But, as it can be concluded from the Validation Report [RD.1], it is strongly recommended to the user to provide as many fixed pressure levels as possible with the most uniform and widest vertical distribution from the selected NWP models to feed the NWC/GEO package. If possible, it is recommended the use of GRIB files on hybrid levels as input to the GEO-iSHAI.

2.2.3   Real satellite BT bias correction

Brightness temperature bias adjustment is very important for product quality. The original satellite measurements must be bias BT adjusted to account for the bias between the satellite observation and the synthetic radiative transfer model BTs. Since synthetic RTTOV BTs have been used to train the algorithm, differences between synthetic and measured clear-sky BTs must be mitigated with a real satellite BT bias correction. The biases are caused by both measurement problems and errors in the radiative transfer model. The bias BT correction is based on finding the differences between the observed real satellite BTs and those simulated from the radiative transfer model (here synthetic RTTOV BTs) with robust regression. Usually there are two ways for brightness temperature bias estimation:

    (1) using collocated NWP analysis and real brightness temperature measurements,
    (2) using quality controlled radiosonde observations (RAOBs) and collocated brightness temperature measurements.

To calculate the BT bias correction, the use of collocated RTTOV BTs calculated from NWP analysis and real satellite BTs has been chosen. An issue in brightness temperature bias calculation is the emissivity estimation. Due to the emissivity uncertainty, brightness temperature bias estimation on window channels might not be reliable especially on desert pixels. For this reason, the BT bias correction using only sea observations has been done. BT bias correction for water vapour and CO_2 absorption channels should help the retrievals.

The coefficients of the BT bias adjustment's robust regression are read in release 2018 from the common NWC/GEO dataset files using NWCLIB library.

2.2.4   Use regression as first guess

The GEO-iSHAI algorithm uses non-linear regressions as first guess (FG). The predictands are the temperature and the logarithm of specific humidity profiles at each one of the RTTOV pressure levels and the skin temperature. For each predictand is calculated a non-linear regression.

The regressions use real bias corrected satellite IR BTs and background NWP forecast as basic predictors. Since GEO imager instruments only has a few sounding IR channels, the temperature/moisture profiles from numerical weather prediction (NWP) forecast model are used as additional predictors. Here, the temperature and the logarithm of specific humidity profiles interpolated to the RTTOV pressure levels, the surface pressure, the skin temperature from a forecast, the latitude and the fraction of land in pixel are included as additional predictors.

The dependence of the atmospheric attenuation on the satellite zenith angle has been taken into account in practically all algorithms that have been implemented to obtain derived products from IR satellite data. Here, 76 regression coefficient sets are generated for each parameter using the predictors of Eq.1. Each coefficient set corresponds to a local zenith angle ranging from 0 to 75 degree. In GEO-iSHAI the regression coeeficients sets for T, q, ozone and SKT have been divided in separated files. There is a FG regression coefficients file that contains the 76 by the number of RTTOV pressure levels coefficients regressions for every zenith angle and every T at each one of the RTTOV pressure levels There is a similar set *76 x number_RTTOV_pressure_levels* of FG regression coefficients for log(q) profile. In the case of SKT there are 76 regressions for every zenith angle.

The regression equation has the following format for every one of the 76 fixed zenith angles:

$$z = \sum_{j=1}^{N} A_j \cdot BT_j + \sum_{j=1}^{N} B_j \cdot BT_j^2 / 250 + C \cdot P_{sfc} + D \cdot latitude + E \cdot rate_{land} + \sum_{l=1}^{NRTTOV} F_l \cdot T_l + \sum_{l=1}^{NRTTOV} G_l \cdot \log(q_l) + H \cdot T_{skin} + I_0 \qquad \text{Eq. } 1$$

Where:

    - Z is one of the following parameters: temperature or specific humidity at each one of the RTTOV pressure levels or Skin temperature

    - BT is the real bias corrected satellite brightness temperature;

    - T and **q** are background NWP forecast temperature and specific humidity profile at the RTTOV pressure levels respectively;

    - **Psfc** is the surface pressure;

    - T_{skin} is the Skin temperature from the ECMWF

    - **Rate**$_{land}$ is the fraction of land in pixel (0 : sea pixels and 1 : land pixels).

    - A, B, C, D, E, F, G, H and I$_o$ are regression coefficients;

    - N, is the total number of real satellite IR channels used as predictors.

In the case of ozone profile, the regressions include also as predictors the IR channel nearest to 9.7 μm and the log(ozone) profile.

$$z = \sum_{j=1}^{N+IR9.7} A_j \cdot BT_j + \sum_{j=1}^{N+IR9.7} B_j \cdot BT_j^2 / 250 + C \cdot P_{sfc} + D \cdot latitude + E \cdot rate_{land} + \sum_{l=1}^{NRTTOV} F_l \cdot T_l + \sum_{l=1}^{NRTTOV} G_l \cdot \log(q_l) + \sum_{l=1}^{NRTTOV} H_l \cdot \log(ozone_l) + I \cdot T_{skin} + J_0$$

$$\text{Eq. } 2$$

Based on several tests made and not shown here, the combination of FG regression plus physical retrieval has better results that use as FG directly the background NWP plus physical retrieval. Due to the fact that FG regression steps could be enough in a great proportion of pixels and this speeds up the process avoiding the time consuming task of jacobian and inversion matrix calculations, it has been decided to maintain in GEO-iSHAI the combination of FG non-linear regression step plus physical retrieval if the residual (in non-window channels) is greater than a configurable threshold.
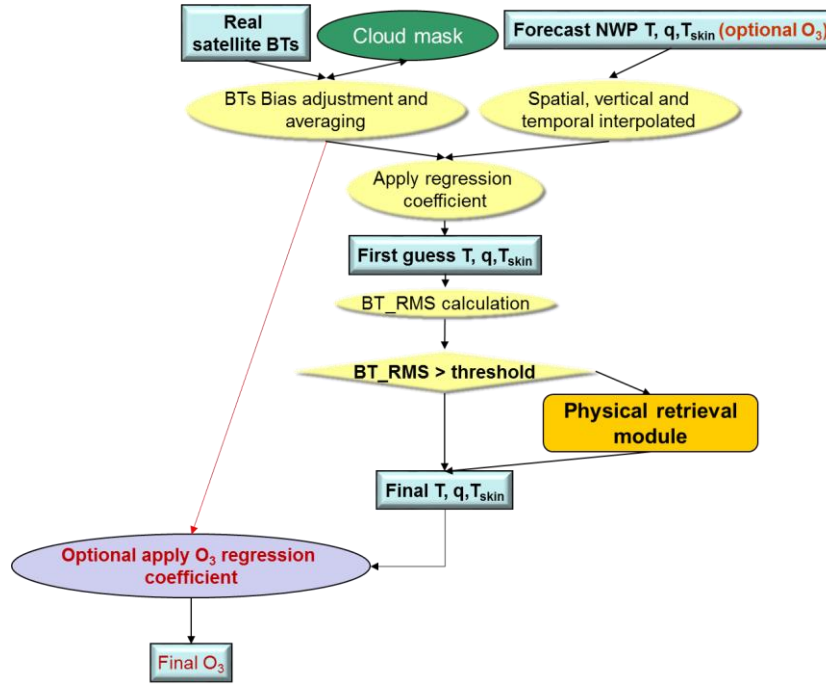
Figure 5: Regression Flowchart of the GEO-iSHAI retrieval process

2.2.5 Mathematical Description of Physical Retrieval module

In this section the Physical retrieval module is described. In the GEO-iSHAI algorithm, the physical retrieval module is executed only if the error between the real bias corrected satellite BTs and the RTTOV BTs calculated using the FG profiles is greater than a configurable threshold on the non-window channels (i.e. in SEVIRI case the WV6.2, WV7.3 and IR13.4 channels).

The GEO-iSHAI approach uses an optimal method of combining observations with a background (in GEO-iSHAI from the FG regression) which accounts for the assumed error characteristics of both. The variational retrieval is performed by adjusting the atmospheric profile state, X, from the First Guess, X^{FG}, to minimize a cost function (Rodger 1976; Li and Huang 1999; Li et al. 2008). The regularization parameter (also called smoothing factor) is introduced for convergence and solution stability. The cost function is defined by

$$J(X) = \left[Y^m - F(X)\right]^T E^{-1}\left[Y^m - F(X)\right] + \left[X - X^{FG}\right]^T \gamma B^{-1}\left[X - X^{FG}\right] \quad \text{Eq. 3}$$

where γ is the regularization parameter; **B** and **E** are the error covariance matrices of background, $\mathbf{X}^{FG}$, and the observation (brightness temperatures) vector, $\mathbf{Y}^m$, respectively; $\mathbf{F(X)}$ is the forward radiative transfer model operator and superscripts ^{T} and $^{-1}$ are the matrix transpose and inverse, respectively.

By using the Newtonian iteration

$$X_{n+1} = X_n + J''(X_n)^{-1} \cdot J'(X_n) \qquad \text{Eq. 4}$$

The following Quasi-Nonlinear iterative form is obtained

$$\delta X_{n+1} = \left(F_n'^T \cdot E^{-1} \cdot F_n' + \gamma B^{-1}\right)^{-1} \cdot F_n'^T \cdot E^{-1} \cdot \left(\delta Y_n + F_n' \cdot \delta X_n\right) \qquad \text{Eq. 5}$$

Where:

> **X** is the vector of temperature and humidity profile to be solved; **n** is the iteration step, **n**=0 denotes first guess or background profile,

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$$\delta X_n = X_n - X^{FG};$$
$$\delta Y^m = Y^m - F(X_n)$$

F' is the tangent linear operative (Jacobian) of forward model **F**. The RTTOV is used for forward model (**F**) and Jacobian (**F'**) calculations.

The regularization parameter γ is adjusted in each iteration according to the discrepancy principal (Li and Huang 1999; Li et al. 2000). The reason to introduce the regularization parameter is to balance the contributions from background and satellite observations in the solution, which is important when the background (e.g., forecast) error is not Gaussian or it is only locally Gaussian distributed.

Since there are correlations among atmospheric variables, only a limited number of variables are needed to explain the vertical structure variation of an atmospheric profile (Smith, 1976). The number of independent structure functions can be obtained from a set of global atmospheric profile samples.

Assume

$$X - X^{FG} = \Phi A, \qquad\qquad Eq.\ 6$$

Where $A = (\alpha_1, \alpha_2, ..., \alpha_M)$, and

$$\Phi = \begin{bmatrix} \Phi_T & 0 & 0 \\ 0 & \Phi_q & 0 \\ 0 & 0 & \Phi_{Ts} \end{bmatrix}$$

Φ_T is the matrix of the first $\tilde{N}_T$ empirical orthogonal functions (EOFs) of the temperature profile; Φ_q is the matrix of the first $\tilde{N}_q$ EOFs of the logarithm of specific humidity profiles, $\Phi_{Ts} = 1$, and $M = \tilde{N}_T + \tilde{N}_q + 1$. In GEO-iSHAI version 2018: 3 temperatures EOFs, 3 specific humidity EOFs and 1 skin temperature EOF are used.

It is obvious that $\Phi^T \Phi = I$. Defining $\tilde{F}' = F' \cdot \Phi$, Eq. (5) becomes

$$A_{n+1} = (\tilde{F}_n'^T \cdot E^{-1} \cdot \tilde{F}_n' + \gamma B^{-1})^{-1} \cdot \tilde{F}_n'^T \cdot E^{-1} \cdot (\delta Y_n + \tilde{F}_n' \cdot A_n) \qquad Eq.\ 7$$

where $A_0 = 0$, and

$$\left\| F(X_n) - Y^m \right\|^2 = \sigma^2, \qquad\qquad Eq.\ 8$$

where σ is the observation error of real satellite BTs, define $\left\| X \right\|^2 = \dfrac{1}{N} \sum_{i=1}^{N} x_i^2$, $X = (x_1, x_2, ..., x_N)$

Eq.(6) and Eq.(7) are applied to derive the solution from real satellite brightness temperatures.

In the GEO-iSHAI retrieval, the water vapour is expressed as the logarithm of the specific humidity due to the fact that the latter is more linear to the infrared brightness temperatures than the specific humidity itself. The matrix dimensions in Eq. (5) are (2* *number_RTTOV_pressure_levels* +1)²; but matrix dimensions in Eq. (7) are *number_of_EOF* x *number_of_EOF* (by default 7 = 3 EOF for T +3 EOF for log(q) + 1 EOF for Skin temperature). This allows speeding up the process and reducing the CPU time.

In the User Manual [RD.2] it is described how the user can configure several parameters of the GEO-iSHAI related to the physical module. More specifically the key parameters in the physical retrieval are controlled through the following keywords of the model configuration file:

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- The threshold used to decide if the physical retrieval is executed it is fixed in the keyword BT_RMS_THRESHOLD (maximum allowed difference between real bias corrected satellite BTs and RTTOV BTs calculated from the first guess in the non-window channels).

- In the "check iteration" step the maximum number of iterations is fixed with the keyword MAX_ITERATIONS.

- In the "check iteration" step the allowed residual threshold is fixed with the keyword MAX_RESIDUAL.

2.2.5.1 Observed brightness temperatures (Y^m)

The bias-adjusted observed brightness temperatures vector $\mathbf{Y^m}$ represents the satellite measured brightness temperatures in $\mathbf{N}$ channels.

- In the case of SEVIRI on board MSG satellites, the 6.2 µm, 7.3 µm, 10.8 µm, 12 µm, and 13.4 µm channels are used.
- In the case of AHI on board Himawari satellites, the 6.25 µm, 6.95 µm, 7.35 µm, 10.45 µm, 11.20 µm, 12.35 µm and 13.30 µm channels are used.
- In the case of ABI, the 6.19 µm, 6.93 µm, 7.34 µm, 10.33 µm, 11.21 µm, 12.29 µm and 13.28 µm channels are used.

2.2.5.2 RTTOV as radiative transfer model

RTTOV version 11.2 has been used in the GEO-iSHAI v4.0 algorithm implementation. Calculations are based on the atmospheric profile, surface skin temperature and surface emissivity in clear skies. RTTOV is maintained and supplied by the NWP SAF.

2.2.5.2.1 Synthetic brightness temperature (Y_n)

The synthetic brightness temperatures $\mathbf{Y_n = F(X_n)}$ are computed from the atmospheric profile vector for iteration step $\mathbf{n}$ with the radiative transfer model.

$\mathbf{Y_n}$ must be computed as a vector for all $\mathbf{N}$ IR channels.

RTTOV model is used for the radiative transfer calculations. The profile parameters are represented at L levels; it has been used L = *number_RTTOV_levels* because it is the number of RTTOV pressure levels. The radiation model needs the profile parameters at L prescribed pressure levels so that the first guess profile must be appropriately interpolated to these levels. Each profile is interpolated in space, time and vertically to fit the time and location of the real satellite observation.

As a surface value, the First Guess skin temperature is used in the retrieval. Thus, the observation vector has a length of 2*L + 1; i.e. L temperature values, L logarithm of specific humidity values and the surface skin temperature.

2.2.5.2.2 Weighting function (Jacobian) matrix (F')

The weighting function or Jacobian matrix $F_n^{'}$ (the subscript n denotes the nth iteration in the physical retrieval procedure) really describes the change of the brightness temperature at the top of the atmosphere (TOA) with a changed atmospheric parameter:

$$F_n^{'} = \frac{\delta Y_n(i)}{\delta X_n(j)} \qquad\qquad Eq.\ 9$$

Where *i* is the channel index in the brightness temperature vector ($\mathbf{Y}$) and *j* is the parameter index in the profile vector ($\mathbf{X}$).

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If there are a total of **N** channels used for physical retrieval, the matrix has thus **N** columns and 2*L+1 rows (L for temperature, L for humidity and 1 for the skin temperature).

Such two-dimensional partial derivatives are also referred to as Jacobians. It is indeed the computation of these Jacobians what is a substantial factor in the computational load of the retrieval equation. Since Jacobian from RTTOV is based on specific humidity directly, the Jacobian should be multiplied by specific humidity in order to obtain the Jacobian for natural logarithm of specific humidity.

The software takes into account two different types of surfaces: land and sea. Over land pixels, emissivity values are read from precomputed monthly emissivity atlases for each channel of the NWC/GEO satellites (see 2.3.3.7). Over sea pixels, the emissivity values used are the default of RTTOV for sea surface and this option is selected by fixing a value of 0.0 in the call to RTTOV.

2.2.5.3 Discrepancy principle for regularization parameter

The reasons to introduce the regularization parameter γ (also called smoothing factor) are:

(1) to speed up the convergence, and
(2) to stabilize the solution in case the background error is not Gaussian distribution, or only locally Gaussian distribution.

The factor γ is used to weight the contribution of background and satellite observations for the solution.

If γ is too large, more weight is given to background and the solution tends to be background or only a moderate modification of background.

However, if γ is too small, more weight is given to satellite observations. Since the inverse problem is ill-posed and there are only a few channels (equations), the solution could be unstable.

Objective selection of γ is important to obtain an accurate and stable solution. The discrepancy principal is used to select this regularization parameter (Li and Huang 1999) which is reflected by Eq. (8), where

$$\sigma^2 = \sum_{k=1}^{N} e_k^2 \qquad\qquad Eq.\ 10$$

e_k is the square root of the diagonal of **E** or the observation error of channel k

Usually σ^2 can be estimated from the instrument noise and estimated radiative transfer model error but in version 2018 it has been calculated from the root mean square between real satellite BTs after bias correction and synthetic RTTOV BT on sea pixels.

For simplicity, a numerical approach (Li et al. 2000) is adopted for solving Eq. (8); γ is changed in each iteration according to

$$\gamma_{n+1} = q_n \gamma_n, \qquad\qquad Eq.\ 11$$

where q is a factor for γ to increase or decrease.

q is obtained in each iteration by satisfying the following conditions:

$q_0 = 1.0$

If $\left\| F(X_n) - Y^m \right\|^2 \le \sigma^2$, then $q_n = 1.1$;

If $\left\| F(X_n) - Y^m \right\|^2 > \sigma^2$, then $q_n = 0.9$;

The q factor was found from empirical experiments to ensure that the solution is stable between iterations. Thus, γ continues to change until the iteration stops.

2.2.5.4 Iteration checking and residual estimation

In the retrieval processing, several checks are made for retrieval quality control. The quantity $Rs_n = \left\| F(X_n) - Y^m \right\|^2$ is computed to check the convergence or divergence,

If $\text{MAX\_RESIDUAL} < Rs_{n+1} < Rs_n$, iteration is convergent, continue to next iteration.

If $Rs_{n+1} < \text{MAX\_RESIDUAL}$ or $\left| Rs_{n+1} - Rs_n \right| < 0.025$ stop iteration.

If $Rs_{n+1} > Rs_n$, iteration is divergent, stop iteration, use first guess as final retrieval.

The degree of convergence of each iteration depends on the accuracy of the previous atmospheric and surface state.

The maximum number of iterations and $MAX\_RESIDUAL$ parameters are configurable by the user just by changing the values in the GEO-iSHAI configuration file. (Keywords: `MAX_ITERATIONS` and `MAX_RESIDUAL`).

2.2.6 Other considerations

For computation efficiency, the following transform can be performed for Eq. (7):

$$\overline{F}_n^{'} = E^{-\frac{1}{2}} \cdot \tilde{F}_n^{'}$$

$$\delta \overline{Y}_n = E^{-\frac{1}{2}} \cdot \delta Y_n \qquad\qquad Eq.\ 12$$

Then Eq. (7) becomes

$$A_{n+1} = \left(\overline{F}_n^{'T} \cdot \overline{F}_n^{'} + \gamma B^{-1} \right)^{-1} \cdot \overline{F}_n^{'T} \cdot \left(\delta \overline{Y}_n + \overline{F}_n^{'} \cdot A_n \right) \qquad\qquad Eq.\ 13$$

Using Eq. (13) instead of Eq. (7) will avoid some matrix multiplication and reduce computation time. The software has been codified using Eq. (13).

2.2.7 Quality control

To check the product quality, several flags have been added to the product outputs:

- Clear air flag: Derived from the cloud mask product (CMA). This first flag allows differentiating between cloud free and cloudy pixels

- Quality flags

  - Flag to indicate if the FOR has been processed with Physical retrieval or only first guess retrieval was performed.

  - Flag to indicate the FOR where convergence have failed.

  - Residual of the profile.

  - Number of iterations done (maximum number of iteration is three).

  - BT_residual: root mean square of differences between the real bias corrected satellite and calculated brightness temperature.

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2.2.8 Post-processing

2.2.8.1 Fill clear pixels of FOR with the calculated value

The main post-processing task is to fill with a value all clear air pixels inside the FOR. The selection of the post-processing method is made in the GEO-iSHAI configuration file. Copying to all clear pixels the same value calculated at the FOR is the default method (POST_PROC_METHOD 1).

The other option (POST_PROC_METHOD 0) is not to fill clear pixels and it can be used to display the pixels where physical retrieval has been calculated inside the FOR. It can be useful in cloudy regions to display where the physical retrieval has been really calculated when real satellite BTs at the warmest clear pixel in the cleanest IR window channel has been selected.
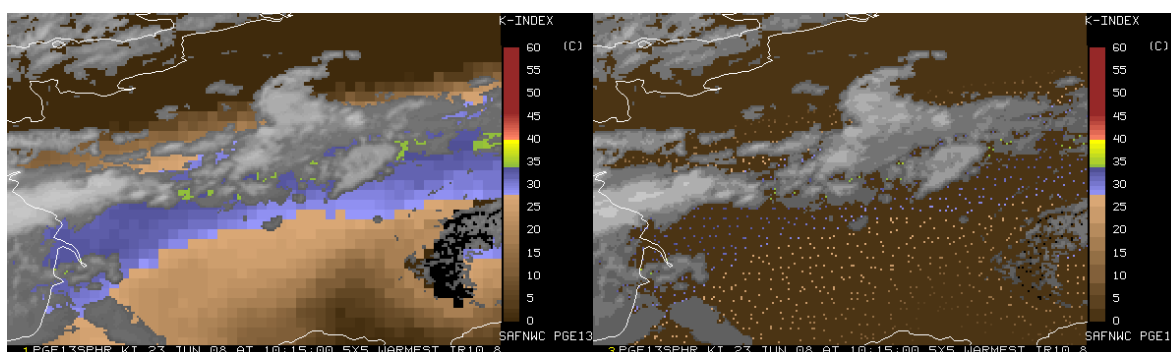
Figure 6: Zoom of K-Index processed with BT at warmest pixel in the IR10.8. The default post-processing "filling FOR" option (left) and the "not filling FOR" option (right).

2.2.8.2 Writing of outputs on netCDF file

In the NWC/GEO release 2018, the GEO-iSHAI parameter outputs at each clear air FOR are written in the netCDF as 16-bit integer after scaling and offsetting from their original float values.

The units of precipitable water (TPW and LPW) parameters are kg/m^2 while the units of stability indices are Kelvin (mm and degrees Celsius are more familiar in operational meteorology). The same units are used for fields with differences between parameter calculated with the physical retrieval and with the background NWP profiles.

For cloudy pixels, determined by CMA, an IR channel is also stored as a byte field degraded to 7 bits (range [0 – 127]) values for the IR channel selected in the configuration file. This IR channel is only different to missing value at cloudy pixels. It can be used to generate operational images in which cloudy pixels appear as grey scaled pixels and clear pixels appear as colour scaled pixels (see section 2.4.3 for example) or CIMSS images. In GEO-iSHAI this process must be made by the user.

The quality flags are written using bits fields.

2.3 ALGORITHM INPUTS, COEFFICIENTS AND FILES

This section describes briefly the inputs and coefficients files needed to process the GEO-iSHAI and it provides a guide on how they have been obtained. These files are available in the NWC/GEO software package and they are needed by the GEO-iSHAI software. In the User Manual [RD.2] it is provided detailed information about size, name of files, format, etc.

The list of inputs, files and coefficients needed is the following:

- **Inputs**
    - i) Real satellite BTs.

ii) Cloud Mask.

iii) NWP GRIB files from range [*t+00, t+24*] hours forecasted.

- **Geographical data from NWCSAF functions**

    a. Longitude.

    b. Latitude.

    c. Zenith angle.

- **Coefficients**

    1. Bias BT corrections coefficients.

    2. FG regression coefficient files.

    3. Inverse of error covariance matrix of background and first guess (B^{-1}).

    4. Inverse of error covariance of observation matrix (E^{-1}).

    5. Empirical Orthogonal Functions coefficients.

    6. RTTOV coefficients for the GEO supported satellites are also needed.

- **Geographical static data files**

    1. Precomputed monthly emissivity atlases for each channel of the NWC/GEO satellites generated from the 2007 IREMIS dataset (U. Wisconsin) RTTOV-11.2 emissivity atlases remapped to the supported NWG/GEO full-disk projections.

    2. Topographic data.

- **Configuration File of GEO-iSHAI**

2.3.1 Inputs

2.3.1.1 Real satellite BTs

Several IR channels from the NWC/GEO supported satellites are the main input to GEO-iSHAI.

In the case of SEVIRI on board MSG, the following IR channels are needed at full IR spatial resolution:

BT6.2μm	BT7.3μm	BT9.7μm	BT10.8μm	BT12.0 μm	BT13.4 μm
Mandatory	Mandatory	Mandatory	Mandatory	Mandatory	Mandatory

Table 3: List of SEVIRI IR channels used in GEO-iSHAI version 2018.

In the case of AHI on board Himawari, the following IR channels are needed at full IR spatial resolution:

BT6.25μm	BT6.95μm	BT7.35μm	BT9.6μm	BT10.45μm	BT11.20μm	BT12.35μm	BT13.30μm
Mandatory	Mandatory	Mandatory	Mandatory	Mandatory	Mandatory	Mandatory	Mandatory

Table 4: List of AHI IR channels used in GEO-iSHAI version 2018.

In the case of ABI on board GOES-R class satellites, the following IR channels are needed at full IR spatial resolution:

BT6.20μm	BT6.93μm	BT7.34μm	BT9.6μm	BT10.33μm	BT11.21μm	BT12.29μm	BT13.20μm
Mandatory	Mandatory	Mandatory	Mandatory	Mandatory	Mandatory	Mandatory	Mandatory

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Table 5: List of AHI IR channels used in GEO-iSHAI version 2018.

In this version, the BT of 9.7µm region is only used in to estimate the ozone profile using non-linear regressions if user activates the TOZ calculation. The rest of channels are used as predictors for temperature, humidity and skin temperature retrieval.

Considering the emissivity issues and the small added value, the channels in 8.7 µm region are not used in this version of GEO-iSHAI algorithm.

Considering the diurnal changes in the BTs, the channel in the 3.9 µm region are not used in this version of the GEO-iSHAI algorithm.

2.3.1.2 Cloud Mask (GEO-CMA)

GEO-iSHAI is only generated in clear sky pixels and one Cloud Mask is a mandatory input to GEO-iSHAI. The Cloud Mask product for the region and slot must exists and for this reason GEO-CMA must be executed before GEO-iSHAI. NWC/GEO Task Manager synchronises the execution of the products and the first product that is generated upon the arrival of a new image is the cloud mask GEO-CMA.

2.3.1.3 Background NWP data

Background numerical weather profiles forecast from range [*t+00*, *t+24*] hours are needed as mandatory input to GEO-iSHAI. These NWP data are later spatially, temporally and vertically interpolated to get background NWP data collocated with the real satellite data.

Note: the user could increase the t+24 limit.

To maintain continuity with the NWP GRIB files dataset managed by the NWCLIB software, version 4.0 of GEO-iSHAI can be executed in the default P mode. Users can use their own model and choice for the NWP supply. In real time operational mode, once the NWP GRIB files are received, the NWC/GEO software package has predefined tools (coordinated by the NWC SAF Task Manager daemon) which check every minute for new NWP data making automatically the spatial remapping to the predetermined regions to process. This avoids spending time in every call to one processor to make the remapping process. See [RD.2] for details.

As in GEO-iSHAI release 2016 and PGE13 SPhR version 2013, GEO-iSHAI release 2018 allows the use of ECMWF GRIB files in hybrid levels when executing in HYB mode. This has been proved with ECMWF model and ECMWF GRIB files on hybrid levels from *t+00* to *t+24* hours forecast could be also used as inputs.

As an attempt to get experience and the user's feedback, it is also possible to use as input other NWP models GRIB files on hybrid levels. In release 2018, the identification codes of section 1 of GRIB header for T, q, Ozone, SKT and P_{sfc} are now configurable parameters. That means that users could try to use their own NWP models with hybrid GRIB files as input to GEO-iSHAI in HYB mode. It is needed that their hybrid GRIB files must have regular longitude-latitude representation and a structure similar to the ECMWF hybrid GRIB files. The feedback of the users is expected in order to improve for future versions.

2.3.2 Geographical data from NWCSAF functions

Longitude, latitude and satellite zenith angles associated to selected region are provided by functions available on the NWCLIB library.

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2.3.3 Coefficients

2.3.3.1 BT bias correction coefficients

In GEO-iSHAI, BT bias correction coefficients are considered as common coefficients available for all the products and specific coefficient files and functions in the NWCLIB to access them are available.

GEO-iSHAI uses this common BT bias correction coefficients and functions to get the optimal BT bias corrections and then apply them to the real satellite BTs before being used in the First-Guess regression and/or Physical retrieval steps.

In a best effort basis the BT bias correction coefficients are being updated monthly for MSG and the ECMWF model in the NWCSAF web in this link *http://www.nwcsaf.org/web/guest/bias-bt-correction-coefficients*. Similar process is being established for AHI and ABI and they will be also published.

2.3.3.2 Regression coefficients to calculate First Guess profiles

In GEO-iSHAI algorithm, instead of using directly the background NWP data as First Guess it is used as First Guess a set of non-linear regressions with the real bias corrected satellite BTs and background NWP data (as main inputs). Since forecast profile is used together with real bias corrected satellite IR brightness temperatures as predictors, the regression should not be worse than the forecast. The regression derived profile is used as the first guess for physical retrieval iterations.

The FG nonlinear regression coefficients have been generated offline using a training dataset and they are read from binary files by GEO-iSHAI. To train the FG regressions several options are available. In the Jun Li's VSA, to generate the FG regression coefficient, a global radiosonde dataset with surface skin temperature and surface IR emissivities physically assigned (Seemann et al. 2003; 2007) was used.

For version 2018, the FG regression coefficients files have been calculated using the 2017 year of the GEO-iSHAI training and validation dataset as described in the Validation Report [RD.1]. Similar approach was made for the versions 2013 and 2016.

The structure of the FG regression coefficients files is described on [RD.2]. The FG regression coefficient files can be changed by the users editing the name of the regression coefficient files on the GEO-iSHAI configuration file.

In GEO-iSHAI release v2018 the same FG regression coefficient files can be used for P and HYB modes. This fact is due to the improved extrapolation below P_{sfc} in HYB mode.

2.3.3.3 The inverse background error covariance matrix and first guess (B^{-1})

Background error covariance matrix for temperature and humidity profiles and skin temperature has been calculated using the GEO-iSHAI training and validation dataset (for the 2017 year period) with the errors of collocated ECMWF model outputs for $t+12$ forecast and analysis. The assumption of no correlation existing between temperature and moisture in the error covariance matrix has been made. The water vapour is expressed as logarithm of specific humidity when calculating the background error covariance matrix.

The statistical error of the background is represented by the matrix B (see Table 6).

L pressure levels are used to represent temperature and moisture profiles. In our case, as RTTOV uses a set of *number_RTTOV_levels* predefined pressure levels, L is equal to the number of RTTOV pressure levels (in the case of RTTOV-11.2 the number is 54 levels).

This (2*L+1) by (2*L+1) element matrix represents the correlation of the background error between a parameter and the same parameter in another level. The pairs of errors for temperature, logarithm of

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specific humidity and skin temperature are assumed to be uncorrelated. The levels correspond to the RTTOV pressure levels.

Schematically, the matrix has thus the below form, where the value in the lower right corner is the error of the skin temperature to itself.
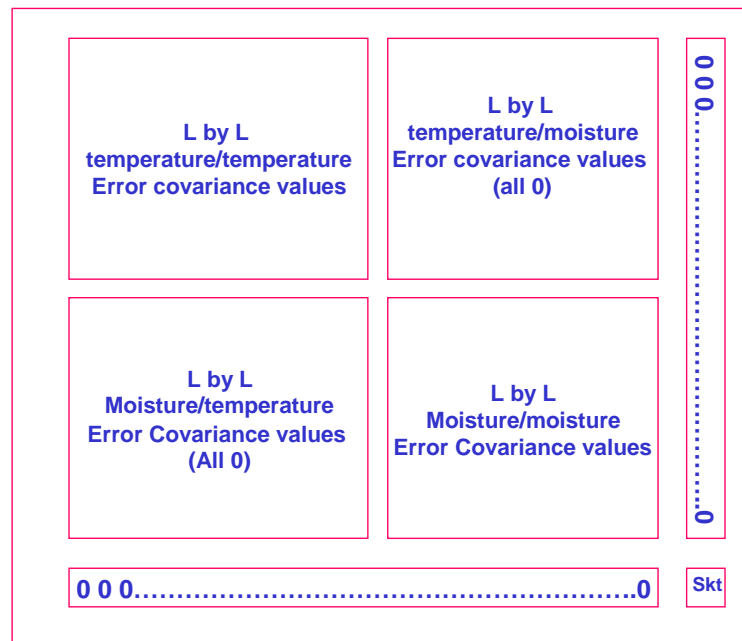

Table 6: The background error covariance matrix

For the calculation of B^{-1} all the profiles have been interpolated at the 54 RTTOV pressure levels from the original hybrid levels (137 hybrid levels). The filename with the B^{-1} matrix is written in the default GEO-iSHAI configuration file. The ECMWF model has been used because most of the users rely on this European model and/or many European limited area models use the ECMWF as a reference (contour conditions at initialization and validation process or cross validation with ECMWF).

2.3.3.4 The inverse of observation error covariance matrix (E^{-1})

The errors of the observed brightness temperatures and the errors of the radiative transfer model are represented altogether by the matrix **E**. There are several ways to estimate it.

In the first way, the elements describe the covariance of the brightness temperature error of the instrument and an assumed uncertainty of the radiative transfer model is added to that value. As the covariance of any two different channels is not known, this matrix has only diagonal elements.

The (assumed) error of the radiative transfer model could merely be added to these diagonal elements. In versions before 2013 it was calculated using the SEVIRI instrument noise and the forward model error for each SEVIRI IR channel.

In second way and in the case of SEVIRI, for the calculation of E in version 2018 (same in version 2013 and version 2016), the diagonal element was the square of observation error and it was calculated using real bias corrected satellite BTs and synthetic RTTOV BTs (profiles at the RTTOV pressure levels interpolated from the ECMWF hybrid levels) on sea pixels of the GEO-iSHAI training and validation dataset. In version 2018 it has been used the 2017 year period. The default observation error covariance matrix is a diagonal matrix.

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Since the generation of GEO-iSHAI training validation datasets to AHI and ABI instruments is being made the initial E^{-1} matrix in GEO-iSHAI version 2018 has been estimated but it will be improved and calculated using real satellite data. And they will be distributed later on the NWC SAF web.

In the coefficients file is written the square root of the inverse of E following Eq 12.

$$
E = \begin{pmatrix}
e_1^2 & 0 & 0 & .... & 0 \\
0 & e_2^2 & 0 & .... & 0 \\
0 & 0 & e_3^2 & .... & 0 \\
.... & .... & .... & .... & .... \\
0 & 0 & 0 & 0 & e_N^2
\end{pmatrix}
$$

2.3.3.5 Empirical orthogonal Functions (EOF) representation for temperature and moisture profiles

Since there are correlations among atmospheric variables, only a limited number of variables are needed to explain the vertical structure variations of an atmospheric profile (Smith, 1976). The recommend number of independent structure functions (EOFs) was obtained from a set of global atmospheric profile samples in Jun Li's 2007 VSA.

See Eq. (6) for the EOF representation of a profile. Using EOF representation is convenient because of the limited number of infrared channels used. The advantages of using EOF representation for a profile are:

    (1) to reduce the number of unknowns in the solution, which makes the solution more stable
    (2) to significantly reduce the time of computation in retrieval process; study shows that using EOF representation will not degrade the retrieval accuracy in profile retrieval with real satellite BTs

In the physical retrieval process of GEO-iSHAI version 2018, 3 temperature profile EOFs, 3 logarithm of specific humidity profile EOFs and 1 SKT EOF for all NWC/GEO satellite is used.

Until PGE13 SPhR 2011, profiles from NOAA 88 global radiosonde training dataset were used for EOFs calculations. EOFs were supplied by Jun Li and they were generated based on NCEP model and a global radiosonde base.

Trials to generate new EOFs using PGE13 SPhR training and validation dataset from ECMWF profiles were successful. EOFs from ECMWF were included since the PGE13 SPhR 2013 version.

For GEO-iSHAI v2016 the process to manage the RTTOV pressure levels and to use 2013 year from hybrid ECMWF GRIB profiles in GEO-iSHAI validation dataset to calculate 2016 default EOFs was made. For GEO-iSHAI v2018 similar approach but with the 2017 year period of the GEO-iSHAI training and validation dataset has been used. The filename with the EOFs is written in the GEO-iSHAI configuration file and thus are one configurable parameter of iSHAI.

2.3.3.6 RTTOV coefficients

In addition, a clear sky fast and accurate radiative transfer model is needed in the retrieval process. In GEO-iSHAI the RTTOV radiative transfer model provided by NWP SAF is used (Eyre, 1991; Saunders and Matricardi, 2008). RTTOV-11.2 is used in version 2018.

2.3.3.7 Use of predetermined surface IR emissivity atlas

Emissivity determination for retrieval remains as a critical issue. Handling surface IR emissivity is very important since an emissivity error of 0.01 in long wave IR window region could result in

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approximately 0.5 K brightness temperature changes. The emissivity values from database or regression equation can be attempted.

Usually there are four ways to handle surface IR emissivity in physical retrieval:

(1) Use emissivity from database:
      a. Advantage: monthly global coverage.
      b. Disadvantage: at MODIS channels.
(2) Use regression based emissivity:
      a. Advantage: dynamic emissivity, at real satellite channels.
      b. Disadvantage: rely on emissivity in training data, might create false diurnal variation in real satellite emissivity retrievals.
(3) Use independent retrieved emissivity with time continuity, assume skin temperature is temporally variable and emissivity is not changed because emissivity is very slowly varying:
      a. Advantage: avoid false diurnal feature in emissivity retrievals.
      b. Disadvantage: algorithm has not been tested, still in concept stage.
(4) Use emissivity from LEO hyperspectral IR radiances:
      a. Advantage: emissivity can be updated routinely and can be at any channels.
      b. Disadvantage: the need to obtain by users external emissivity data regularly.

Regression for emissivity is simple but usually brings false diurnal change of emissivity, which result in additional error in water vapour retrieval.

There is also other option such as IR emissivity model. The emissivity model over ocean is quite reliable but is difficult and much less accurate over land.

A realistic way is to use emissivity values from a database. As example the emissivity database developed at CIMSS by combining Moderate-Resolution Imaging Spectroradiometer (MODIS) emissivity measurements and laboratory measured hyperspectral emissivity spectra. The database can be used for real satellite physical retrieval of profile using emissivity values spectrally, temporally and spatially interpolated to the each satellite IR channel. Some information about the emissivity database can be obtained from the following link: http://cimss.ssec.wisc.edu/iremis/

In GEO-iSHAI release 2018, the option to use emissivity atlases have been adopted and they are provided by the common NWCLIB datasets. After decision of NWC SAF Project Team to consider emissivity dataset as common software elements and the incorporation of management functions on the NWC/GEO NWCLIB, fixed IREMIS dataset has been selected from year 2007 using the RTTOV-11.2 emissivity atlases. Thus, in GEO-iSHAI version 2018 are used the precomputed monthly emissivity atlases for each channel of the NWC/GEO satellites generated from the 2007 IREMIS dataset (U. Wisconsin) RTTOV-11.2 emissivity atlases.

See in NWC/GEO documents for details about emissivity atlas files naming and format.

2.3.3.8 Ancillary data sets

The elevation mask atlas, remapped onto satellite images, is also a mandatory file. Atlas and sea/land mask datasets covering the whole GEO supported disk in the default satellite projection at full GEO supported horizontal resolution are available within the NWC/GEO software package.

In 2018 version, the elevation dataset is used to distinguish between land and sea pixels (sea pixels are those which elevation value equal to missing code). Then, in the case of land pixels the emissivity values are read from the emissivity datasets.

2.3.3.9 GEO-iSHAI Model Configuration File

GEO-iSHAI has been built as a modular and configurable by the user as possible software. GEO iSHAI model configuration file contains all the coefficients file names and some keywords required by GEO-

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iSHAI product. The model configuration file is an ASCII file and then it can be easily modified with any text editor. See the User Manual [RD.2] for details.

2.4 GEO-ɪSHAI OUTPUTS

Together with the main clear air parameters calculated directly from the retrieved profile, it was considered as adequate at 2007 Madrid Workshop to provide as other outputs the difference between the retrieved profiles and the background NWP model. Following this idea, the differences between the parameters obtained with the retrieved profile and the same parameters obtained with the background NWP model profile are included as additional outputs.

2.4.1 Main outputs: GEO-iSHAI netCDF files description.

In this version, the following **fields** are calculated for clear pixels:

- o **iSHAI_tpw**: Total precipitable water ($P_{Surface}$ - top) from the retrieved specific humidity profiles in kg/m^2.
- o LPW Precipitable water in three layers from the retrieved specific humidity profiles in kg/m^2:
    - o **iSHAI_bl**: layer $P_{Surface}$ to 850 hPa
    - o **iSHAI_ml**: layer 850 to 500 hPa
    - o **iSHAI_hl**: layer 500 to 0 hPa).
- o **iSHAI_li**: Lifted Index from the retrieved profiles of temperature and humidity in Kelvin.
- o **iSHAI_shw**: Showalter Index from the retrieved profiles of temperature and humidity in Kelvin.
- o **iSHAI_ki**: K-Index from the retrieved profiles of temperature and humidity in Kelvin.
- o **iSHAI_difftpw:** Difference between TPW from retrieved profile and TPW from background NWP profiles in kg/m^2.
- o **iSHAI_diffbl, iSHAI_diffml, iSHAI_diffhl**: Difference between LPWs from retrieved profile and LPWs from background NWP profiles in kg/m^2.
- o **iSHAI_diffli, iSHAI_diffki, iSHAI_diffshw**: Difference between stability indices from retrieved profile and stability indices from background NWP profiles.
- o **iSHAI_skt** and **iSHAI_diffskt**
- o **iSHAI_toz** and **iSHAI_difftoz**: if user activated calculation TOZ.
- o **iSHAI_residual:** root mean square of differences between the real bias corrected satellite and RTTOV calculated brightness temperatures.
- o Quality Flags: **iSHAI_quality, iSHAI_sflag** fields.
- o Configurable IR channel BT degraded to 7 bits only in cloudy pixels.

The format of the file is netCDF and it is described in [AD.6]. In release 2018, the outputs are not image like fields and are data fields. It is the responsibility of the user to use adequate tools to generate images.

It is important to highlight that, as GEO-iSHAI retrieves the complete profiles of temperature and humidity, it is possible in future versions to implement new stability indices after user requirements or to modify the limits and thickness of the atmospheric layers where precipitable water is computed.

2.4.2 Optional binary files outputs.

Since GEO-iSHAI is executed locally by the users, GEO-iSHAI can generate optional binary files with the whole temperature, humidity and ozone profiles outputs. They allow to debug their local installations or create new parameters or stability indices. There are two keywords in the GEO-iSHAI configuration file to activate the writing temperature, humidity and optionally ozone profiles on binary files at different steps of the algorithm (from the background NWP data supplied by the users to the final retrieved profiles used to calculate the main outputs).

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The users can activate the options to write the binary files editing the ASCII GEO-iSHAI model configuration file. The main advantage of these binary files is that all temperature, humidity and ozone profiles are spatially, temporally and vertically collocated with satellite data. See User Manual [RD.2] for details on how to manage the keywords. The format of the binary files is also described on [RD.2].

Debugging activities, vertical cross sections, 3D visualizations, and generation of validation dataset are only a few among other applications where they can be used. As an example, the GEO-iSHAI validation and training dataset described in Validation Report [RD.1] has been built using these binary files.

At the present time, the generation of tools for conversion from binary to netCDF format is in progress. These tools are being generated from the IDL prototypes at the best effort basis.

The structure of the netCDF format has been designed to be used directly in application as IDV, McIDAS-V, IDL, MATLAB, etc. for one easy management of the GEO-iSHAI binary files for generation of all kinds of visualizations. As one example of the possibilities you can see Figures 7 and 8 taken from Martinez 2013. More examples can be seen in Martinez&Calbet 2018, Martinez&Calbet 2016[a,b], Martinez 2015 and Martinez 2013.

In order to show examples of the important applications of the optional binary file for change in temperature and humidity monitoring see the loops and animations in the presentations Martinez&Calbet 2018 and in Martinez 2015 at 2015 NWC SAF workshop.
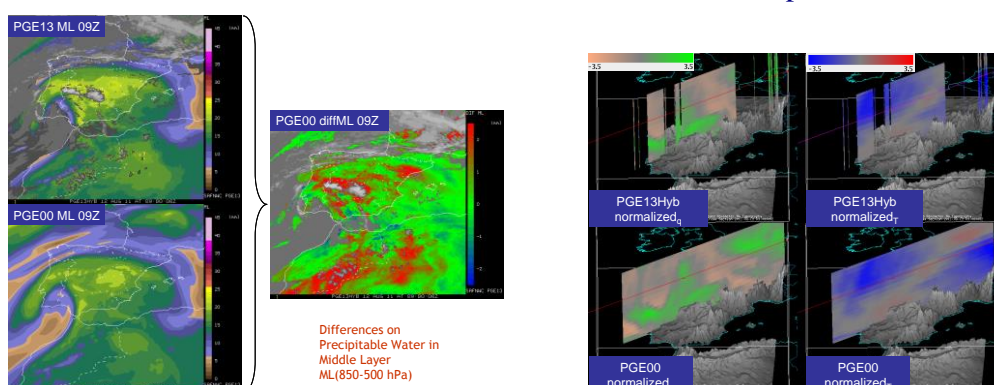

Figure 7: PGE13Hyb parameters diffML (precipitable water 850-500 hPa). Difference of precipitable water content between PGE13Hyb ML and ECMWF ML at 9 UTC on 12th August 2011. Vertical cross sections using McIDAS-V of normalized 3D arrays of T and q for 9 UTC on 12th August 2011 from PGE13Hyb and ECMWF (PGE00Hyb). To normalize them it has been subtracted the mean on every level for the t+12 ECMWF forecast in the region and divided by the standard deviation on the level for this slot.
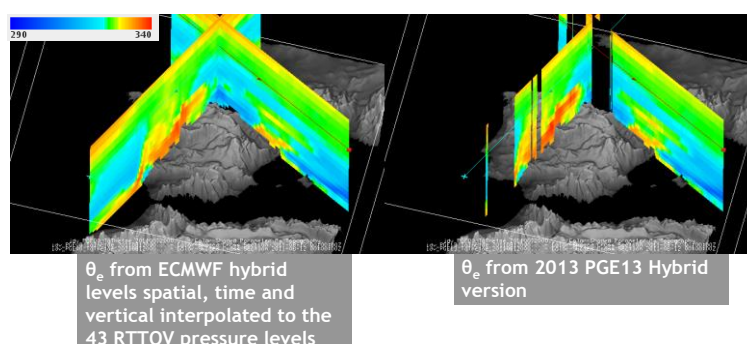

Figure 8: PGE13Hyb and ECMWF (PGE00Hyb) vertical cross sections of θ_e for 9 UTC on 12th August 2011.

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In [Martinez 2015](#)several examples on the use for nowcasting for case studies 12th August 2011 and 20th June 2013 were presented. Also the ideas for generalization to other GEO satellites and the extension to MTG-IRS applications in nowcasting are shown in this presentation.

2.4.3 Examples of GEO-iSHAI visualisation

Graphic displays of GEO-iSHAI product generated at the AEMET NWCSAF/MSG Reference System area will be available on real-time in the web of the NWC SAF Help Desk (http://nwc-saf.eumetsat.int).

For the display of the clear air outputs, a set of colour enhancement tables (similar to the ones used by CIMSS for the visualisation of the GOES derived TPW and LI product) has been selected. (See http://cimss.ssec.wisc.edu/goes/rt/sounder-dpi.php).

The best way to use GEO-iSHAI products is with adequate displays and using loops of images. In the NWC SAF web site it will be available near real time images and animations. Also images and animations from selected case studies will be provided. In the NWCSAF web, in the description of GEO-iSHAI version there is [web page](#) with a summary of the case study 10th August 2016 used in Martinez 2016a and other example of vertical cross sections. This is a sample of web pages for iSHAI version 2018 with full case studies analysis when the NWCSAF web server with the description of version 2018 will be updated.

The images corresponding to the 10th August 2016 at 12UTC from SEVIRI on MSG-3 are shown as an example in the Figures below.
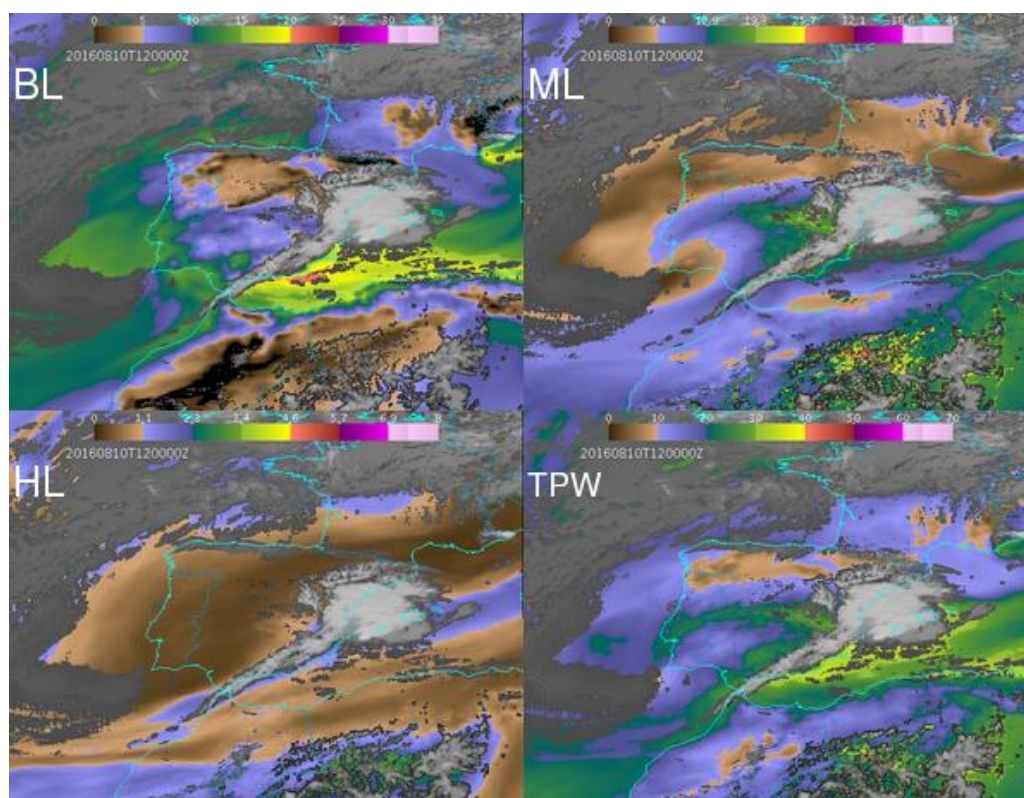

Figure 9: Example of GEO-iSHAI BL, ML, HL and TPW from 12 UTC on 10 August 2016 produced from SEVIRI on MSG-3.
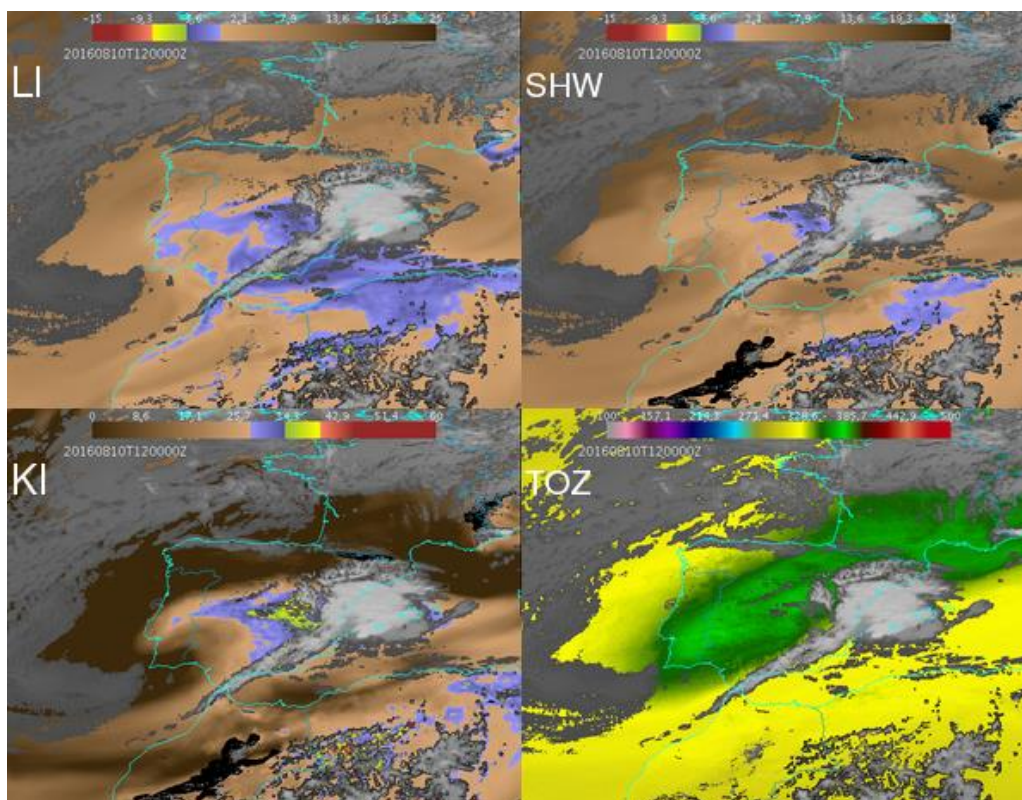
Figure 10: Example GEO-iSHAI LI, SHW, KI and TOZ from 12Z 10 August 2016 produced from MSG-3.
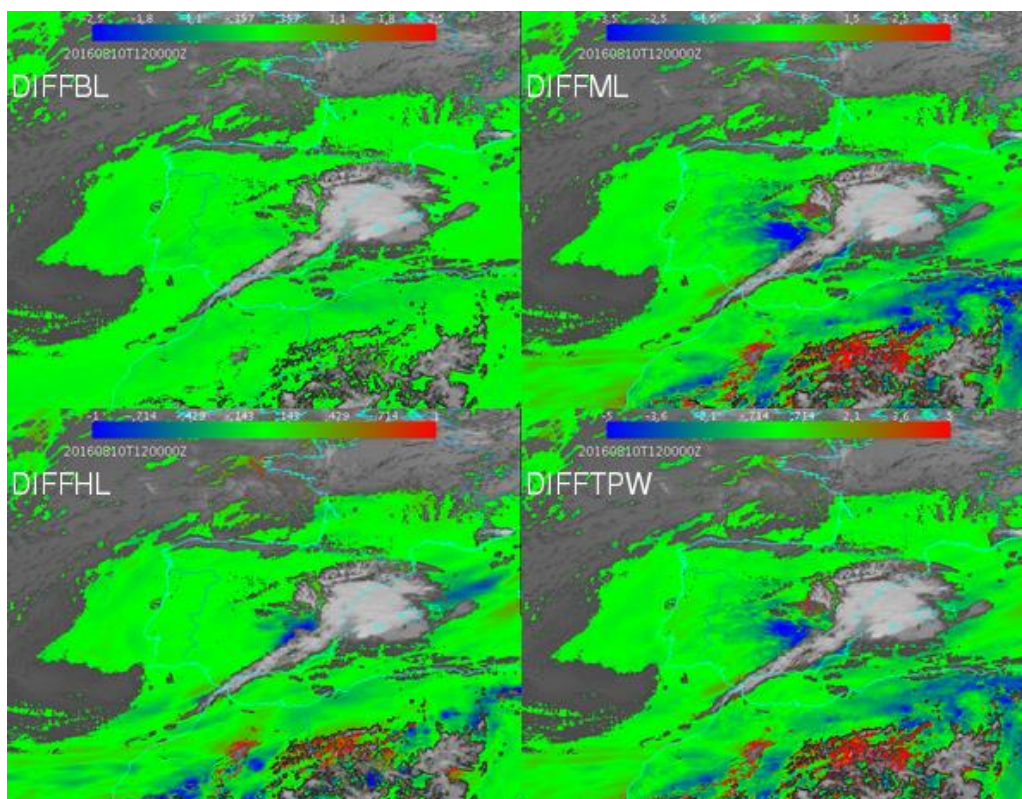

Figure 11: Example GEO-iSHAI diffBL, diffML, diffHL and diffTPW from 12z on 10 August 2016 produced from MSG-3.

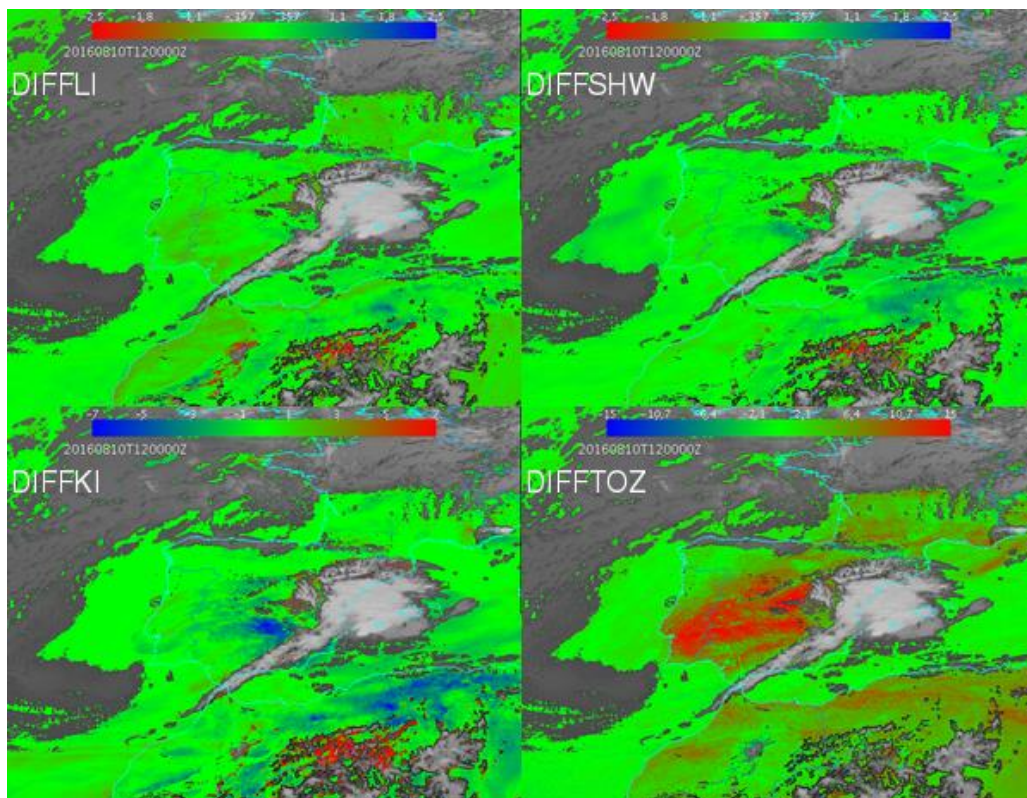|		Code:	NWC/CDOP2/GEO/AEMET/SCI/ATBD/iSHAI
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Figure 12: Example of GEO-iSHAI diffLI, diffSHW,diffKI and diffTOZ from 12 UTC on 10 August 2016 produced from MSG-3.
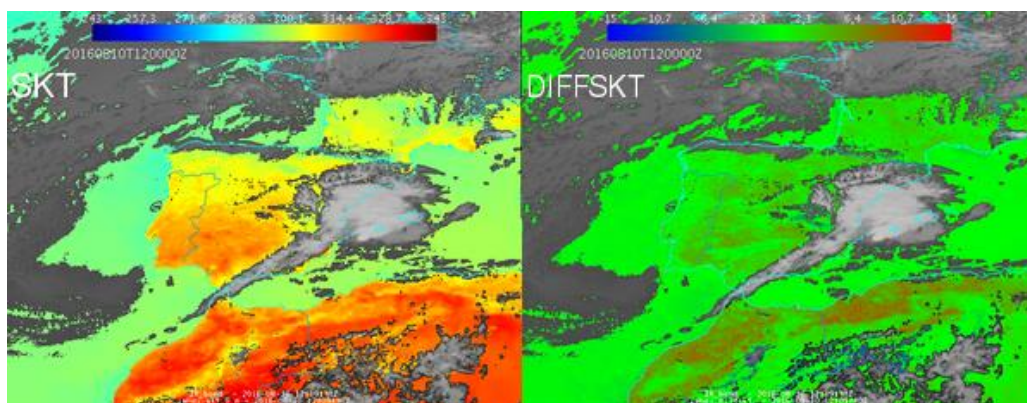

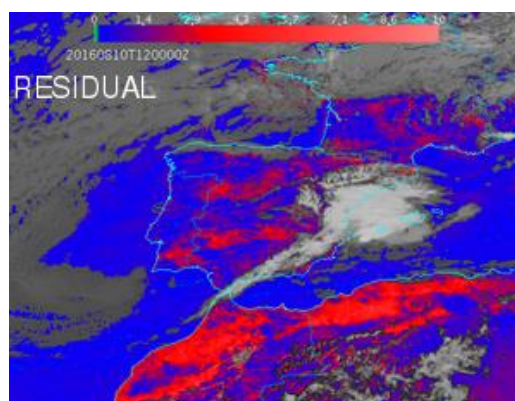*Figure 13: Example of GEO-iSHAI SKT and diffSKT 12 UTC on 10 August 2016 produced from MSG-3.*

Figure 14: Example GEO-iSHAI residual from 12Z on 10 August 2016 produced from SEVIRI on MSG-3.

		Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/iSHAI
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In the description of GEO-iSHAI version 2016 web page it has been created a web page with a summary of the case study 10th August 2016 used in Martinez&Calbet 2016b and other example of vertical cross sections is available.

http://www.nwcsaf.org/HTMLContributions_v2016/iSHAI/summary_of_case_study_21060810.html

This is a sample of future web pages with full iSHAI case studies analysis when the NWCSAF web server will be updated with version 2018.

The images corresponding to the 31 December 2017 at 12UTC from AHI instrument on Himawari-8 are shown as an example in the Figures below.
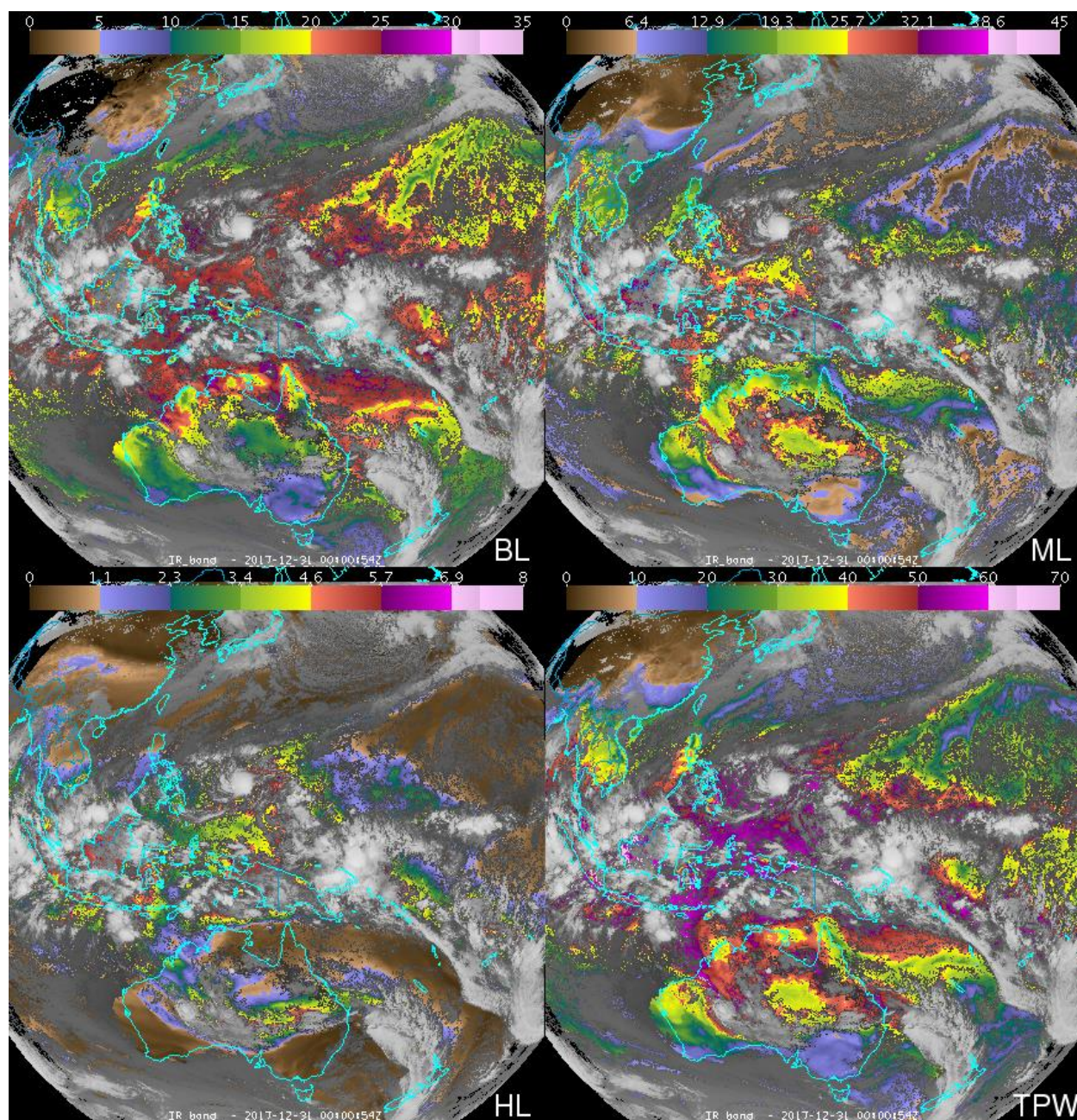

Figure 15: Example of GEO-iSHAI BL, ML, HL and TPW from 12 UTC on 31 December 2017 produced from AHI on Himawari-8.
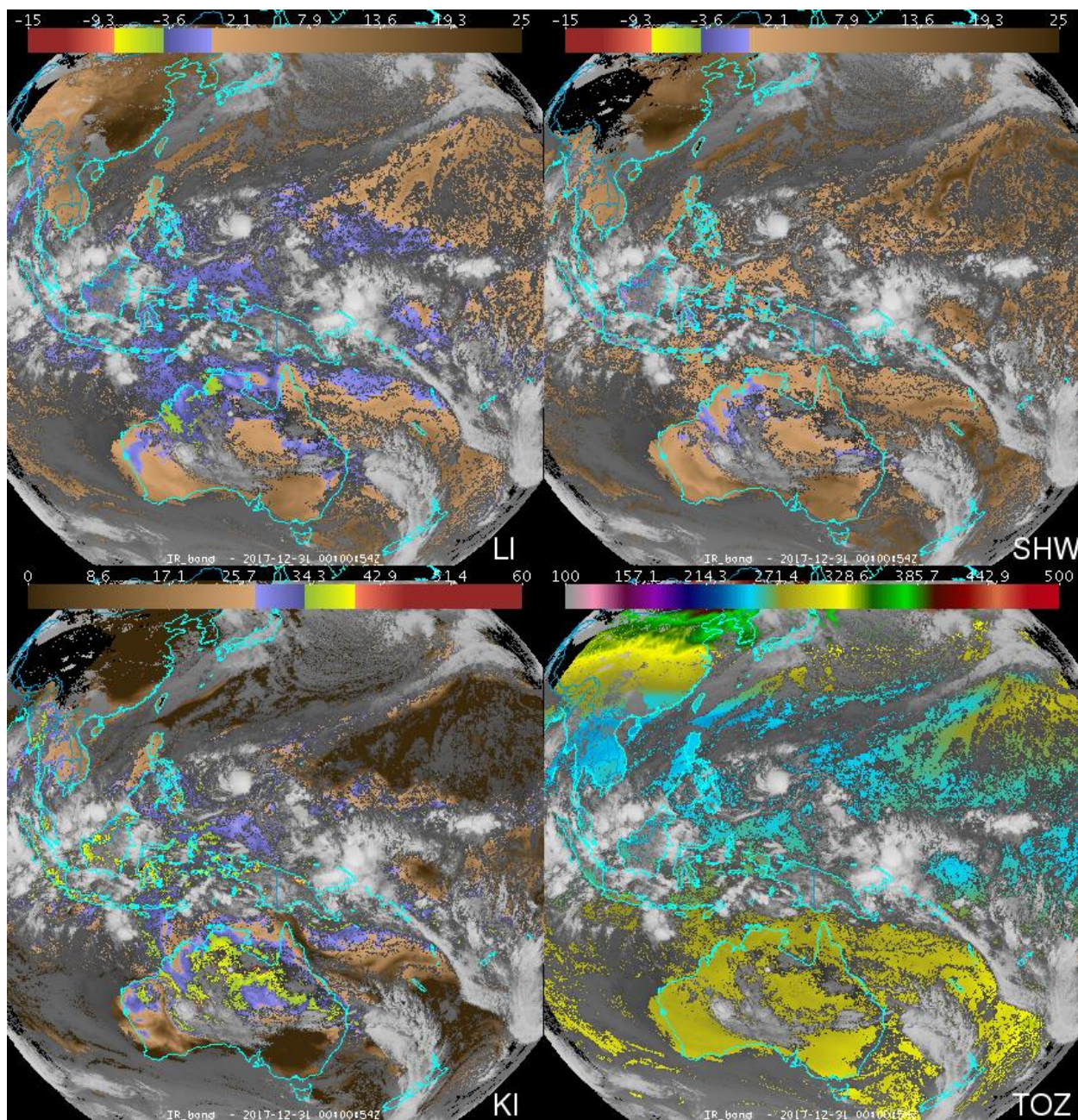
Figure 16: Example of GEO-iSHAI LI, SHW, KI and TOZ from 12 UTC 31 December 2017 produced from AHI on Himawari-8.

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3. PRACTICAL CONSIDERATIONS

3.1 PROGRAMMING AND PROCEDURAL CONSIDERATIONS

The GEO-iSHAI requires information from the cloud mask within each FOR. The GEO-iSHAI is implemented sequentially (pre-processing, regression step followed by iterative physical retrieval step and post-processing). GEO-iSHAI is purely a FOR by FOR algorithm. It could then be parallelised in future versions for processing with several CPUs.

In P mode, the spatial and temporal interpolation of background NWP profiles is made outside GEO-iSHAI and just the vertical interpolation/extrapolation to the RTTOV pressure levels is made inside GEO-iSHAI code. In this case, the spatial and temporal interpolation of background NWP profiles is made by the *AllMappingNWP* tool executed automatically by the Task manager in NRT or directly by the users on reprocessing.

In HYB mode; the spatial, temporal and vertical interpolation to get NWP data collocated with the real satellite data is fully made inside the GEO-iSHAI. GEO-iSHAI made the process directly from the hybrid GRIB files.

3.2 EXCEPTION HANDLING

Algorithm cannot be run if any of the mandatory IR channels data or the Cloud Mask (CMA) is bad or missing.

The GEO-iSHAI code does check for conditions where the iSHAI cannot be performed.

3.3 ASSUMPTIONS

(1) The surface pressure used in the iSHAI comes from the background NWP model. Better spatial resolution of the background NWP implies a better surface pressure field. The better surface pressure is the lower the error will be.
(2) The emissivity is fixed. After decision of NWC SAF Project Team to consider emissivity datasets as common software elements and the incorporation of management functions on the NWC/GEO NWCLIB the NWCSAF precomputed monthly emissivity atlases for each channel of the NWC/GEO satellites are generated from the 2007 IREMIS dataset (U. Wisconsin) RTTOV-11.2 emissivity atlases.

3.4 LIMITATIONS

(1) iSHAI products are available over "clear" FORs only.
(2) Since physical retrieval is an iterative process, computation is relatively expensive and an increase in the width of the FOR could be necessary when processing large regions on machine with light power CPU.
(3) The result can exhibit errors over mountain regions with large differences between the real topography and the background NWP topography. The same happens in desert pixels, where the difference of skin temperature between the background NWP and the real skin temperature could be high. Similar behaviour is expected on very hot or cold pixels over non-desert land pixels. From our experience, changes in the supply of the background NWP have improved clearly the quality of the GEO-iSHAI outputs. As example it was improved the request to MARS for ECMWF model supply in the internal AEMET chain from ECMWF GRIBs every 6 hours from *t+00* to *t+24* with 0.5°x0.5° resolution to every 1 hour from *t+00* to *t+24* with 0.125°x0.125°resolution. **It is strongly recommended to feed GEO-iSHAI with GRIBs files**

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with temperature and humidity profiles with as many fixed pressure levels as possible. In general, the more accurate the background profile is the more accurate the retrieval will be.

(4) In case to use as background NWP the ECMWF model: it is strongly recommended to the GEO-iSHAI users to use ECMWF on hybrid levels as background NWP; although this implies that the user needs to download the GRIB files on hybrid and fixed pressure levels (the latter needed for the Cloud Mask and the other products). The best quality is achieved using as input to GEO-iSHAI GRIB files on hybrid levels and the execution of GEO-iSHAI in HYB mode. As example, at the present time ECMWF GRIB files on fixed pressure levels have available only 25 fixed pressure levels but ECMWF GRIB on hybrid levels files have 137 hybrid levels.

(5) Effect of emissivity temporal variation is not handled. Precomputed monthly emissivity atlases for each channel of the NWC/GEO satellites are generated from the 2007 IREMIS dataset (U. Wisconsin) RTTOV-11.2 emissivity atlases.

3.5 IMPLEMENTATION OF GEO-iSHAI

Three main steps are identified. The user manually interacts with the GEO-iSHAI software during the installation step, and the GEO-iSHAI preparation and execution steps are automatically monitored by the Task Manager (if real-time environment is selected).

3.5.1.1 The GEO-iSHAI installation step

Previous condition and licences

The right to use, copy or modify this software is in accordance with EUMETSAT Policy for the NWC/GEO software package.

Installation and building of the executable

The software installation procedure does not require special resources. It is restricted to decompress the distribution file (a gzip-compressed tar file) and to successfully build the executables of the GEO-iSHAI-v4.0 to be stored into the *$SAFNWC/bin* directory.

After the steps shown in [AD.7], GEO-iSHAI-v40 of the NWC/GEO is installed and configured in the system. The operational use of NWC/GEO requires the definition of some configuration files in order to select the regions to be processed and some configuration parameters of the corresponding configuration file.

A set of default GEO-iSHAI model configuration file (extension *.cfm) is provided with the software package. There are default GEO-iSHAI model configuration file for any NWC/GEO supported satellite and for P and HYB modes. As all configuration files, it is an ASCII file, so further modification can be easily performed with a text editor. The configuration file manages all processes in the executable file.

The automatic set of pre-defined time scheduling (of the preparation step) relies on Programmed Task Definition Files.

3.5.1.2 The GEO-iSHAI preparation step

An output CMA netCDF file for the same slot and region is mandatory as input to GEO-iSHAI and for this reason it has to be executed *GEO-CMA-v50* before *GEO-iSHAI-v40* execution.

Also NWP spatial preprocessing should be done by the Task Manager or with the *AllMappingNWP* tool if the GEO-iSHAI is executed in P mode

If GEO-iSHAI is executed in *HYB* mode (configurable in the iSHAI configuration file using the keyword *NWP_EXEC_MODE* fixed to *HYB*) the NWP spatial preprocessing is needed only for GEO-

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CMA generation but it is not needed for GEO-iSHAI. In HYB mode, GEO-iSHAI opens and manages directly the hybrid GRIB files.

3.5.1.3 The GEO-iSHAI product execution step

The execution step is the real-time processing of real satellite images over the region. This process consists of the launch of the command *GEO-iSHAI-v40* along with the required parameters (slot, region file name and model configuration file) by the Task manager after the GEO-CMA-v50 has finished. The *GEO-iSHAI-v40* is then performed following the corresponding configuration file. The use of the *GEO-iSHAI-v40* is very easy on scripts. Here, an example of execution is provided:

GEO-iSHAI-v40 YYYY-MM-DDThh:mm:00Z *region*.cfg *configuration_file*.cfm

Where:

YYYY-MM-DDThh:mm:00Z is the date (YYYY-MM-DD) and hour (hh:mm:00Z) of the GEO satellite image

region.cfg is the name of file with region to use

configuration_file.cfm is the name of the ASCII file with the configurable parameter that GEO-iSHAI needs.

GEO-iSHAI has been designed as much modular and configurable by the user as possible. In order to configure it, the configurable options are collected in the GEO-iSHAI configuration file. In the User Manual [RD.2] more details about this are provided.

3.6 VALIDATION

An extensive validation for the year 2017 has been done. The applied methodology and the results are available in the Validation Report [RD.1].

The validation is based on the comparison of GEO-iSHAI parameters with the calculated from ECMWF model analysis from hybrid GRIB files.

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4. SUMMARY

The availability of GEO-iSHAI allows an easy processing of NWC/GEO supported satellite (MSG, Himawari and GOES-R) data in an operational environment to get estimations of several parameters related with precipitable water and stability on clear air pixels.

The NWC/GEO Task Manager allows a synchronization of all tasks involved in the process (launching of events, reading of real satellite files, navigation, geographical and ancillary management, management of forecast NWP GRIB files, etc.).

The software of GEO-iSHAI has been designed in order to be as configurable by the user as possible. Then, the user could easily adapt it to its region, NWP availability and choose between several configurations (as processing with large FOR's width on a large regions and with small FOR's width on small regions centred in its country). Also there is the possibility to use GRIB files on hybrid levels (at least ECMWF) as input to GEO-iSHAI v4.0. This fact is a great advance continuation of PGE13Hyb version 2013 module and GEO-iSHAI version 2016. In future releases, it should be studied to have full support by NWCSAF library of NWP models on hybrid levels for other products.

The validation of GEO-iSHAI using as input hybrid profiles has confirmed the recommendation to feed GEO-iSHAI with the best background NWP profiles as possible. It is strongly recommended to make the effort to use as background NWP GRIB files with the best spatial, temporal and vertical resolution as possible.

The availability of the former PGE13 SPhR and GEO-iSHAI has allowed creating a huge PGE13 and GEO-iSHAI training and validation dataset since 2009. As the generation of training/validation dataset shows, the use of GEO-iSHAI allows generating spatially, temporally and vertically collocated dataset of satellite data with NWP models, RAOB soundings, GPS stations, hyperspectral satellite, etc.; this is very important in order to improve the operational version 2018 and for the developing of new ones

This version also serves as basis for the developing of GEO-iSHAI for future MTG-FCI satellites.

Since AHI and ABI instruments have three water vapor channels and three channels in the split window regions, it will allow the execution of tests to determine the added value of the individual WV and IR channels; this experiments will be taken into account in the MTG era. Thus, this fact will make possible to test some improvements not included in this version and it will allow testing the improvements needed for evolution of the physical retrieval algorithms in the MTG era. It will be basic for future releases of GEO-iSHAI to improve the generalization of the process to generate training and validation dataset to other GEO satellites (future MTG-FCI and MTG-IRS).

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