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EUMETSAT
NWC SAF

SUPPORT TO NOWCASTING AND VERY SHORT RANGE FORECASTING

User Manual for iSHAI Product Processors of the NWC/GEO: Science Part

NWC/CDOP3/GEO/AEMET/SCI/UM/iSHAI, Issue 1, Rev.1

18 December 2019

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

Prepared by Agencia Estatal de Meteorología (AEMET)

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REPORT SIGNATURE TABLE

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DOCUMENT CHANGE RECORD

Version	Date	Pages	CHANGE(S)
1.1	*18 December 2019*	48	Updated version for GOES-R support.
1.1	*21 January 2019*	48	Updated version after NWC/GEO v2018 DRR and ORR2018.
1.0d	*31 October 2018*	46	Draft for version 2018 DRR.

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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 SCOPE OF THE DOCUMENT

This document is the User Manual (UM) for the iSHAI Product Processor of the NWC/GEO software package release 2018. GEO-iSHAI (imaging Satellite Humidity And Instability) is the name of Product Processor to estimate some parameters of interest in nowcasting in clear air pixels.

This document contains practical information on the use and configuration of GEO-iSHAI. It describes the characteristics, how to configure and how to execute the GEO-iSHAI processor; including the needed input files and the resulting outputs. It also provides comprehensive information on the algorithm implementation.

1.2 SOFTWARE VERSION IDENTIFICATION

This document is the User Manual of GEO-iSHAI version v4.0 included in the NWC/GEO software package release 2018.1 after delivery of the patch for GOES-R class satellite support.

1.3 SUMMARY OF CHANGES WITH RESPECT TO PREVIOUS VERSION

GEO-iSHAI algorithm remains based in Jun Li's algorithm for GOES Sounder physical retrieval algorithm (physical iterative 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 SEVIRI. In version 2018.1 the supported GEO imager instruments are SEVIRI on board METEOSAT Second Generation satellites, AHI on board Himawari satellites and ABI instrument on board GOES-R satellites.

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.

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. 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.

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Thus, neither the physical retrieval step nor the iSHAI retrieved profile (result of FG or physical retrieval step depending on BT_RMS_THREHOLD 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.

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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
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

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TM	Task Manager
UM	User Manual
VR	Validation Report
VSA	Visiting Scientist Activities
WV	Water Vapour Channel

1.5 REFERENCES

1.5.1 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	Date
[AD.1]	Proposal for the Third Continuous Development and Operations Phase (CDOP-3) March 2017-February 2022	NWC SAF: CDOP-3 proposal	1.0	11/04/2016
[AD.2]	Project Plan for the NWCSAF CDOP3 phase	NWC/CDOP3/SAF/AEMET/MGT/PP	1.3	12/07/2019
[AD.3]	Configuration Management Plan for the NWCSAF	NWC/CDOP3/SAF/AEMET/MGT/CMP	1.0	21/02/2018
[AD.4]	NWCSAF Product Requirements Document	NWC/CDOP3/SAF/AEMET/MGT/PRD	1.1	21/12/2018
[AD.5]	The Nowcasting SAF glossary	NWC/CDOP2/SAF/AEMET/MGT/GLO	2.1	03/02/2017

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	21/01/2019
[RD.2]	Algorithm Theoretical Basis Document for iSHAI Product Processors of the NWC/GEO	NWC/CDOP2/GEO/AEMET/SCI/ATBD/iSHAI	2.1	21/01/2019
[RD.3]	Data Output Format for the NWC/GEO	NWC/CDOP3/GEO/AEMET/SW/DOF	1.1	01/10/2019
[RD.4]	System and Components Requirements Document for the NWC/GEO	NWC/CDOP2/GEO/AEMET/SW/SCRD	2.2	01/04/2019
[RD.5]	Interface Control Document for Internal and External Interfaces of the NWC/GEO	NWC/CDOP3/GEO/AEMET/SW/ICD/1	1.1	01/10/2019
[RD.6]	Interface Control Document for the NWCLIB of the NWC/GEO	NWC/CDOP3/GEO/AEMET/SW/ICD/2	1.1	01/10/2019
[RD.7]	User Manual for the NWC/GEO: Software Part	NWC/CDOP3/GEO/AEMET/SW/UM	1.1	01/10/2019

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2. DESCRIPTION OF GEO-iSHAI PRODUCT

2.1 GOAL OF GEO-iSHAI PRODUCT

GEO-iSHAI version 4.0 product aims to provide information about water vapour and instability distributions on clear air pixels from version 2018 supported satellites infrared channels and NWP fields. Products are generated at high spatial and temporal resolution to support real time meteorological applications.

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 and must be activated by the users and the 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, 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.

Besides the above main output parameters, GEO-iSHAI can be optionally configured to save intermediate results (writing as binary files of structures with T/q/ozone profiles together with some surface and ancillary parameters) that can be useful for debugging purposes or to feed new user applications.

GEO-iSHAI products are useful in nowcasting applications, used in synergy with other data available to the forecaster. Since the physical basis of temperature and humidity retrieval is based in the minimization of the error between the real bias corrected satellite BTs and the synthetic BTs calculated from the profiles and taking into account the limited number of channels and the spectral information of the supported NWC/GEO imager satellite instruments, GEO-iSHAI mainly improve the humidity profiles of the background NWP in middle and high levels. Despite of this, the retrieved fields have a higher spatial resolution compared with the forecast. This fact must be taken into account by the users when the GEO-iSHAI outputs are used in nowcasting applications.

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2.2 GEO-iSHAI PROCESSING OUTLINE

As a whole, GEO-iSHAI code is designed in a modular way, so that it can be easy to handle and modify. The algorithm of the GEO-iSHAI is based in the calculation of First-Guess using non-linear regressions followed by physical retrieval and it is described in [RD.2]. In this section only a brief outline and the points related in how to configure the process of the data is provided.

For the selected region, the initialization gives access to real satellite BTs, Cloud Mask (GEO-CMA product), satellite zenith angle and ancillary files (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 the GEO-iSHAI parameters are calculated for this pixel or FOR.

If user activates it, also TOZ is calculated using only First-Guess 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 ozone profile.

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 a land-sea mask as static input information and land emissivity maps pre-computed for each IR channel and for every month of the year.

- In the case of MSG satellites are used the SEVIRI infrared channels centred at 6.2, 7.3, 9.7, 10.8, 12.0 and 13.4 μm.
- In the case of Himawari satellites are used the AHI infrared channels centred at 6.2, 7.0, 7.3, 9.6, 10.4, 11.2, 12.3 and 13.3 μm.
- In the case of GOES-R class satellites are used the ABI infrared channels centred at 6.2, 6.9, 7.3, 9.6, 10.3, 11.2, 12.3 and 13.3 μm

A Cloud Mask computed by GEO-CMA processor 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.
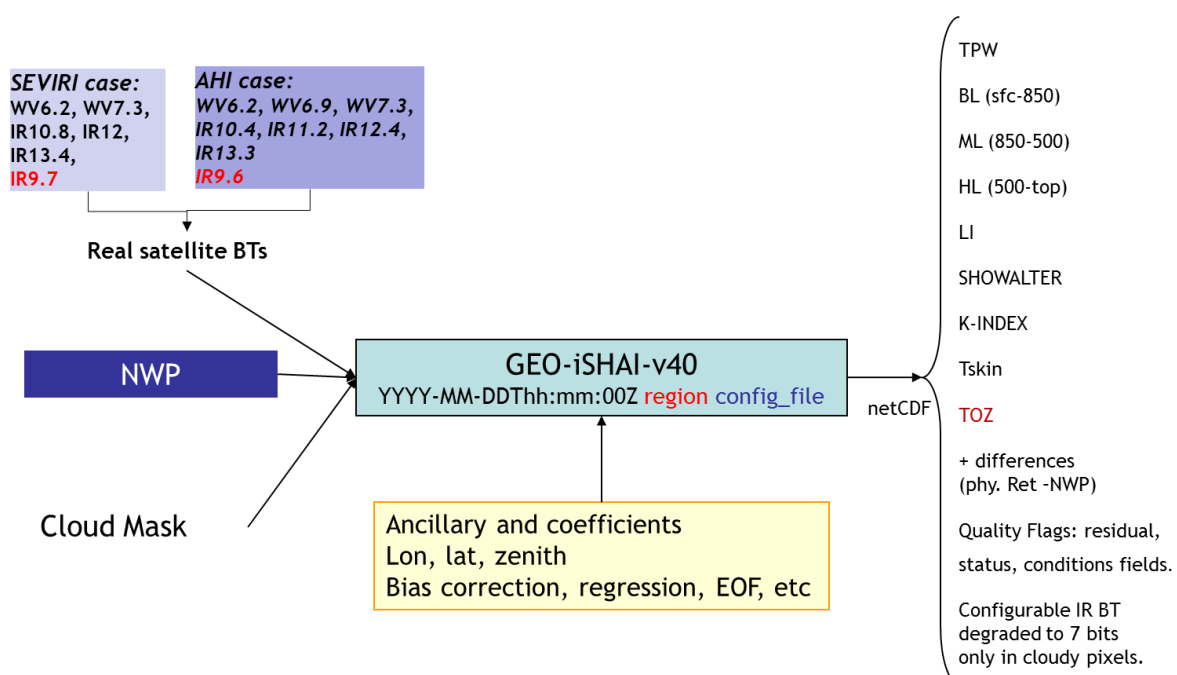

Figure 1: GEO-iSHAI inputs and outputs scheme

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Below, the main steps in the algorithm are described; in the GEO-iSHAI ATBD [RD.2] there is a similar description where the theoretical aspects 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-11.2, getting real satellite BTs, associated geographical ancillary files, IR emissivity maps and CMA for region to process.

   The second argument in GEO-iSHAI program is the name of region to process.

   The configuration file (extension *.cfm*) is an ASCII file that contains all coefficient file names, processing options, etc. The name of the configuration file is the third argument in GEO-iSHAI program. See in Section 4.3.1 the content and options in the configuration file.

   The keywords with the name of coefficients files are:
   `FG_reg_T_filename`, `FG_reg_logq_filename`, `FG_reg_logOzone_filename`, `FG_reg_SKT_filename`, `EOF_FILENAME`, `Binverse_covariance_matrix_filename`, `Einverse_covariance_matrix_filename`

   Optional thinning of real satellite BTs to process on FOR of M x N pixels (M and N is a configurable parameter in the configuration file). The default number is 3x3. Keywords: `LSIZE_FOR`, `CSIZE_FOR`

   Two methods are available to calculate BTs of the FOR: 1) mean value of clear pixels BTs on FOR (default) or 2) BTs of the warmest clear pixel at the cleanest channel in the IR window. The keyword `FOR_METHOD` is used to select this.

     In the case of SEVIRI the cleanest channel in the IR window is IR10.8.

     In the case of AHI the cleanest channel in the IR window is IR10.4.

     In the case of ABI the cleanest channel in the IR window is IR10.3.

- To 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 (and optionally ozone) profiles to the pixel position and time.

   Depending on the vertical representation of temperature and moisture profiles there are two execution modes. The selection of the mode is made with keyword `NWP_EXEC_MODE`. The default mode is P.

   In the case of P mode: The spatial (horizontal) and temporal interpolation is made outside of GEO-iSHAI reading the files generated by the pre-processing tool *AllMappingNWP* with common functions of NWC/GEO NWCLIB library. The vertical interpolation to 54 pressure levels of RTTOV is made from the user profile at fixed levels. The selection of the fields to use is made using the keywords `NWP_PARAM`. There are several "`NWP_PARAM*`" keywords with three arguments to select the parameter, the spatial thinning and spatial interpolation. See more details in Section 4.3.1. Conversion from relative humidity to specific humidity is made by the *AllMappingNWP* tool.

   In the case of HYB mode: all the NWP process is made inside the GEO-iSHAI code. GEO-iSHAI open directly the previous and next ECMWF GRIB files on hybrid levels to the time of the image, makes the vertical interpolation on ECMWF position to the 54 RTTOV-11.2 pressure levels, makes the temporal interpolation to the date

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of the image and finally makes the spatial interpolation just over the clear air processed FOR. The selection of the fields to use is made using the keywords `NWP-HYB_*`. There are several "`NWP-HYB_*`" keywords with two arguments to select the parameter and GRIB code. See more details in Section 4.3.1. 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.

- Bias adjustment of the real satellite BTs. The bias BT correction regression coefficients are read from the common NWC/GEO files and BT bias correction is made.

- Execution of non-linear regression to calculate the first guess profiles of temperature and specific humidity using as main inputs: a) real bias corrected satellite BTs and b) the background NWP temperature and specific humidity profiles spatially, temporally and vertically interpolated. Same to calculate the first guess of the skin temperature. In the GEO-iSHAI ATBD [RD.2] are described the non-linear regressions used to calculate the Firs-Guess. The structure of the files is described in section 4.2.2.

   The keywords with the name of coefficients for the FG regression coefficients files are: `FG_reg_T_filename`, `FG_reg_logq_filename` and `FG_reg_SKT_filename`

- Calculation of synthetic RTTOV BTs from first guess profile.

2.   Processing:

- If the calculated error between the synthetic RTTOV BTs from first guess profile and the satellite bias corrected BTs (over non window channels) are greater than a predefined threshold the Physical Retrieval module is executed (keyword: `BT_RMS_THRESHOLD`).

- In the Physical Retrieval Module the physical retrieval is an optimal estimation iterative process (see GEO-iSHAI [RD.2]); the physical retrieval iterative process is executed while the error between corrected satellite BTs and synthetic RTTOV calculated from the (T, q) profile and SKT after the iteration is greater than a threshold (keyword: `MAX_RESIDUAL`) and while the maximum number of iterations is not reached (keyword: `MAX_ITERATIONS`)

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

   To activate the calculation of TOZ, it is needed to change keyword `TOZ_CALCULATION` to 1 and to include an ozone profile in the GRIB files supplied to NWC/GEO in fixed pressure levels or hybrid levels. The keyword with the name of ozone regression coefficients files is `FG_reg_logOzone_filename`

- The software performs a direct calculation of TPW, LPWs, LI, SHW and KI parameters at FOR from the retrieved profiles of T and q. SKT is one parameter in the structure with profiles.

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

- The software computes the differences between the products (TPW, LPWs, LI, SHW and KI) calculated from retrieved profiles of T and q, and the ones calculated

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from the background NWP profiles of T and q. Calculate the difference between SKT and the background NWP SKT.

- 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 is possible. Also other parameters as surface pressure, skin temperature, real satellite BTs, ancillary files, etc are written. The profiles are written at the 54 RTTOV levels at the different algorithm steps (after physical retrieval, after iterations, after First-Guess or the background NWP). If activated in the configuration file these optional binary files are written in the `$SAFNWC/tmp`. The keywords to activate the optional binary files are:

  `SAVE_PROFs_in_BINARY_files`, `SAVE_iSHAI_in_BINARY_file`.

  See section 2.3.3 for details.

3. Post-processing:

   - Quality control: Several quality flags have been added to the output product.

   - Filling clear pixels inside the FOR:

     The default method is to copy the same value to all clear pixels in the FOR.

     The other configurable option is to write the output only at the clear pixel or FOR position. That means the warmest pixel in the case of the BTs of the warmest clear pixel at the cleanest channel in the IR window. Keyword: `POST_PROC_METHOD`

   - Over cloudy pixels, one IR BT channel degraded to 7 bits (range [0 – 127]) values is stored. This will be later used to generate adequate images in which cloudy pixels are grey scaled and clear pixels are colour scaled. The number of the IR BT channel is configurable using the keyword `BAND_CLOUDY`;

     By default in the SEVIRI case is 16, which means IR10.8 channel.

     By default in the AHI case is 15, which means IR10.4 channel.

     By default in the ABI case is 15, which means IR10.3 channel.

   - The outputs are written in a netCDF format file.

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2.3 DESCRIPTION OF GEO-iSHAI OUTPUTS

The main outputs provided are parameters informing about the water vapour content in the vertical column (total and in selected layers) and about the atmospheric thermal instability. These parameters are computed using the final retrieved temperature and humidity profiles. Since NWC/GEO release 2016, also the Skin Temperature (SKT) and Total Ozone (TOZ) are additional outputs.

As additional outputs, GEO-iSHAI also provides the differences between the above parameters, computed from the final retrieved profiles, and similar ones computed from the forecasted background profiles. These deviations are important for (1) signalling areas with discrepancies between model forecast and the observations and (2) showing the added value of real satellite observations.

Optionally, GEO-iSHAI can be configured to keep the final retrieved profiles and the intermediate profiles. This allows users (1) to feed new applications or to compute specific stability indices at their own and (2) to debug, test and monitor GEO-iSHAI performances.

2.3.1 GEO-iSHAI main outputs description.

2.3.1.1 Introduction: Humidity and Stability Indices parameters

2.3.1.1.1 Humidity parameters

An evaluation of humidity distribution is critical in order to determine the possibilities of convection, severe weather and heavy precipitation. Storms usually develop where humidity is already high or where some mechanism makes it to increase. Precipitable water is a measurement of the water vapor mass contained in a vertical column of atmosphere of unit section and thickness limited between two pressure levels. The units are kg/m^2 (mm are commonly used in operational meteorology)

Four different precipitable water parameters, defined as function of two selected pressure levels, are considered of interest:

> Total Precipitable Water, TPW: $p_{max} = p_{surface}$ and $p_{min} = 0$
>
> Low Layer Precipitable Water, BL: $p_{max} = p_{surface}$ and $p_{min} = 850$ hPa
>
> Medium Layer Precipitable Water, ML: $p_{max} = 850$ hPa and $p_{min} = 500$ hPa
>
> High Layer Precipitable Water, HL: $p_{max} = 500$ hPa and $p_{min} = 0$

Most of the contribution to TPW comes from a layer between surface and 500 hPa.

2.3.1.1.2 Stability indices parameters

Stability indices were developed in the past to support storms and severe weather forecast using as main input local radiosonde profiles of temperature and humidity. It is important to remark as introductory note that the use of these indices needs to be supported by previous experience in the use of the more appropriate ones to each specific region and weather regimes. Among all the stability indices, Lifted Index (Galway, 1956) and (Miller, 1972), the Showalter Index (Showalter, 1947) and the K-Index (George, 1960) have been chosen to be codified in the 2010 version. These indices are widely used in operational meteorology.

There are several stability indices defined as the difference between the air environment temperature at 500 hPa and the temperature of an air parcel representative of the properties of low levels, lifted up to the 500 hPa. These indices have negative values when the lifted parcel arrives warmer than the environment as it means buoyancy and hence instability. The units are Kelvin (but ºC is commonly used also in operational meteorology).

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$$\text{Thermal Stability Index} = T_{env}^{500} - T_{parc}^{500}$$

In the case of Lifted Index (LI), the temperature and humidity of the virtual lifted parcels are the average of the lowest 100 hPa (or 1000 m).

The following table provides empirical relation between LI values and the stability degree:

LI value	
$V > 0$	Stable
$-3 <= v < 0$	Slightly Unstable
$-6 <= v < -3$	Unstable
$-9 <= v < -6$	Very Unstable
$v < -9$	Extremely Unestable

In the case of Showalter Index (SHW), the lifted parcel represents the environment at 850 hPa.

The following table provides empirical relation between SHW values and the stability degree:

Showalter value	
$v > 0$	Stable
$-3 <= v < 0$	Marginal instability
$-6 <= v < -4$	Large instability
$v < -6$	Extreme instability

K Index (KI) measures the thermal stability in function of the vertical gradient of temperature and humidity content in low levels.

$$KI = (T^{850} - T^{500}) + (T_d^{850} - DD^{700})$$

where: $DD^{700} = (T^{700} - T_d^{700})$

The following table provides empirical relation between KI values and storm probability:

K-Index value	Storm probability
$v < 15$	$\approx 0\%$
$15 < v <= 20$	$< 20\%$
$21 < v <= 25$	$20 – 40 \%$
$26 < v <= 30$	$40 – 60 \%$
$31 < v <= 35$	$60 – 80 \%$
$36 < v <= 40$	$80 – 90 \%$
$v > 40$	$> 90 \%$

2.3.1.2 **SKT and TOZ**

2.3.1.2.1 **Skin temperature (SKT) and diffSKT**

SKT and diffSKT=(SKT$_{retrieved}$ − SKT$_{nwp}$) were introduced in version 2016. In any case, GEO-iSHAI SKT does not pretend to be an alternative to SST or LST products because more temporal and spatial controls are required. They have been introduced in order the users and forecasters can use them as nowcasting parameters. The temporal evolution and spatial gradients of SKT and the diffSKT could be used in several nowcasting applications as monitoring of pixel not well screened out by cloud mask, detection of fogs, advice for very fast increase of SKT as triggering convection mechanism, advice users of bad SKT, etc

2.3.1.2.2 **Total Ozone (TOZ) and diffTOZ**

TOZ and diff(TOZret − TOZnwp) have been also introduced as optional parameters since release 2016. That means that user must activate them and provide NWP GRIB file with ozone profiles.

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Users can activate them editing keyword `TOZ_CALCULATION` to 1 and including ozone profile in the GRIB files supplied to NWC/GEO in fixed pressure levels or hybrid levels.

For these reasons the IR channel in spectral region 9.7 µm is also a mandatory channel. The retrieval of TOZ is based on statistical retrieval using non-linear regression from ozone profile, satellite corrected bias BTs from the IR channels (including the BTs of IR channel in spectral region 9.7 µm) and the retrieved GEO-iSHAI T,q profiles and SKT.

Temporal changes and spatial gradients of TOZ are nowcasting interest parameters due to the relation between TOZ fields and the detection of tropopause breaks and vorticity maxima.

diffTOZ is useful to detect the disagreement between NWP TOZ and retrieved TOZ.

2.3.2 GEO-iSHAI main outputs: 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 NWP profiles in kg/m^2.
- o **iSHAI_diffbl, iSHAI_diffml, iSHAI_diffhl**: Difference between LPWs from retrieved profile and LPWs from NWP profiles in kg/m^2.
- o **iSHAI_diffli, iSHAI_diffki, iSHAI_diffshw**: Difference between stability indices from retrieved profile and stability indices from 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_status_flag, iSHAI_conditions** fields.
- o Configurable IR channel BT degraded to 7 bits only in cloudy pixels.

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.

The format of the file is netCDF and it is described in [RD.3]. 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.

The netCDF format files scales have the following minima and maxima values. They are fixed in the *$SAFNWC/import/Aux_data/iSHAI/S_NWC_PRODIO_iSHAI.cf*

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Parameter	minimum	maximum
iSHAI_bl	0	35
iSHAI_ml	0	45
iSHAI_hl	0	8
iSHAI_tpw	0	70
iSHAI_li	-15	40
iSHAI_ki	0	60
iSHAI_shw	-15	40
iSHAI_skt	243	343
iSHAI_toz	100	500
iSHAI_diffbl	-2.5	2.5
iSHAI_diffml	-3.5	3.5
iSHAI_diffhl	-1.0	1.0
iSHAI_difftpw	-5	5
iSHAI_diffli	-2.5	2.5
iSHAI_diffki	-7	7
iSHAI_diffshw	-2.5	2.5
iSHAI_diffskt	-15	15
iSHAI_difftoz	-30	30
Residual	0	600

Table 2: Maximum and Minimum values for each parameter

The detailed structure of the netCDF output for the NWC/GEO iSHAI product is described in the "Data Output Format for the NWC/GEO" (document [RD.3]). Together with the main output fields described in Table 2 there are a set flags and a set of common global netCDF attributes described in the "Data Output Format for the NWC/GEO" (document [RD.3]).

The iSHAI flags are:

- `ishai_conditions:` contains the common processing conditions.
- `ishai_quality:` contains the common Quality Indicator filled in function of the residual.
- `ishai_status_flag:` describes the GEO-iSHAI Specific Processing Conditions in the processing pixel of the processed clear FOR. It is a 8 bit-mask indicating the processing status:

Bit #	8th	7th	6th	5th	4th	3rd	2nd	1st
Data	[Reserved]	[Reserved]	Pixel processed with 3rd retrieval iteration	Pixel processed with 2nd retrieval iteration	Pixel processed with 1st retrieval iteration	Pixel processed with first guess	Pixel Processed	Cloudy flag

Where

Cloudy flag (1st bit):
> (0) Cloudy pixel.
> (1) Cloud free pixel
>> *Note: only cloud free pixel are processed*

Status Pixel Processed flag (2nd bit):
> (0) Pixel has not been processed.
> (1) Pixel has been processed without error.

Status Pixel processed with first guess regression flag (3rd bit):
> (3rd bit) First guess regression step has been applied.

Status Pixel processed with physical retrieval and number of iterations (4th to 6th bits):
> (4th bit) 1st iteration of physical retrieval has been done
> (5th bit) 2nd iteration of physical retrieval has been done
> (6th bit) 3rd iteration of physical retrieval has been done

The "Common attributes" are global netCDF attributes:

- The "product_quality" is the "mean Quality index" of all (Field of Regards) or MxM boxes written in the netCDF output file. This parameter gives a percentage value (from 0% to 100%) of the FOR with residual lower than 4 with respect of all processed clear FORs.

- The "product_completeness" is the "percentage of the FOR (Field of Regards) or MxM boxes processed OK, with respect to the number of processed clear FOR. This parameter gives an idea of how many clear FOR were successfully calculated, defined also as a percentage value (from 0% to 100%).

The name of the iSHAI netCDF output file is:

S_NWC_iSHAI_*satid_nameregion*-*resolution*_*yyyyMMDD*T*hhmm*00Z.nc

where:

> *satid* is one string that identifies the satellite series and the number of the satellite. The *satid* is read from the keyword `SATELLITE` from `$SAFNWC/config/sat_conf_file`.

> *nameregion* is the name of the region used to execute GEO-iSHAI (second argument)

> *resolution* spatial resolution of the channels in relation with the highest resolution

> *yyyyMMDD*T*hhmm*00Z is the date and hour of the satellite image.

Examples of iSHAI netCDF output filenames:

> MSG: *S_NWC_iSHAI_MSG3_LargeIberica-VISIR_20160810T120000Z.nc*

> Himawari: *S_NWC_iSHAI_HIMA08_FullDiskHimawari-NR_20171231T000000Z.nc*

> GOES-R: *S_NWC_iSHAI_GOES16_Conus-NR_20171231T000000Z.nc*

The netCDF output files are stored in `$SAFNWC/export/iSHAI`.

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2.3.3 GEO-iSHAI optional binary files.

Since GEO-iSHAI is executed locally by the users, the collocated temperature, specific humidity and ozone profiles with satellite data can be written in optional binary files at different steps of the algorithm. The main advantage to get spatial, temporal and vertically collocated (T, q, ozone) profiles with satellite data is to allow debugging activities or generating new parameters or stability indices or generation of 3D displays as vertical cross sections or 3D visualizations or generation of validation datasets. These applications are only a few among other applications that could be used.

At the present time, the generation of tools for conversion from binary to netCDF format is in progress. There are a variety of software packages that can read the netCDF format and can be used by the users to a wider and deeper exploitation of the GEO-iSHAI binary files.

These conversion tools from GEO-iSHAI binary files to netCDF format are being generated at the best effort basis from the IDL prototypes. One possibility it use the GNU version of IDL called GDL; the IDL prototypes will tested and adapted to be compatible with GDL if possible. The other possibility it to develop FORTRAN, C or Python versions; these could be written using the API netCDF library and the IDL versions as 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 an example, tools freely available as IDV, McIDAS-V could be used to get all kind of interactive 2D and 3D visualization. As an example of the possibilities you can see Figures 2 and 3 taken from Martinez 2013. More examples can be seen in Martinez&Calbet 2018, Martinez&Calbet 2016[a,b], Martinez 2015 and Martinez 2013.
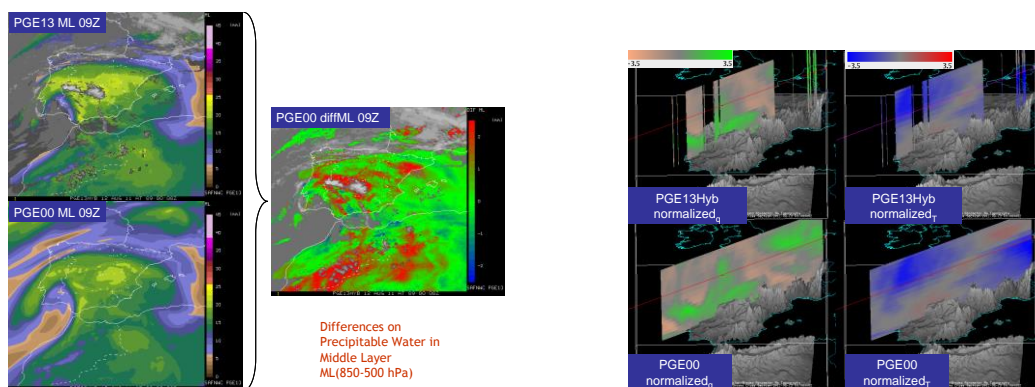
Figure 2: PGE13Hyb parameters diffML (precipitable water 850-500 hPa). Difference of precipitable water content between PGE13Hyb ML and ECMWF ML at 9 UTC on 12th August 2011. Vertical cross sections using McIDAS-V of normalized 3D arrays of T and q for 9 UTC on 12th August 2011 from PGE13Hyb and ECMWF (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.

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θ$_e$ from ECMWF hybrid levels spatial, time and vertical interpolated to the 43 RTTOV pressure levels

θ$_e$ from 2013 PGE13 Hybrid version

Figure 3: PGE13Hyb and ECMWF (PGE00Hyb) vertical cross sections of θ$_e$ for 9 UTC on 12th August 2011.

Note: IDV is available at http://www.unidata.ucar.edu/software/idv/ and McIDAS-V is freely available at http://www.ssec.wisc.edu/mcidas/software/v/

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.

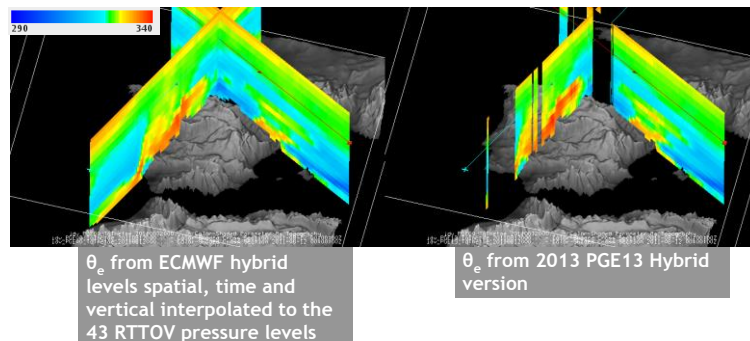There are two keywords in the GEO-iSHAI model configuration file to activate writing temperature and humidity profiles on binary files at different steps of the algorithm (from the background NWP files supplied by the users to the final retrieved profiles used to calculate the main outputs). The users can activate any combination of the two keywords to start writing the optional binary files editing the ASCII GEO-iSHAI model configuration file. Once any of the keywords are activated in the configuration file, the GEO-iSHAI optional binary files will be written in the `$SAFNWC/tmp` directory in the next execution of GEO-iSHAI.

These keywords are:

- `SAVE_PROFs_in_BINARY_files` this keyword activates the writing of background NWP and FG structures. The number of pixels written depends on the value. 1 means the structures are written only at clear air FOR or pixels. 2 means the structures are written in ALL pixels.

- `SAVE_iSHAI_in_BINARY_file` this keywords activates the writing of end profile structures. End profile is the result of physical retrieval or FG non-linear regressions depending on processing options and the convergence of the physical retrieval. The number of pixels written depends on the value. 1 means the structures are written only in clear air FOR or pixels. 2 means the structures are written in ALL pixels.

Using the allowed values of these keywords, users can select to activate the possibilities in Table 3. See sections 2.3.3.1 to 2.3.3.4 for details about names and contents of the corresponding GEO-iSHAI optional binary files:

keyword	Value = 0	Value = 1	Value = 2
`SAVE_PROFs_in_BINARY_files`	Not written	Written **only at clear air** FOR or pixels	Written in **ALL** FOR or pixels
`SAVE_iSHAI_in_BINARY_file`	Not written	Written **only at clear air** FOR or pixels	Written in **ALL** FOR or pixels

Table 3: combinations for optional binary GEO-iSHAI binary files generation.

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Due to the huge size of the GEO-iSHAI optional binary files for large regions (as example full disc region), users should be careful on activation of options when all pixels are written. For this reason it is recommend to use **only the option to write at clear air FOR.**

The content of the optional binary are records that contains C or Fortran-90 structures repeated for every pixel written. Besides the profiles (that means [T[54], q[54], ozone[54], SKT]), the GEO-iSHAI parameters, the synthetic and real satellite BTs, ancillary files, the errors between the real satellite BTs after bias correction and the synthetic RTTOV BTs, etc. are also written. Every record contains now the complete set of parameters of the profile used for the calculations of the GEO-iSHAI outputs. The amount of bytes written in each record depends on the satellite (the number of channels is different in MSG than in Himawari or GOES-R class).

For all the files and for every pixel (or FOR) the structures `inputs&ancillary` and `iSHAI_profile` declared in `$SAFNWC/src/iSHAI/iSHAI_*/iSHAI.c` are written. The members of the structures are all Float (4 bytes) and the name of the members are described in the tables 4 and 5:

line	column	latitude	longitude	zenith_angle	emissivity[nchannels]	land_sea_type	topo

$+$

bt_satellite[$n_{channels}$]	bias_offset[$n_{channels}$]	bias_scale[$n_{channels}$]

$+$

bt_rms_threshold	max_residual	max_iterations	emissivity_IR97	bt_satellite_IR97	bias_offset_IR97	bias_scale_IR97

Table 4: *members in* `"inputs&ancillary"` *structure*

bt_rttov[$n_{channels}$]	SKT	p_{sfc}	z_{sfc}	T_{sfc}	q_{sfc}	p[54]	T[54]	q[54]	O$_3$[54]	BL	ML	HL	TPW	LI	KI	SHW	TOZ	Bt_rms	residual	iteration	qc_flag

Table 5: *members in* `"iSHAI_profile"` *structure*

The units of q profiles at the 54 RTTOV pressure levels are ppmv. Same for Ozone profile. The position on region coordinates (i=element, j=line) are included in every record together with ancillary parameter (longitude, latitude, etc) in order to geolocate the FOR. For BT_SATELLITE and BT_RTTOV arrays with dimension $n_{channels}$ and the order is from lower to higher wavelength.

For synthetic or simulated brightness temperature binary files, RTTOV BTs for channels are stored in the BT_RTTOV arrays and have been obtained after applying RTTOV forward to the stored retrieved profiles.

The fields on the GEO-iSHAI binary files have been unified for HYB and P mode and just differ in the name of the binary file because the GEO-iSHAI execution mode has been included in the name.

2.3.3.1   END PROFILE at clear FOR (`SAVE_iSHAI_in_BINARY_file 1`)

Fixing `SAVE_iSHAI_in_BINARY_file` to 1, the final retrieved profiles (T, q, ozone profile at the 54 RTTOV levels) and other parameters are written only at clear FOR or pixels. These are the profiles used to calculate TPW, LPW, stability indices and TOZ together with the difference with background NWP profiles. The name of END PROFILE at clear air FOR optional binary file is:

iSHAI_mode_END_____CLEAR_nameregion_Clinc_colc_Ssizi_sizc_YYYY-MM-DDThh:mm:00Z.bin

where:

- **CLEAR** indicates only at clear air FOR
- mode processing mode P or HYB

- ▪ `nameregion` name of region
- ▪ C`linc_colc` S`sizl_sizc` position of region centre (C`linc_colc`) and size of region (S`sizl_sizc`)
- ▪ `YYYY-MM-DDThh:mm:00Z` is the date (YYYY-MM-DD) and hour (hh:mm:00Z) of satellite image

Example:

iSHAI_HYB_END_____CLEAR_LargeIberica_C1748_0558_S0665_0511_2016-08-10T12:15:00Z.bin

In this case the binary file is a 1D array [*number_clear_FOR*] containing values of the structures written on the clear air FOR or pixels where the GEO-iSHAI algorithm has been really executed.

The size of this file is *(size_of_record x number_clear_FOR)*. The GEO-iSHAI optional binary files are always written at *$SAFNWC/tmp* directory.

2.3.3.2 END PROFILE at ALL pixels (`SAVE iSHAI in BINARY file 2`)

Fixing `SAVE_iSHAI_in_BINARY_file` to 2, the final retrieved profiles (T, q, ozone profile at the 54 RTTOV levels) and other parameters **are written for all the pixels**. At clear FOR or pixels these profiles are the profiles used to calculate GEO-iSHAI parameters and for cloudy or not processed pixels dummy structures filled all members with missing value (-9999.0) are written. The name of END PROFILE at all pixels optional binary file is:

iSHAI_mode_END_____nameregion_Clinc_colc_Ssizl_sizc_YYYY-MM-DDThh:mm:00Z.bin

where:

- ▪ `Mode` processing mode P or HYB
- ▪ `Nameregion` name of region
- ▪ C`linc_colc` S`sizl_sizc` position of region centre (`linc`, `colc` are the line and column coordinates of the centre of the region/(0-based)) and size of region (S`sizl_sizc` are the size of the region (number of lines and number of columns)).
- ▪ `YYYY-MM-DDThh:mm:00Z` is the date (YYYY-MM-DD) and hour (hh:mm:00Z) of satellite image

Example:

iSHAI_HYB_END_____LargeIberica_C1748_0558_S0665_0511_2016-08-10T12:15:00Z.bin

In this example LargeIberica is a region of 665 lines x 511 columns centred in (558, 1758) by this reason the name of binary file contains C1748_0558_S0665_0511

In this case the binary file is a 2D array [ncols, nlines] containing values of the structures written on **all pixels**. These binary files are adequate for small to medium regions when processing in 1x1 FOR and in applications as vertical cross sections, 3D visualizations, etc.

Note: users must take into account the huge size of the binary files that could be generated and the very expensive CPU time of the pixel by pixel processing for large regions.

The size of this file is *(size_of_record x ncols x nlines)*

2.3.3.3 Background NWP and FG profiles at clear FOR (`SAVE PROFs in BINARY files 1`)

Fixing `SAVE_PROFs_in_BINARY_files` to 1, the background NWP and after FG non-linear regressions profiles (T, q, ozone profile at the 54 RTTOV levels) and other parameters are written only at clear FOR or pixels. These are the profiles used to calculate TPW, LPW, stability indices

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and TOZ together with the difference with end GEO-iSHAI profiles. The name of background nwp and FG at clear air FOR optional binary files are respectively:

iSHAI_mode_nwp_____CLEAR_nameregion_Clinc_colc_Ssizl_sizc_YYYY-MM-DDThh:mm:00Z.bin

iSHAI_mode_FG_____CLEAR_nameregion_Clinc_colc_Ssizl_sizc_YYYY-MM-DDThh:mm:00Z.bin

where:

- **CLEAR** indicates only at clear air FOR
- `Mode` processing mode P or HYB
- `Nameregion` name of region
- `Clinc colc Ssizl sizc` position of region centre (`Clinc_colc`) and size of region (`Ssizl_sizc`)
- `YYYY-MM-DDThh:mm:00Z` is the date (YYYY-MM-DD) and hour (hh:mm:00Z) of satellite image

Examples:

iSHAI_HYB_nwp_____CLEAR_LargeIberica_C1748_0558_S0665_0511_2016-08-10T12:15:00Z.bin

iSHAI_HYB_FG_____CLEAR_LargeIberica_C1748_0558_S0665_0511_2016-08-10T12:15:00Z.bin

In this case the binary files are a 1D array [number_clear_for] containing values of the structures written on the clear air FOR or pixels where the GEO-iSHAI algorithm has been really executed.

The size of this file is *(size_of_record x number_clear_FOR)*.

2.3.3.4 Background NWP and FG profiles at ALL pixels (`SAVE iSHAI in BINARY file 2`)

Fixing `SAVE_iSHAI_in_BINARY_file` to 2, the background NWP and after FG non-linear regressions profiles (T, q, ozone profile at the 54 RTTOV levels) and other parameters **are written for all the pixels**. These are the profiles used to calculate GEO-iSHAI parameters at clear FOR or pixels and dummy structures filled all members with missing value (-9999.0) for cloudy or not processed pixels.

The name of background nwp and FG at all pixels optional binary files are respectively:

iSHAI_mode_nwp_____nameregion_Clinc_colc_Ssizl_sizc_YYYY-MM-DDThh:mm:00Z.bin

iSHAI_mode_FG_____nameregion_Clinc_colc_Ssizl_sizc_YYYY-MM-DDThh:mm:00Z.bin

where:

- `Mode` processing mode P or HYB
- `Nameregion` name of region
- `Clinc colc Ssizl sizc` position of region centre (`Clinc_colc`) and size of region (`Ssizl_sizc`)
- `YYYY-MM-DDThh:mm:00Z` is the date (YYYY-MM-DD) and hour (hh:mm:00Z) of satellite image

Examples:

iSHAI_HYB_nwp_____LargeIberica_C1748_0558_S0665_0511_2016-08-10T12:15:00Z.bin

iSHAI_HYB_FG_____LargeIberica_C1748_0558_S0665_0511_2016-08-10T12:15:00Z.bin

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In this case the binary file are a 2D array [ncols, nlines] containing values of the structures written on **all pixels**. It is more useful when processing in 1x1 FOR.

Note: users must take into account the huge size of the binary files that could be generated and the very expensive CPU time of the pixel by pixel processing for large regions.

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3. IMPLEMENTATION OF GEO-ISHAI

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

3.1 THE GEO-iSHAI INSTALLATION AND PREPARATION 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

Once the user has obtained the necessary permissions to download the software package, 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 GEO-iSHAI-v4.0 to be stored into the *$SAFNWC/bin* directory.

After the steps shown in [RD.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.

3.2 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 *GEO-CMA-v50* has to be executed 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-CMA generation but it is not needed for GEO-iSHAI. In HYB mode, GEO-iSHAI opens and manages directly the hybrid GRIB files.

3.3 THE GEO-iSHAI EXECUTION STEP

The execution step is the real-time processing of real satellite images over one 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).

It could be done interactively by the user or automatically in near real time by the Task manager. The execution of GEO-iSHAI cannot be till GEO-CMA-v50 has finished for the same slot and region. 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:

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> **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 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 modular and configurable by the user as possible. In order to configure it, the configurable options are collected in the GEO-iSHAI configuration file (see section 4.3.1). GEO-iSHAI model configuration file allows an easy management of all GEO-iSHAI keywords that can be changed by the user. Each model configuration file is an ASCII file, so further modifications can be easily performed with a text editor.

The GEO-iSHAI running in near real time scheduling relies on the Programmed Task Definition File. This process consists in running `GEO-iSHAI-v40` command along with the required parameters (slot, region file and model configuration file) by the Task Manager.

Since the model configuration file is the third argument required by the GEO-iSHAI program, to change the configuration used to execute the GEO-iSHAI code is as easy as to change the third argument when the GEO-iSHAI is executed or edit it. Thus, several GEO-iSHAI configuration files can be available by the user in the `$SAFNWC/config` and GEO-iSHAI can be executed on real time with different configuration depending on the region to process, the hour of the image, etc. As an example, users can execute GEO-iSHAI with a large FOR's width in a full-disc or large region with only one iteration and execute GEO-iSHAI over a small region centred in their countries with FOR's width 1x1 or 3x3 and three iterations.

When setting up the execution conditions, users must look for a balance among the region size, the computer resources and the following configurable keywords of the configuration file: `BT_RMS_THRESHOLD`, `LSIZE_FOR`, `CSIZE_FOR` and `MAX_ITERATIONS` (see in section 4.3.1 for a wider discussion on how to choose them).

Also this mechanism allows to change the GEO-iSHAI execution mode (P or HYB) editing or using different configuration file changing the `NWP_EXEC_MODE` keyword.

In the GEO-iSHAI configuration file there is not one specific keyword to choose the satellite to process. **GEO-iSHAI-v40** is indeed one ksh script that reads the *satid* of the satellite to process from the keyword `SATELLITE` from the `$SAFNWC/config/sat_conf_file`. Then, the ksh **GEO-iSHAI-v40** will run the real executable program `GEO-iSHAI-MSG-v40` for MSG satellites, `GEO-iSHAI-AHI-v40` for Himawari satellites and `GEO-iSHAI-ABI-v40` for GOES-R class satellites.

4. DESCRIPTION OF INPUTS, COEFFICIENTS FILES AND CONFIGURABLE PARAMETERS

In this section a description of the inputs, coefficients files content and user configurable parameters is made.

Concerning the coefficients files, more specific scientific information can be found in the GEO-iSHAI Algorithm Theoretical Basis Document [RD.2].

4.1 DESCRIPTION OF INPUTS FOR GEO-ɪSHAI

A region configuration file and a GEO-iSHAI model configuration file (with the diverse parameters and options that are indicated by the user for calculation, see section 4.3) are needed as mandatory parameters in order to execute the GEO-iSHAI command. Both must be located in the `$SAFNWC/config` directory.

4.1.1 Region configuration file

The region configuration file sets the dimensions and positions where GEO-iSHAI product will be obtained (as an example "`Spain.cfg`" defines a region of 1500 x 1500 km centred at (40ºN, 4ºW)). Any valid region configuration file could be used for the GEO-iSHAI generation. See details on how to create valid region configuration files in [RD.7].

Since the region configuration file sets the name of the region, dimensions and position, these parameters are used later to build the ancillary files (geographical, topography, emissivity atlas, etc) and they are part of the name of the optional GEO-iSHAI binary output file.

In release 2018 the size of the region in the configuration file is expressed in kilometres relatives to the size of the pixel at the centre position. Since it is difficult to know the size (lines x columns) and centre position in the name of GEO-iSHAI optional binary files, the position of centre and the size in lines and columns are written (Clinc_**colc**_S**sizl**_**sizc**) in the name of the optional GEO-iSHAI binary files.

This has been done in order users to know the size and position of the region if they need to allocate 2D or 3D arrays before read the files and/or for the generation of netCDF or HDF-5 files.

4.1.2 Real satellite BTs.

The following real satellite IR BTs values are needed at full IR spatial resolution:

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 6: 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 7: List of AHI IR channels used in GEO-iSHAI version 2018.

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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

Table 8: List of ABI IR channels used in GEO-iSHAI version 2018.

The GEO-iSHAI checks the availability of all the mandatory channels for the configured satellite in each pixel. No results are produced for pixels where one or more channels are missing. The NWCSAF library reads BTs from real satellite files and extracts the region to process. The real satellites files for the image to process must be located by the user in `$SAFNWC/import/Sat_data` .

In this version, the IR BTs in region 9.7 μm is only used to estimate the ozone profile using non-linear regressions if the user activates the TOZ calculation. But it is a mandatory IR channel.

In the version 2018 GEO-iSHAI code, BTs of IR channels in regions 8.7 or IR3.9 μm are not used. See the Algorithm Theoretical Basis Document [RD.2] for details.

4.1.3 Cloud Mask (GEO-CMA).

GEO-iSHAI is only generated in clear sky pixels. A cloud mask is a mandatory input to GEO-iSHAI. The Cloud Mask product for the region and slot must exist 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.

The Cloud Mask netCDF file for the satellite, image and the region to process must be located in `$SAFNWC/export/CMA` directory.

4.1.4 Background NWP GRIB files.

Background numerical weather prediction GRIB files from *t+00* to *t+24* hour forecast are needed as another input. These NWP data need to be spatially, temporally and vertically interpolated to get NWP data collocated with real satellite data. Since it is not adequate to provide specific error matrices, EOFs, regression coefficients, etc for the great number of combination in user pressure levels, the interpolation of different NWP model to 54 RTTOV-11.2 pressure levels is performed.

The selection of P mode or HYB mode is a GEO-iSHAI configurable parameter. Users can choose between mode P or HYB editing in the GEO-iSHAI configuration file the keyword `NWP_EXEC_MODE`.

In the case of executing GEO-iSHAI in P mode: This is the default mode to maintain continuity with others products of the NWC/GEO package. The same NWP GRIB files at fixed pressure levels used by other products can be used. This fixed pressure levels GRIB files are fully supported and managed by the NWCLIB software.

The spatial interpolation and the calculation of the specific humidity from relative humidity are made outside the GEO-iSHAI code with the tools existing in the NWCLIB of NWC/GEO package. This step is made executing the *AllMappingNWP* tool interactively or is made automatically on real time by the NWC SAF's Task Manager. This is made using the usual NWC/GEO management of NWP:

> ➢ Users select their preferred NWP model to be used as input using the `$SAFNWC/config/nwp_conf_file`

> ➢ When executing *AllMappingNWP* tool or *MappingNWP* tool with cfs file, it is executed the spatial interpolation and generation of derived parameter for all keywords `NWP_PARAM` in all the product configuration files included in all the cfr files of the cfs file.

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> ➢ In the case of the GEO-iSHAI configuration files the NWP_PARAM keywords are:

```
NWP_PARAM NWP_T        1   BLI
NWP_PARAM NWP_Q        1   BLI
NWP_PARAM NWP_OZ       1   BLI
NWP_PARAM NWP_SP       1   BLI
NWP_PARAM NWP_ST       1   BLI
NWP_PARAM NWP_SGEOP    1   BLI
NWP_PARAM NWP_2T       1   BLI
NWP_PARAM NWP_2Q       1   BLI
```

The parameter requested are: T, q and optionally Ozone profiles, surface pressure, Skin Temperature, surface geopotential, NWP topography and 2 metres T and q. The third and fourth arguments mean that all the fields are requested at satellite resolution using bilinear interpolation.

As the fixed pressure levels GRIB files contain relative humidity profile 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 relation to TOZ it must be taken into account that: if users want TOZ they must activate fixing to 1 the keyword TOZ_CALCULATION and the GRIB files must include ozone profile.

Temporal interpolation is made at user supplied NWP pressure levels between previous and following available NWP files close to the time of the image. It is made using functions of the NWCLIB library.

The NWP GRIB files must be located in *$SAFNWC/import/NWP_data* with names:

S_NWC_NWP_*YYYY-MM-DD***T***hh*:mm:00Z_*FFF*.grib

where: *FFF* is the number of hours ahead of the forecast ($t+FFF$)

This way GEO-iSHAI is able to use background NWP GRIB files with any number and distribution of fixed pressure levels if they can be managed by the NWC/GEO software packages. Then GEO-iSHAI 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 really 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.

As it can be concluded from the reading of the Validation Report [RD.1], it is strongly recommended to users to provide as many fixed pressure levels with the most uniform and widest vertical distribution as he can provide from the selected NWP model to feed the NWC/GEO package.

In the case of executing GEO-iSHAI in HYB mode: In the case of GEO-iSHAI release 2018, ECMWF GRIB files on hybrid levels could be also used as inputs.

GEO-iSHAI allows the use of ECMWF GRIB files on hybrid levels as background NWP input. In this case the keyword NWP_EXEC_MODE is fixed to **HYB** in the configuration file (cfm extension)

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 to the time of the image, makes the vertical interpolation on ECMWF position to the 54 RTTOV-11.2 pressure levels, makes the temporal interpolation to the date of the image and finally makes the spatial interpolation just over clear air processed FOR.

The hybrid levels GRIB files must be located in *$SAFNWC/import/NWP_data* with names:

S_NWC_NWP**-Hyb_***YYYY-MM-DD***T***hh*:mm:00Z_*FFF*.grib

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Since the specific humidity profile is read from the ECMWF GRIB files on hybrid levels the conversion from relative humidity to specific humidity is not needed.

If activated the TOZ calculation (keyword `TOZ_CALCULATION`), also the ozone profile is needed.

As it can be concluded from the Validation Report [RD.1], it is strongly recommended to the users to provide as many fixed pressure levels as possible with the most uniform and widest vertical distribution from the selected NWP model to feed the NWC/GEO package. Thus, if possible it is recommended the use of GRIB files on hybrid levels for feed GEO-iSHAI.

As in PGE13 SPhR v2013 and GEO-iSHAI version 2016, GEO-iSHAI version 2018 allows the use of ECMWF GRIB files in hybrid levels when executing in HYB mode. In the case of ECMWF the list of parameters needed to request to MARS for ECMWF GRIB files on hybrid levels is:

Field	MARS code	levels
T	130	Number of Hybrid levels
q	133	Number of Hybrid levels
lnsp	152	1st Hybrid level
skt	235	surface

As an attempt to get experience and the user's feedback, in release 2018 the identification codes 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. Thus, it is also possible to use as input GRIB files on hybrid levels with NWP models on regular representation (equidistant lon-lat) configuring in GEO-iSHAI configuration files the codes of section 1 of GRIB header to identify T, q, O_3, SKT and P_{sfc} fields. It is also needed that users hybrid GRIB files have the half levels coefficients in every grid as in the ECMWF hybrid GRIB files. For this reason it has been added the below keywords `NWP-HYB_??` in the GEO-iSHAI configuration file. As one example, the keywords for the hybrid levels ECMWF GRIB files are:

```
NWP-HYB_T        T       130
NWP-HYB_Q        q       133
NWP-HYB_OZ       o3      203
NWP-HYB_ST       skt     235
NWP-HYB_SP       sp      152
NWP-HYB_GEOP     z       129
```

The feedback of the users is expected in order to improve for future versions.

Note: GRIB files on fixed pressure levels are always needed in order to execute CMA before execution of GEO-iSHAI code.

4.1.5 Geographical files from NWCSAF functions.

Longitude, latitude and satellite zenith angles associated to selected region are computed on real time by functions available on the NWCSAF library.

As many NWC SAF PGEs need this geographical information, NWCLIB computes and archives it on `$SAFNWC/tmp` binary files avoiding to repeat the calculation. If these files are erased or a new region is needed, new binary files are created automatically by the first PGE that needs them.

4.2 DESCRIPTION OF COEFFICIENTS FOR GEO-ɪSHAI

The GEO-iSHAI coefficients files are described here together with a brief summary of some characteristics that the user must know and take into account for proper operation of the GEO-iSHAI. The scientific aspects about how these coefficients files were obtained can be seen in the ATBD [RD.2].

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4.2.1 BT bias correction coefficients.

The real satellite measurements must be bias-adjusted to account for the bias between the satellite observation and the synthetic radiative transfer model BTs.

In NWC/GEO package, 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 use this common BT bias correction coefficients and functions to get the optimal BT bias corrections and then applies them to the real satellite BTs before they are 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.

4.2.2 GEO-iSHAI First-Guess regression coefficients files

These files contain the non-linear regression coefficients used to generate the First Guess from the Background NWP fields and the bias corrected satellite IR BTs (see ATBD [RD.2]).

Also contain the non-linear regression coefficients used if activated by the users to generate the statistical retrieval of ozone profile to calculate the TOZ and diff_TOZ parameters.

The names of the files can be configured editing in the GEO-iSHAI configuration file the keywords `FG_reg_*_filename`.

Although the users can specify any valid file name, the NWC SAF will use the following naming convention for the distribution of the FG coefficients files. The default name is composed of:

> **FG_reg**_*parameter*_**GEO_iSHAI_v2018_rttov11**_*satid*_**date**_*<month><year>*.**bin**

Where:

> *parameter* is the name of the predictand parameter. By default can be *T* or *logq* or *logOzone* or *SKT*.

> *satid* is the name of satellite. By default in the coefficients file supplied by the NWC SAF can be *msg*, for SEVIRI, *AHI* or *ABI*. As example if *satid* is *msg* that indicates that have been calculated with synthetic RTTOV-11.2 BTs for MSG satellites.

> As example, in release 2018 the default values of FG coefficients file for MSG are:

keyword	Default name FG non-linear regression coefficients file
FG_reg_T_filename	FG_reg_T_GEO_iSHAI_v2018_rttov11_msg_date_sep2018.bin
FG_reg_logq_filename	FG_reg_logq_GEO_iSHAI_v2018_rttov11_msg_date_sep2018.bin
FG_reg_logOzone_filename	FG_reg_logOzone_GEO_iSHAI_v2018_rttov11_ms3_date_sep2018.bin
FG_reg_SKT_filename	FG_reg_SKT_GEO_iSHAI_v2018_rttov11_msg_date_sep2018.bin

> *<month><year>* is the string with the month and year of the distribution of the coefficient file and it indicates a reference date to identify the FG regression coefficient file.

The FG coefficients files must be located at *$SAFNWC/import/Aux_data/iSHAI*

The files contain regression coefficients for every zenith degree between 0º to 75º. There is a regression for each one of the output variables and every satellite zenith angle from [0º, 75º]. Since the number of RTTOV-11.2 RTTOV pressure levels is 54 then the number of regressions inside the T, logq and logozone coefficients file is 76x54.

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In the case of `FG_reg_SKT_filename` there are just 76 regressions every satellite zenith angle from [0º, 75º].

Keyword	Dimensions			
	Number zenith angles	Number of levels	Number of predictors	Number of bytes
`FG_reg_T_filename`	76	54	$(n_{channels}*2+3+54*2+1+1)$	4
`FG_reg_logq_filename`	76	54	$(n_{channels}*2+3+54*2+1+1)$	4
`FG_reg_logOzone_filename`	76	54	$((n_{channels}+1)*2+3+54*3+1+1)$	4
`FG_reg_SKT_filename`	76	1	$(n_{channels}*2+3+54*2+1+1)$	4

$n_{channels}$ is the number of IR channels used in the regressions. In the case of MSG satellites $n_{channels}$ is 5. In the case of Himawari or GOES-R class satellite the "$n_{channels}$" is 7.

In the case of `FG_reg_logOzone_filename` the number of predictors is different because is used also as inputs an IR channel in the 9.7 μm region and the logarithm of the background NWP ozone profile.

All the coefficients files are binary files with Float (4 bytes).

The predictors for each regression can be seen in Eq.1 and Eq.2 of the ATBD [RD.2].

The FG regressions coefficients are the same for P and HYB mode.

4.2.3 GEO-iSHAI Empirical Orthogonal functions (EOF)

As it's explained in the ATBD [RD.2], in the GEO-iSHAI algorithm the minimisation of the error between the real satellite BTs and the synthetic RTTOV BTs is made in the Empirical Orthogonal Functions (EOF) or Principal Components space.

The name of the file that contains the EOFs coefficient file appears in the GEO-iSHAI configuration file and can be configured editing in the GEO-iSHAI configuration file the keyword `EOF_FILENAME`.

Although the users can supply their own EOF coefficient file and specify any valid file name, the default name in version 2018 is:

Keyword	Default name of EOF coefficients file
`EOF_FILENAME`	`EOF_iSHAI_v2018_date_sep2018.bin`

The EOF file must be located in `$SAFNWC/import/Aux_data/iSHAI` directory.

Each EOF file is a float (4 bytes) array of (2*54+1) x (2*54+1) dimensions (47524 bytes).

The order is 2*54+1 elements of first EOF, then the 2*54+1 elements of the second EOF, and so on. In version 2018 in the default distributed EOF coefficients the order on the EOFS has been reorder in order to have first the 3 main EOFs for T, second the 3 main EOFs for Log(q) and then the 1 EOF for SKT.

4.2.4 GEO-iSHAI background NWP inverse covariance matrix B⁻¹

As it's explained in the ATBD [RD.2], the statistical error of the background is represented by the matrix B in the GEO-iSHAI algorithm. In the GEO-iSHAI version 2018, B^{-1} matrix has been computed with the available GEO-iSHAI training and validation dataset with the 2017 year ECMWF model outputs with the covariance error of *t+12* forecast and *t+00* analysis for T and log(q) profiles and skin temperature.

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The name of the file that contains the B^{-1} matrix (inverse covariance matrix) coefficient file appears in the GEO-iSHAI configuration file and can be configured editing in the GEO-iSHAI configuration file the keyword `Binverse_covariance_matrix_filename`.

The default B^{-1} matrix file name in version 2018 is: `Binv_iSHAI_v2018_date_sep2018.bin`

The file is a binary file of 109 x 109 dimensions of floats (4 bytes).

The file with the inverse covariance matrix is located in `$SAFNWC/import/Aux_data/iSHAI` directory. Its size is `47524` bytes `(54*2+1)x(54*2+1)x4`

4.2.5 GEO-iSHAI observation error inverse covariance matrix E^{-1}

As it's explained in the ATBD [RD.2], the errors of the observed brightness temperatures and the errors of the radiative transfer model are represented by the matrix **E** in the GEO-iSHAI algorithm. In GEO-iSHAI 2018 version, E^{-1} matrix has been computed with the available GEO-iSHAI training and validation dataset with ECMWF model outputs.

The name of the file that contains the E^{-1} coefficient file appears in the GEO-iSHAI configuration file and can be configured editing in the GEO-iSHAI configuration file the keyword:

    `Einverse_covariance_matrix_filename`

Since the number of IR channels used in GEO-iSHAI depends on the satellite class, there are default E^{-1} coefficient files for each satellite class. Although the users can supply their own E^{-1} coefficient files and specify any valid file name, the default name in version 2018 are:

Keyword	Default name of EOF coefficients file	Satellite class	bytes
`Einverse_covariance_matrix_filename`	`Einv_iSHAI_v2018_msg_date_sep2018.bin`	MSG	5*5*4
`Einverse_covariance_matrix_filename`	`Einv_iSHAI_v2018_AHI_date_sep2018.bin`	Himawari	7*7*4
`Einverse_covariance_matrix_filename`	`Einv_iSHAI_v2018_ABI_date_sep2018.bin`	GOES-R	7*7*4

Since the generation of GEO-iSHAI training validation datasets from AHI and ABI instruments is being made the initial E^{-1} matrix in GEO-iSHAI version 2018 has been calculated with a limited period but it will be improved and distributed later on the NWC SAF web.

The coefficient files with the E^{-1} matrix are located in `$SAFNWC/import/Aux_data/iSHAI` directory.

4.2.6 Surface IR emissivity atlas files.

In NWC/GEO package version 2018, monthly emissivity atlases are considered as common coefficients available for all the products and specific files and functions in the NWCLIB to access to them are available.

GEO-iSHAI uses these common emissivity atlases and functions to get the emissivity values on land pixels. Precomputed monthly emissivity atlases for each channel of the NWC/GEO satellites are generated from the 2007 IREMIS dataset (See *http://cimss.ssec.wisc.edu/iremis/*) RTTOV-11.2 emissivity atlases. There are monthly emissivity atlas for every IR channel, supported GEO satellite position (example in case MSG: 0º for operational satellite, 9.5º E for Rapid Scan satellite and 41.5º E for MSG-1 in IDOC mission) and for every month.

4.2.7 RTTOV-11.2 coefficients

GEO-iSHAI software strongly relies on a clear sky fast and accurate radiative transfer model. In our case, RTTOV-11.2 software from EUMETSAT NWPSAF is used. RTTOV-11.2 is part of the COTS software installed in the NWC/GEO package installation.

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4.2.8 Ancillary files sets.

The elevation mask remapped onto geostationary satellite image projections is an ancillary file needed to run GEO-iSHAI. The elevation data are used to distinguish between land and sea pixels (sea pixels are those whose elevation value is equal to missing code). Then, in the case of land pixels the emissivity values are read from the emissivity files. Atlas and sea/land mask datasets covering the whole satellite disk in the default satellite projection at full satellite IR horizontal resolution are available within the NWC/GEO software package. They are extracted on the processed region by the GEO-iSHAI software using NWCLIB functions. There are elevation data for every supported GEO satellite position (example in case MSG: 0º for operational satellite, 9.5º E for Rapid Scan satellite and 41.5º E for MSG-1 in IODC mission).

4.3 LIST OF GEO-iSHAI CONFIGURABLE PARAMETERS

GEO-iSHAI has been designed in a highly modular manner and allows a user selectable configuration.

The user configurable parameters are determined through the GEO-iSHAI **model configuration file**. It is the third argument required by the GEO-iSHAI program. Thus, to change the configuration used to execute the GEO-iSHAI code is as easy as changing the third argument when the GEO-iSHAI is run.

Thus, the user can have several GEO-iSHAI model configurations files in the $SAFNWC/config and GEO-iSHAI can be executed on real time with different configurations depending on the region to process, the satellite, the hour of the image, etc. As an example, users can execute GEO-iSHAI on the full disk with a large FOR width and with only one iteration step or, on the other side, to execute GEO-iSHAI over a small region centred in the area of interest with small FOR width and with up to three iterations.

Also users could choose between P or HYB mode using the keyword NWP_EXEC_MODE

4.3.1 GEO-iSHAI Model Configuration File.

A GEO-iSHAI model configuration file contains all the coefficients and some constant values required by GEO-iSHAI software to run. It has by default the extension "*.cfm*". The model configuration file must be placed at the $SAFNWC/config directory.

Below are described all the keywords and the options allowed in the GEO-iSHAI configuration file. They have been grouped by meaning or functions. Also some considerations that the user must take into account to fix them for operational mode:

Keywords with operational or processing impact

- LSIZE_FOR and CSIZE_FOR: the default width of the FOR is 3. But the width of the FOR is configurable by the user.

  For example, changing the width of the FOR from 3x3 to 6x6, the process speed up in a factor of 4. The best resolution is obtained with 1x1 but the price could be the high execution time if the region is large.

- MAX_ITERATIONS number. It establishes the number iterations for one pixel. The default maximum number of iterations is three. Taking into account that in each one of the physical retrieval iterations is one CPU expensive routine, the decreasing of MAX_ITERATIONS can reduce the execution time.

- `BT_RMS_THRESHOLD` and `MAX_RESIDUAL` keywords. These keywords control the level of the desired error between the satellite bias corrected BTs and the synthetic RTTOV BTs.

  Inside GEO-iSHAI is calculated BT_RMS that is the error between the satellite bias corrected BTs and RTTOV BTs (calculated from the profile after FG regression step) at the non window channel (i.e. WV6.2, WV7.3 and IR13.4 in SEVIRI case and WV6.2, WV6.9, WV7.3 and IR13.3 in AHI or ABI case). The physical retrieval module is executed only if BT_RMS is greater than `BT_RMS_THRESHOLD`.

  The `MAX_RESIDUAL` keyword is the threshold used to stop the iteration process in the physical module. `MAX_RESIDUAL` is the allowed error between the satellite bias corrected BTs and the RTTOV BTs.

  Then, if `BT_RMS_THRESHOLD` is fixed to a high value, it speeds up the process because only the FG regression step is applied to a high percent of the FOR. If `BT_RMS_THRESHOLD` is fixed to a low value, the maximum iteration number is applied to a high percent of the FOR slowing the GEO-iSHAI execution (the most CPU expensive routine is RTTOV_K and it is called inside the physical retrieval module).

  Thus, If `BT_RMS_THRESHOLD` is fixed to a low value and if `MAX_RESIDUAL` is fixed to a very low value (example 0.0001) and the number of iterations is fixed to 3, the physical retrieval process will be executed always for every clear FOR and the execution time can increase enormously.

  For an optimal election, the analysis of the histogram the error between the biases corrected satellite bias corrected BTs and the RTTOV BTs could be used; as example, it has been calculated for the ECMWF model in [RD.2].

- `ZENITH_THRESHOLD` Only pixels with satellite zenith angle below or equal to `ZENITH_THRESHOLD` value are processed. Although the FG regressions coefficients are available between [0, 75º] are only validated between [0º, 70º]. For this reason the default value of `ZENITH_THRESHOLD` is 70.

- `BAND_CLOUDY` Over cloudy pixels, one IR BT channel degraded to 7 bits (range [0 − 127]) value is stored as a field in the iSHAI netCDF output file. This field will be later used to generate adequate images in which cloudy pixels are grey scaled and clear pixels are colour scaled. By default is configured the cleanest IR window channel in each satellite.

  In the MSG (SEVIRI) case the default is 16 that means IR10.8 channel.

  In the Himawari (AHI) or GOES-R class case the default is 15 that means IR channel in the 10.4 μm region.

- `FOR_METHOD` This keyword sets the method to calculate the BTs of the FOR. There are two possibilities:

  a) If value is 1 then BT of the FOR is calculated using the mean of all clear pixels. **This is the default value.**

  b) If value is 2 then BT of the FOR is filled with the BTs at the warmest clear pixel in the cleanest IR window channel (IR10.8 in SEVIRI case and IR10.4 in AHI or ABI case).

- `POST_PROC_METHOD` This keyword controls the way that the clear pixels filling inside the FOR is made.

  The default value is 1 and the default method is to copy the same value to all clear pixels in the FOR.

  The other option (value 0) is to write the output only at the clear pixel position.

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This means at the warmest clear pixel in the cleanest IR window channel (IR10.8 in SEVIRI and IR10.4 in AHI or ABI) in case FOR_METHOD is 2 or the centre in FOR_METHOD is 1.

- SAVE_PROFs_in_BINARY_files and SAVE_iSHAI_in_BINARY_file

These keywords control the activation of the optional writing of the GEO-iSHAI binary files. See section 2.3.3 for details.

- TOZ_CALCULATION This keyword makes the activation of calculation of TOZ if fixed to 1.

The default value 0 means that no TOZ calculation is made.

If calculation of TOZ is activated, that implies that the background NWP GRIB files must contain ozone data at same levels that T and humidity profiles.

Keywords with names of coefficients files

- The name of all coefficients files are keywords in the configuration files. Thus, to change a coefficient file it is only needed to change the name of the coefficient file in the model configuration file. The list of the configurable coefficients files is in the table below:

Default configurable coefficients files for MSG satellites in version 2018	
keyword	**Default name of FG non-linear regression coefficients files**
FG reg T filename	FG_reg_T_GEO_iSHAI_v2018_rttov11_msg_date_sep2018.bin
FG reg_logq filename	FG_reg_logq_GEO_iSHAI_v2018_rttov11_msg_date_sep2018.bin
FG reg logOzone filename	FG_reg_logOzone_GEO_iSHAI_v2018_rttov11_msg_date_sep2018.bin
FG reg SKT filename	FG_reg_SKT_GEO_iSHAI_v2018_rttov11_msg_date_sep2018.bin
EOF FILENAME	EOF_iSHAI_v2018_date_sep2018.bin
Binverse_covariance_matrix_filename	Binv_iSHAI_v2018_date_sep2018.bin
Einverse covariance matrix filename	Einv_iSHAI_v2018_msg_date_sep2018.bin

Default configurable coefficients files for Himawari satellites in version 2018	
keyword	**Default name of FG non-linear regression coefficients files**
FG reg T filename	FG_reg_T_GEO_iSHAI_v2018_rttov11_AHI_date_sep2018.bin
FG reg logq filename	FG_reg_logq_GEO_iSHAI_v2018_rttov11_AHI_date_sep2018.bin
FG reg logOzone filename	FG_reg_logOzone_GEO_iSHAI_v2018_rttov11_AHI_date_sep2018.bin
FG reg SKT filename	FG_reg_SKT_GEO_iSHAI_v2018_rttov11_AHI_date_sep2018.bin
EOF FILENAME	EOF_iSHAI_v2018_date_sep2018.bin
Binverse_covariance_matrix_filename	Binv_iSHAI_v2018_date_sep2018.bin
Einverse covariance matrix filename	Einv_iSHAI_v2018_AHI_date_sep2018.bin

Keyword to choose between NWP on fixed pressure levels GRIBs or hybrid levels GRIBs

- NWP_EXEC_MODE The selection of the type vertical representation of GRIB files used as background NWP and then parameters, vertical levels and spatial interpolation is fixed by this keyword. The options are (P) GRIBs at fixed pressure levels or (HYB) GRIB at hybrid levels. The default is P mode but better results are with HYB mode. See Section 4.1.4 for details.

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Keywords with options for hybrid levels GRIBs

- Keywords for establishing the grids to be read by GEO-iSHAI when executed in HYB mode. These keywords are only needed in the case to use as background NWP hybrid levels GRIB files. See full details in Section 4.1.4. These keywords in the case of ECMWF are:

```
NWP-HYB_T          t      130
NWP-HYB_Q          q      133
NWP-HYB_OZ         o3     203
NWP-HYB_ST         skt    235
NWP-HYB_SP         sp     152
NWP-HYB_GEOP       z      129
```

Keywords with options for fixed pressure GRIBs

- Keywords for establishing the parameters to be remapped and the generation of specific humidity profile when the AllMappingNWP tool is executed. These keywords are only needed in the case of using as background NWP fixed pressure levels GRIB files. See full details in Section 4.1.4. These keywords are:

```
NWP_PARAM NWP_T       1  BLI
NWP_PARAM NWP_Q       1  BLI
NWP_PARAM NWP_OZ      1  BLI
NWP_PARAM NWP_SP      1  BLI
NWP_PARAM NWP_ST      1  BLI
NWP_PARAM NWP_SGEOP 1  BLI
NWP_PARAM NWP_2T      1  BLI
NWP_PARAM NWP_2Q      1  BLI
```

As summary, the user must establish a compromise between the computer resources (CPU speed and memory) where the NWC/GEO package will be operated, the region (or regions) to process and the configurable keywords (number of iterations, BT_RMS_THRESHOLD and MAX_RESIDUAL keywords and width of the FOR) in the GEO-iSHAI model configuration.

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5. GEO-ISHAI PRODUCT 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 from hybrid GRIB files.

5.1 GEO-ISHAI PRODUCT ASSUMPTIONS AND LIMITATIONS

5.1.1 Assumptions

(1) The surface pressure used in the GEO-iSHAI comes from the NWP model. The better resolution the surface pressure field is in the background NWP model 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.

5.1.2 Limitations

(1) GEO-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 mountainous regions with large difference between the topography and the NWP topography. The same happens in desert pixels, where the distance on skin temperature between the NWP first guess 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 from ECMWF 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, have improved clearly the quality of the GEO-iSHAI outputs. The GEO-iSHAI HYB mode outputs that uses ECMWF GRIB files on hybrid levels improves the quality. **It is strongly recommended to feed GEO-iSHAI 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 NWP background 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.

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6. EXAMPLES OF GEO-ISHAI VISUALISATION

Graphic displays of GEO-iSHAI product parameters generated at the AEMET NWCSAF/MSG Reference System area are available on real-time in the web site 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*).

In release 2018, the format of the file is netCDF and GEO-iSHAI outputs are not image like fields and they are data fields. Because of this, it is the responsibility of the user to use adequate tools to generate images. Among others, there are some free available tools as McIDAS-V or IDV or HDF-View that can do this using just the GEO-iSHAI netCDF files.

To complete the image on cloudy pixels, and avoid black holes in the images, the BT from the cleanest channel in the IR window has been added to GEO-iSHAI netCDF file. BTs from the cleanest channel in the IR window have been scaled in order to store it in 7 pixels, after scaling, and the values are in the range [0-127] only in cloudy pixels determined by the cloud mask (GEO-CMA product).

As one example, the process with a generic tool to generate an image as the ones shown in Figures 4 to 7 could be the following:

> ➢ open the netCDF file
>
> ➢ read or click over a field parameter
>
> ➢ adjust the range and assign a color palette
>
> ➢ read or click the scaled BT the cleanest channel in the IR window to be displayed on the black holes of cloudy pixels.

In the case of McIDAS-V, the mechanism to represent in a color palette the clear air pixels, and as grey, the cloudy pixels is based in to using a color palette for the parameters shown on clear pixels and to use a gray color palette on cloudy pixels and all pixels where the value is equal to missing code are considered transparent.

In other tools a mechanism to generate separately the clear and cloudy images with different value ranges and fixing to a reserved low value, the missing data value and combine it using a combined color palette with color for clear air range value and grey for cloudy range value could be needed.

Example of MSG satellite visualization

The images corresponding to the 10th August 2016 at 12UTC from SEVIRI on MSG-3 are shown as an example in the Figures 4 to 9. The images have been generated with GEO-iSHAI v4.0 algorithm. One of the best ways to exploit the water vapour and the stability indices generated by GEO-iSHAI software is to take advantage of the high spatial and temporal resolution of GEO satellites and to use loops of images to monitor their evolution.

Graphic displays of GEO-iSHAI product generated at the AEMET NWCSAF/MSG Reference System area will be available on real-time in the web site of the NWC SAF Help Desk (http://nwc-saf.eumetsat.int).
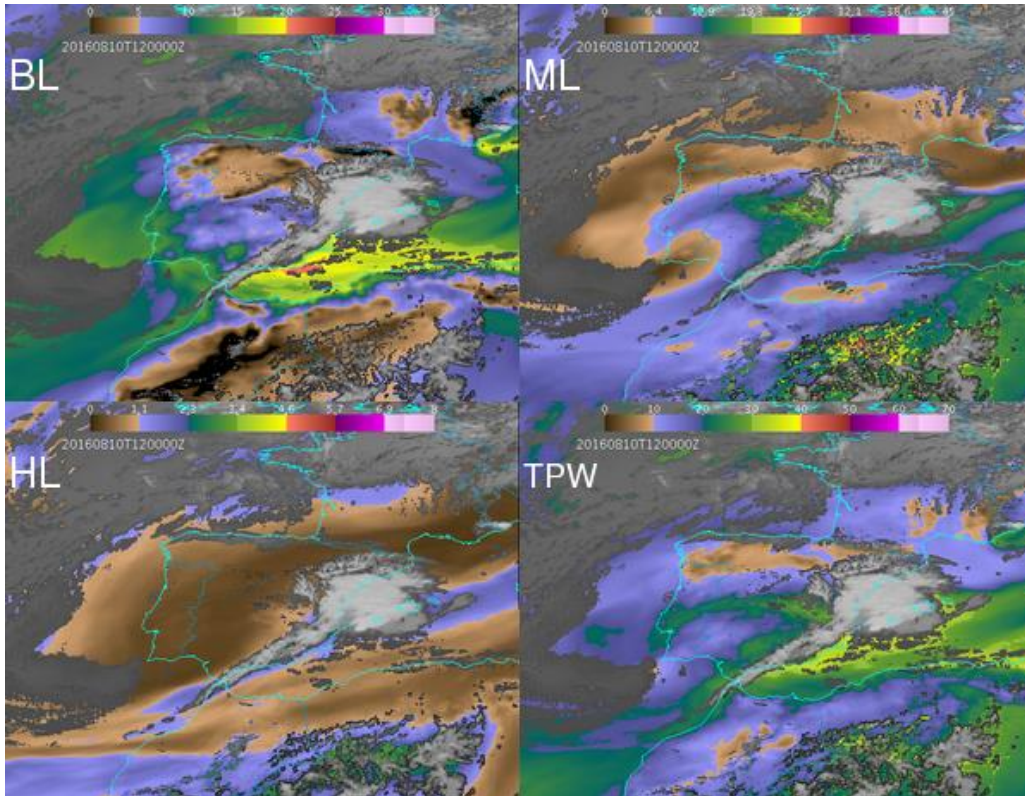
Figure 4: Example of GEO-iSHAI BL, ML, HL and TPW from 12 UTC on 10 August 2016 produced from SEVIRI on MSG-3.

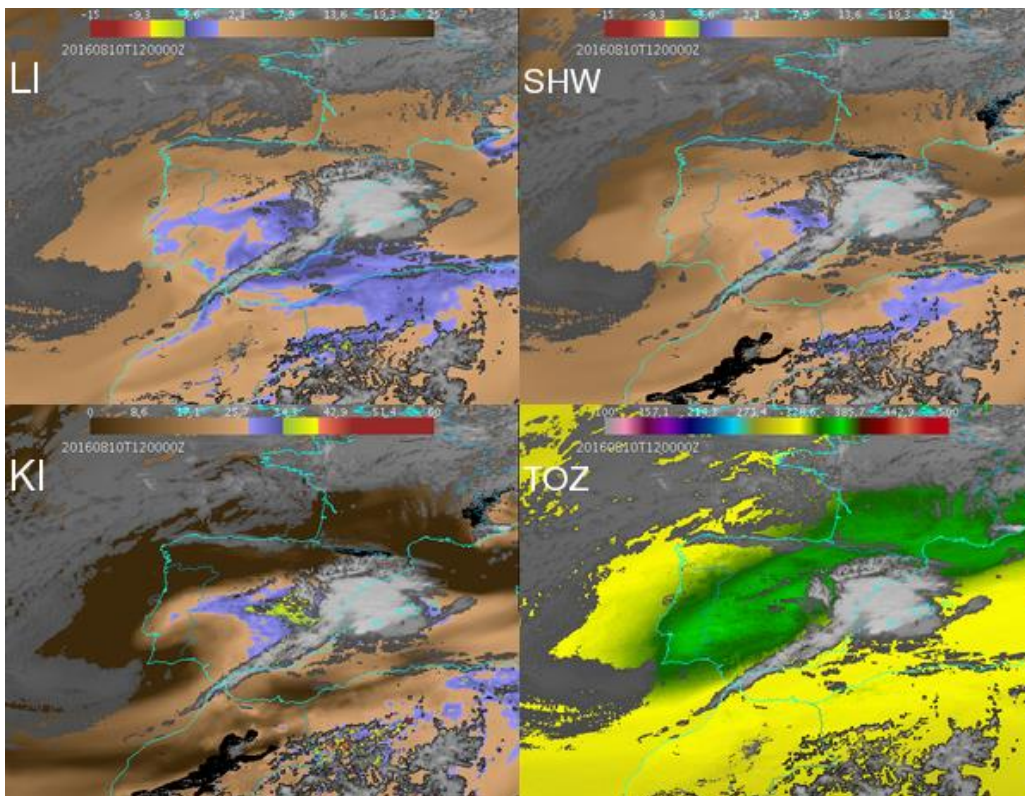*Figure 5: Example GEO-iSHAI LI, SHW, KI and TOZ from 12Z 10 August 2016 produced from MSG-3.*
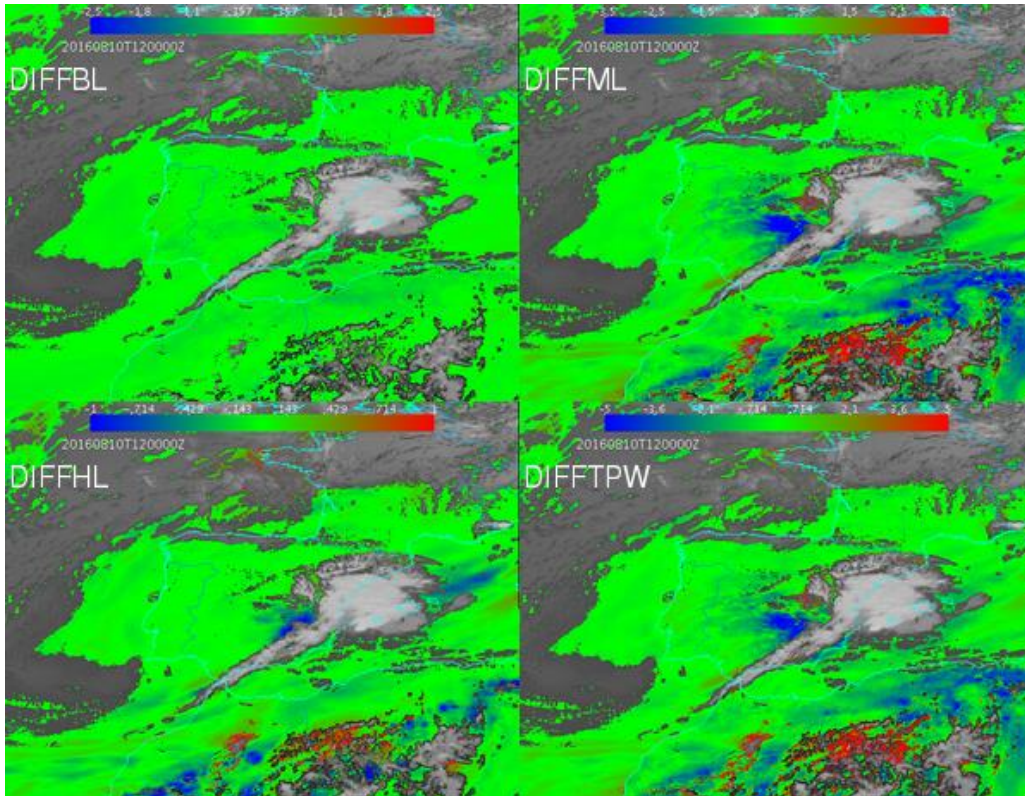
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Figure 6: Example GEO-iSHAI diffBL, diffML, diffHL and diffTPW from 12z on 10 August 2016 produced from MSG-3.
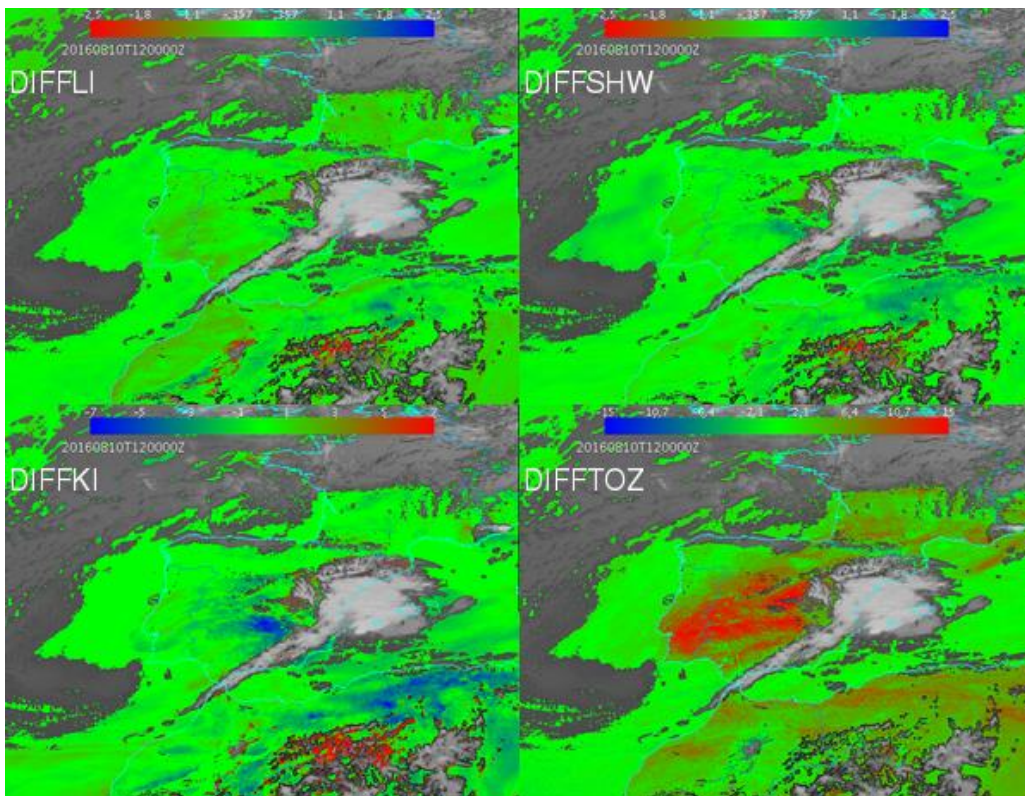
Figure 7: Example of GEO-iSHAI diffLI, diffSHW,diffKI and diffTOZ from 12 UTC on 10 August 2016 produced from MSG-3.

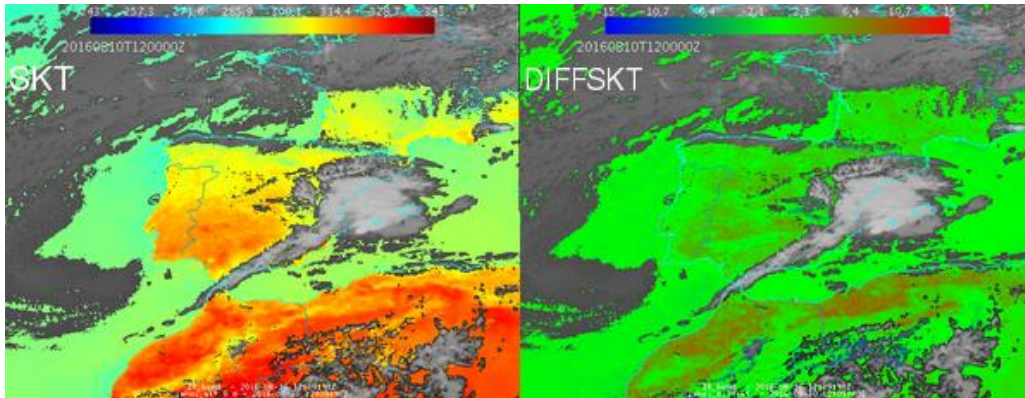|	User Manual for iSHAI Product Processors of the NWC/GEO: Science Part	**Code:** NWC/CDOP3/GEO/AEMET/SCI/UM/iSHAI
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Figure 8: Example of GEO-iSHAI SKT and diffSKT 12 UTC on 10 August 2016 produced from MSG-3.
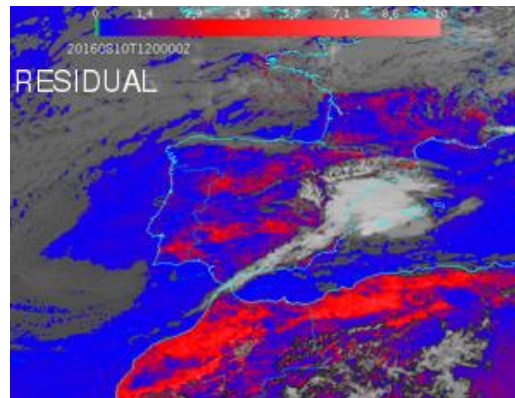
Figure 9: Example GEO-iSHAI residual from 12Z on 10 August 2016 from SEVIRI on MSG-3.

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.

Example of Himawari satellite visualization

The images corresponding to the 31 December 2017 at 12UTC from AHI instrument on Himawari-8 are shown as an example in the Figures 10 and 11.

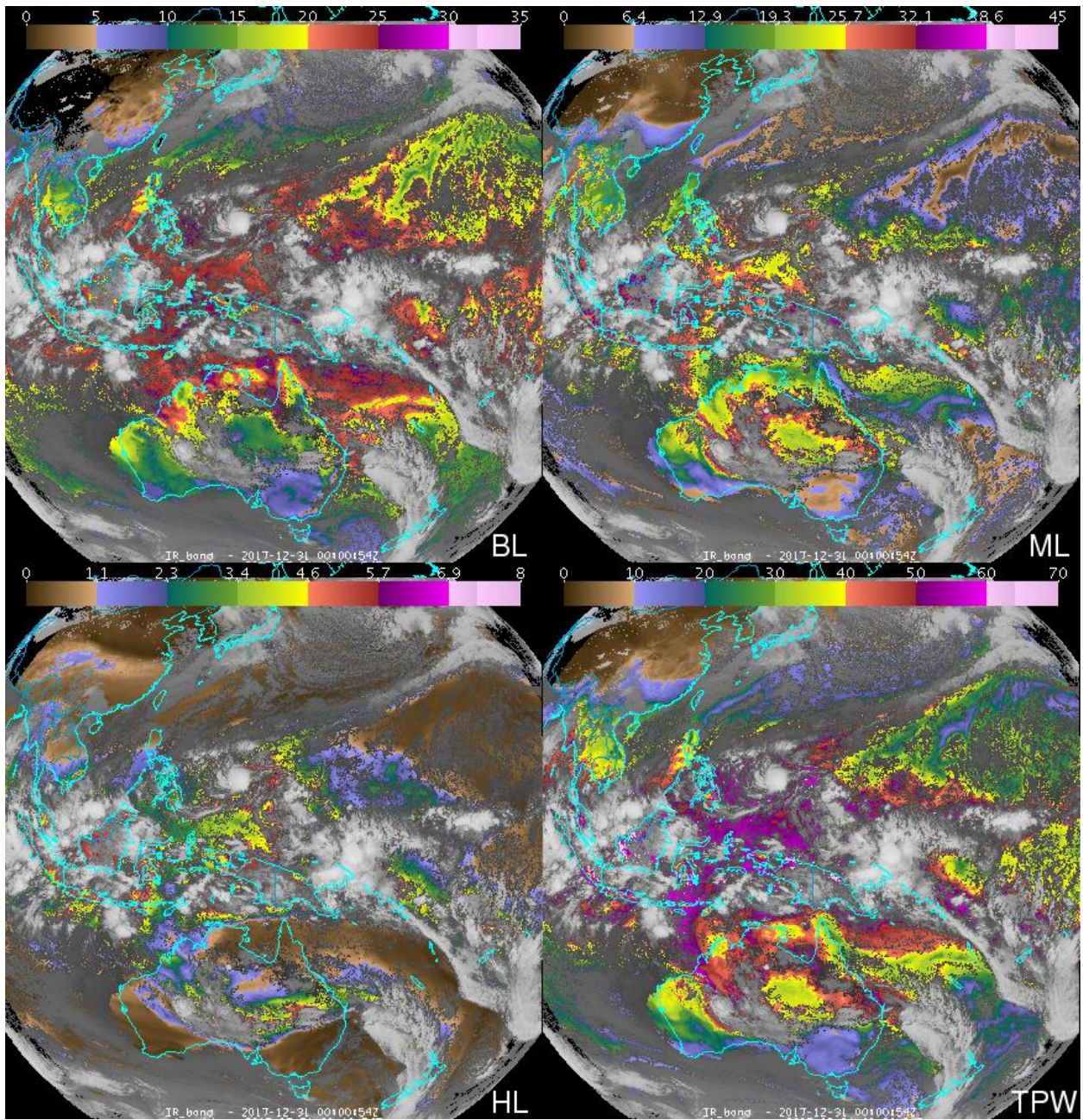|	User Manual for iSHAI Product Processors of the NWC/GEO: Science Part	**Code:** NWC/CDOP3/GEO/AEMET/SCI/UM/iSHAI
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Figure 10: Example of GEO-iSHAI BL, ML, HL and TPW from 12 UTC on 31 December 2017 produced from AHI on Himawari-8.

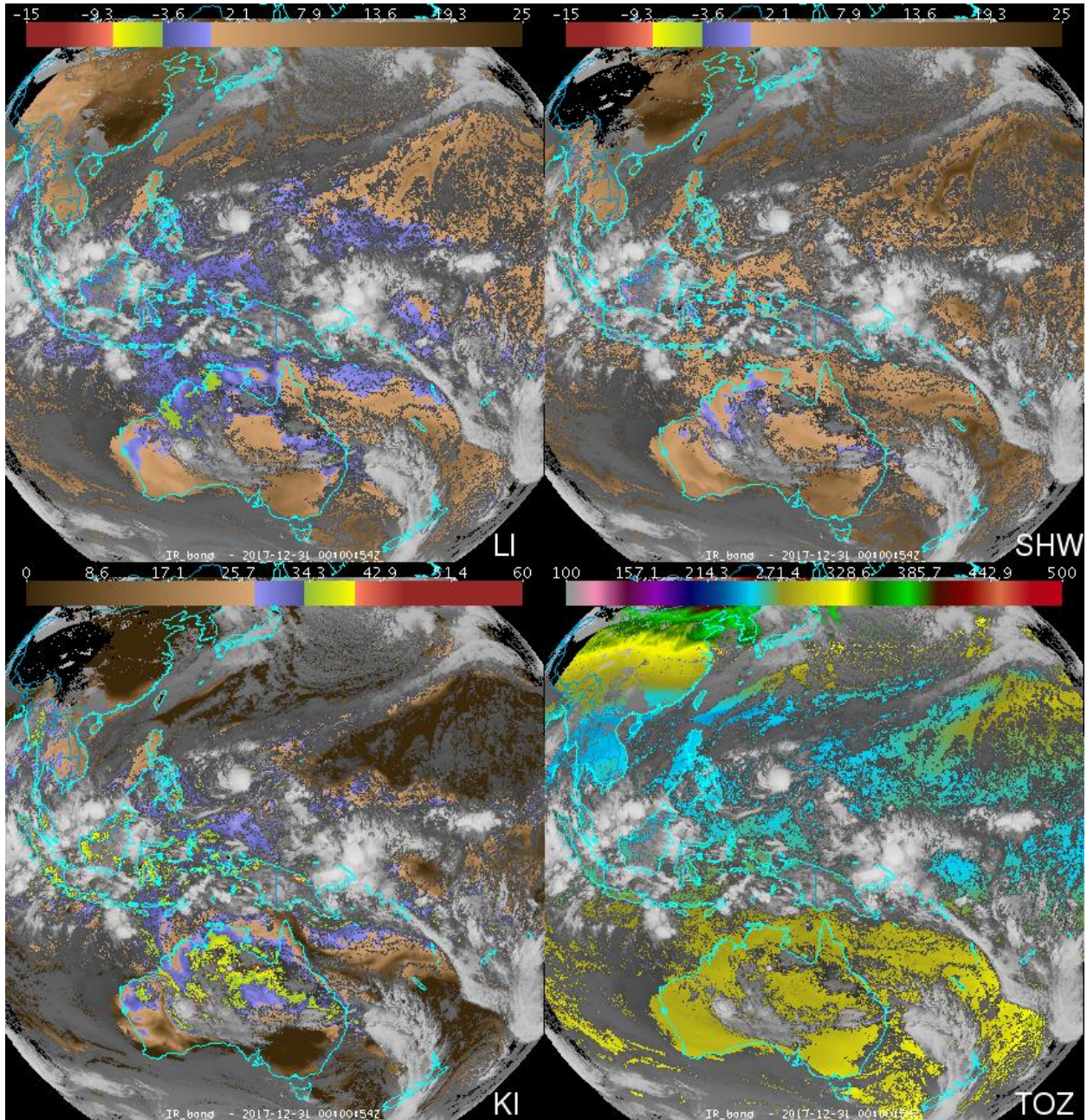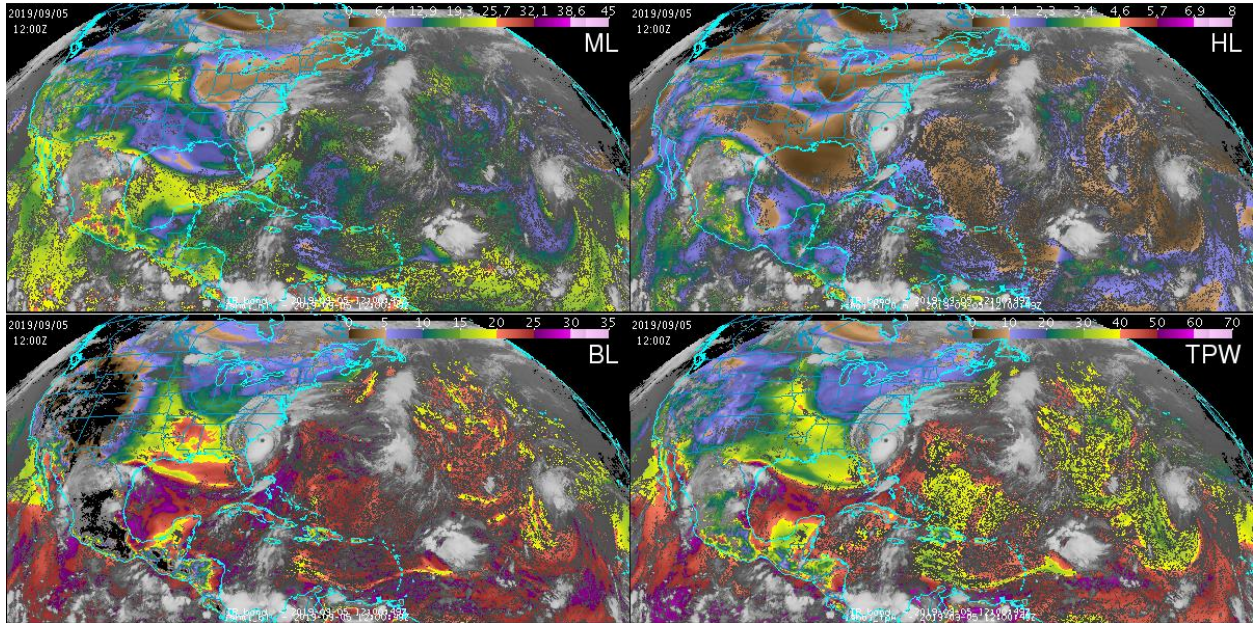|	User Manual for iSHAI Product Processors of the NWC/GEO: Science Part	**Code:** NWC/CDOP3/GEO/AEMET/SCI/UM/iSHAI
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Figure 11: Example of GEO-iSHAI LI, SHW, KI and TOZ from 12 UTC 31 December 2017 produced from AHI on Himawari-8.

Example of GOES-R class satellite visualization

The images corresponding to the 5th September 2019 at 12UTC from ABI instrument on GOES-16 are shown as an example in the Figures 12 and 13. Hurricane Dorian off the Carolinas coasts and TS Gabrielle on the Atlantic can be seen.

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Figure 12: Example of GEO-iSHAI BL, ML, HL and TPW from 12 UTC on 5 September 2019 produced from ABI on GOES-16.
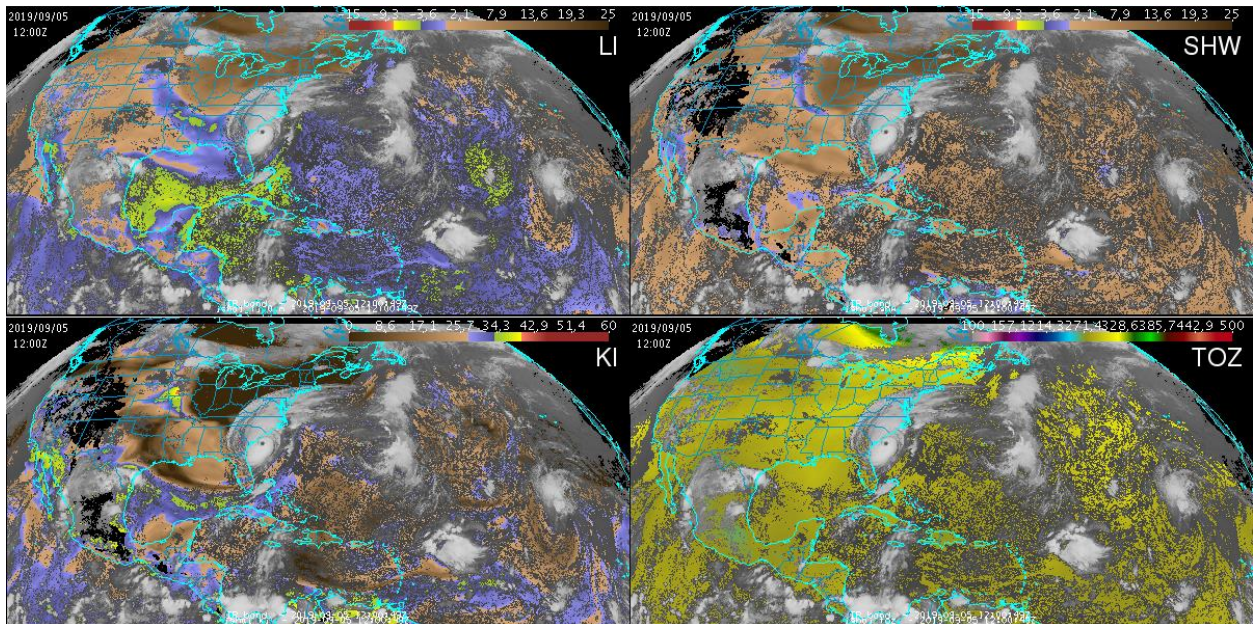
Figure 13: Example of GEO-iSHAI LI, SHW, KI and TOZ from 12 UTC on 5 September 2019 produced from ABI on GOES-16.

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