

 	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 1/47</p>
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Algorithm Theoretical Basis Document for the Clear Air Products Processor of the NWC/GEO

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

15 October 2016

Applicable to GEO-iSHAI v3.0 (NWC-031)

Prepared by Agencia Estatal de Meteorología (AEMET)

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REPORT SIGNATURE TABLE

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DOCUMENT CHANGE RECORD

Version	Date	Pages	Changes
1.0d	<i>15 November 2015</i>	45	Draft version for NWC/GEO GEO-TqPh v3.0 for STRR
1.1	<i>15 October 2016</i>	47	Updated with STRR changes and renamed GEO-TqPH as GEO-iSHAI

Table of Contents

1. INTRODUCTION	7
1.1 PURPOSE AND SCOPE OF THE DOCUMENT	7
1.2 SOFTWARE VERSION IDENTIFICATION	7
1.3 IMPROVEMENTS FROM PREVIOUS VERSIONS	8
1.4 DEFINITIONS, ACRONYMS AND ABBREVIATIONS	9
1.5 REFERENCES	12
1.5.1 <i>NWC SAF Applicable Documents</i>	12
1.5.2 <i>Reference Documents</i>	12
2. GEO-ISHAI PRODUCT ALGORITHM	13
2.1 GEO-ISHAI PROCESSING OUTLINE	14
2.2 GEO-ISHAI ALGORITHM DESCRIPTION	17
2.2.1 <i>Use of Field of Regards (FOR)</i>	18
2.2.2 <i>NWP data Interpolation to 54 RTTOV-11.2 levels of NWP profiles</i>	21
2.2.3 <i>SEVIRI BT bias correction</i>	22
2.2.4 <i>Use regression as first guess</i>	22
2.2.5 <i>Mathematical Description of Physical Retrieval module</i>	24
2.2.5.1 Observed brightness temperatures (Y^m)	26
2.2.5.2 RTTOV-11.2 as radiative transfer model	26
2.2.5.3 Discrepancy principle for regularization parameter	27
2.2.5.4 Iteration checking and residual estimation	28
2.2.6 <i>Other considerations</i>	29
2.2.7 <i>Quality control</i>	29
2.2.8 <i>Post-processing</i>	29
2.2.8.1 Fill clear pixels of FOR with the calculated value	29
2.2.8.2 Writing of outputs on netCDF file	30
2.3 ALGORITHM INPUTS, COEFFICIENTS AND FILES	30
2.3.1 <i>Inputs</i>	31
2.3.1.1 SEVIRI BT	31
2.3.1.2 Cloud Mask (GEO-CMA)	31
2.3.1.3 Background NWP data	32
2.3.2 <i>Geographical data from NWCSAF functions</i>	32
2.3.3 <i>Coefficients</i>	32
2.3.3.1 BT bias correction coefficients	32
2.3.3.2 Regression coefficients to calculate First Guess profiles	32
2.3.3.3 The background error covariance matrix and first guess (B)	33
2.3.3.4 The observation error covariance matrix (E)	34
2.3.3.5 Empirical orthogonal Functions (EOF) representation for temperature and moisture profiles	34
2.3.3.6 RTTOV coefficients	35
2.3.3.7 Use of predetermined surface IR emissivity atlas	35
2.3.3.8 Ancillary data sets	36
2.3.3.9 GEO-iSHAI Model Configuration File	36
2.4 GEO-ISHAI OUTPUTS	36
2.4.1 <i>Main outputs: GEO-iSHAI netCDF files description</i>	36
2.4.2 <i>Optional binary files outputs</i>	37
2.4.3 <i>Examples of GEO-iSHAI visualisation</i>	38
3. PRACTICAL CONSIDERATIONS	41
3.1 PROGRAMMING AND PROCEDURAL CONSIDERATIONS	41
3.2 EXCEPTION HANDLING	41
3.3 ASSUMPTIONS	41
3.4 LIMITATIONS	41
3.5 IMPLEMENTATION OF GEO-ISHAI	42
3.5.1.1 The GEO-iSHAI installation step	42
3.5.1.2 The GEO-iSHAI preparation step	42
3.5.1.3 The GEO-iSHAI product execution step	42
3.6 VALIDATION	44

 	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 5/47</p>
---	--	---

4. SUMMARY..... 45

5. REFERENCES 46

List of Tables and Figures

TABLE 1: LIST OF APPLICABLE DOCUMENTS	12
TABLE 2: LIST OF REFERENCED DOCUMENTS	12
TABLE 3: LIST OF SEVIRI IR CHANNELS USED IN GEO-ISHAI VERSION 2016.....	31
TABLE 4: THE BACKGROUND ERROR COVARIANCE MATRIX.....	33
TABLE 5: SUMMARY OF THE GEO ISHAI STATISTICAL PARAMETERS IN 2013 FOR ODD PIXELS OF GEO ISHAI VALIDATION DATASET USING AS INPUT TO GEO ISHAI ACTUAL SEVIRI BTs BIAS CORRECTED.....	44
FIGURE 1: GEO-ISHAI INPUTS AND OUTPUTS SCHEME.....	15
FIGURE 2: EXAMPLES OF PGE13 SPhR TPW AT 10:15UTC ON 23 JUNE 2008 CALCULATED WITH DIFFERENT SIZE OF FOR. FOR 1x1 (TOP LEFT), FOR 3x3 (TOP RIGHT), FOR 5x5 (BOTTOM LEFT) FOR 7x7 (BOTTOM RIGHT)	19
FIGURE 3: SCATTER PLOTS OF IR13.4 SEVIRI BT VERSUS ECMWF+RTTOV SYNTHETIC BT. ON THE LEFT, MEAN OF SEVIRI BT CLEAR PIXELS IN 0.5° x 0.5° BOX. ON THE RIGHT, SEVIRI BT AT IR10.8 WARMEST CLEAR PIXEL IN 0.5° x 0.5° BOX FOR MSG-N REGION.	20
FIGURE 4: TOP:K-INDEX PROCESSED WITH OPTIONS FOR 5x5 AND BTs FROM IR10.8 WARMEST CLEAR PIXEL BOTTOM: K-INDEX PROCESSED WITH OPTIONS FOR 5x5 AND BTs MEAN OF BTs CLEAR PIXEL.	20
FIGURE 5: REGRESSION FLOWCHART OF THE SEVIRI RETRIEVAL PROCESS	24
FIGURE 6: VARIATIONAL ITERATIVE PHYSICAL FLOWCHART OF THE SEVIRI RETRIEVAL PROCESS.....	26
FIGURE 7: ZOOM OF K-INDEX PROCESSED WITH BT AT WARMEST PIXEL IN THE IR10.8. THE DEFAULT POST- PROCESSING “FILLING FOR” OPTION (LEFT) AND THE “NOT FILLING FOR” OPTION (RIGHT).	30
FIGURE 8: 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.....	38
FIGURE 9: PGE13HYB AND ECMWF (PGE00HYB) VERTICAL CROSS SECTIONS OF θ_e FOR 9 UTC ON 12TH AUGUST 2011.....	38
FIGURE 10: EXAMPLE OF GEO-ISHAI BL, ML, HL AND TPW FROM 12 UTC ON 15 JULY 2015 PRODUCED FROM SEVIRI ON MSG-3.....	39
FIGURE 11: EXAMPLE OF GEO-ISHAI LI AND SHW FROM 12 UTC ON 15 JULY 2015 PRODUCED FROM SEVIRI ON MSG-3.....	39
FIGURE 12: EXAMPLE OF GEO-ISHAI KI FROM 12 UTC ON 15 JULY 2015 PRODUCED FROM SEVIRI ON MSG-3.	40
FIGURE 13: EXAMPLE OF GEO-ISHAI SKT TOZ FROM 12 UTC ON 15 JULY 2015 PRODUCED FROM SEVIRI ON MSG- 3.....	40

	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 7/47
---	---	---

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://www.nwcsaf.org>. This document is applicable to the NWC SAF processing package for geostationary meteorological satellites, NWC/GEO.

1.1 PURPOSE AND SCOPE OF THE DOCUMENT

The purpose of this document is to present the Algorithm Theoretical Basis Document (ATBD) for the Clear Air Product Processor GEO-iSHAI of the NWC/GEO software package release 2016. GEO-iSHAI (imagery Satellite Humidity And Instability) product is a heritage of former PGE13 SEVIRI Physical Retrieval (SPhR) product. The name of the product has been changed to avoid the word SEVIRI because NWC/GEO software package since release 2016 could be used with other GEO imagery instruments than MSG (like ABI and AHI) and in order to be ready for MTG-FCI era.

Note: In CDOP-2 proposal and during the development was used the name GEO-TqPh; but the name has been changed to be coherent with names of NWC SAF products from MTG-FCI and MTG-IRS in CDOP-3.

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

In this version just IR brightness temperatures measured by the SEVIRI flown on Meteosat Second Generation (MSG) meteorological satellites can be used as input. Next versions of GEO-iSHAI could use other GEO imagery instruments having it ready for the MTG-FCI era.

The algorithm retrieves temperature and moisture profiles that are used to derive total precipitable water (TPW), layer precipitable water (LPW), Lifted Index (LI), Showalter Index (SHW) and K-Index (KI) from clear sky brightness temperatures within individual pixels or in a Field of Regard (FOR), which is a region of M x M SEVIRI pixels. Starting with this version, users can optionally activate the estimation of the total ozone (TOZ) parameter and the difference with the TOZ calculated from the NWP background. Also starting with this version, the skin temperature (SKT) and the difference of SKT with the NWP background are new output parameters.

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

1.2 SOFTWARE VERSION IDENTIFICATION

This document describes the theoretical basis of the algorithm implemented in the GEO iSHAI version 3.0 product, to be included in the release 2016 of NWC/GEO software package.

	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 8/47</p>
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1.3 IMPROVEMENTS FROM PREVIOUS VERSIONS

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 SEVIRI. 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 2016 has some major updates due to the introduction of the new NWC/GEO NWCLIB and the use of RTTOV-11.2 in version 2016. The input and output of the GEO-iSHAI processor has been rewritten. Also the integration in the same processor of the management of NWP in GRIB files with fixed pressure levels and with hybrid pressure levels has been introduced.

The use of RTTOV-11.2 (whilst in version 2013 was used RTTOV-9.3) implies that the number of RTTOV pressure levels have increased from 43 to 54. For this reason all the coefficients are now calculated using the GEO-iSHAI validation dataset with vertical dimensions adjusted to the 54 RTTOV-11.2 pressure levels.

NWC/GEO package version 2016 remains with the mandatory use of NWP as background as input for all products as GRIB files with fixed pressure levels. This is due to NWC/GEO NWCLIB in version 2016 maintains the management only in fixed pressure levels and the pre-processing of NWP GRIB files using AllMappingNWP tool is needed.

But together with regular GEO-iSHAI mode (using as background fixed pressure GRIB files), GEO-iSHAI (like PGE13 SPhR in version 2013) allows using as inputs directly ECMWF GRIB files on hybrid pressure levels. As in PGE13 SPhR version, GEO-iSHAI allows the use of ECMWF GRIB files in hybrid levels when executing in HYB mode. To get experience and user's feedback, in release 2016 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; it is needed that their hybrid GRIB files must have regular longitude-latitude representation and a structure similar to the ECMWF hybrid GRIB files (see [RD.2]). The feedback of the users is expected in order to improve future versions.

The software for HYB and P mode is being shared in the same executable program, thus sharing as much as possible the code. Since the lowest RTTOV-11.2 pressure levels have a large value (1050 hPa), the extrapolation below surface pressure level for these low RTTOV-11.2 pressure levels has been improved. This has allowed that the coefficients for hybrid and regular (fixed pressure based) modes could be the same. This fact also means that as the number of vertical levels available in fixed pressure level increases the performance of the fixed pressure mode will converge to the hybrid mode performance. This change has allowed the unification of the processing of vertical interpolation and extrapolation of the profiles from hybrid or P levels to the 54 RTTOV-11.2 pressure levels. Thus the vertical interpolation/extrapolation is the same for both modes and this allows that the FG regression and physical retrieval steps is now the same for the two modes, sharing coefficients and validation.

Besides, all the GEO-iSHAI coefficients have been updated and they have been calculated with a GEO-iSHAI validation dataset from the 2013 period. Similar approach to v2013 has been followed for the 2016 release of GEO-iSHAI: all coefficients have been calculated only using MSG images and ECMWF profiles using the GEO-iSHAI training and validation dataset (former PGE13 validation dataset).

In release 2016, it has been introduced two new output parameters SKT and TOZ.

SKT and $\text{diffSKT} = (\text{SKT}_{\text{retrieved}} - \text{SKT}_{\text{nwp}})$ were calculated internally in previous versions of PGE13 SPhR but they were not available to users as outputs and no validation was made. In any case, GEO-iSHAI SKT does not pretend to be alternatives to SST or LST products because more temporal and spatial controls would be needed. They have been introduced for its use for nowcasting by users and forecasters. The temporal evolution and spatial gradients of SKT and the diffSKT could be used in

several nowcasting applications as monitoring of pixels not well screen out by cloud mask, detection of fogs, advice for very fast increase of SKT as triggering convection mechanism, advice users of bad SKT, etc

TOZ and diff(TOZret – TOZnwp) has been also introduced as optional output parameters. That means that user must activate them and provide NWP GRIB file with ozone profiles. For this reason the IR9.7 channel is also now a mandatory channel. The retrieval of TOZ is based on statistical retrieval using non-linear regression from ozone profile, SEVIRI IR channels (including IR9.7 channel) and the GEO-iSHAI T profile and GEO-iSHAI SKT.

In GEO-iSHAI the channel IR8.7 is not used. Also the emissivity atlases have been changed because emissivities atlases are now common ancillary datasets (see Section 2.3.3.7). The same approach have been made with the bias BT correction coefficients that are now common NWC/GEO files with associated functions in the NWCLIB.

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 imagery 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)
iSHAI	imagery 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
TM	Task Manager
UM	User Manual
VR	Validation Report
VSA	Visiting Scientist Activities

	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 12/47
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WV	Water Vapour Channel
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1.5 REFERENCES

1.5.1 NWC SAF Applicable Documents

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

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

Current documentation can be found at the NWC SAF Helpdesk web: <http://www.nwcsaf.org>.

Ref.	Title	Code	Vers
[AD.1]	Proposal for the Second Continuous Development and Operations Phase (CDOP2)	NWC/CDOP2/MGT/AEMET/PRO	1.0
[AD.2]	NWC SAF CDOP-2 Project Plan	NWC/CDOP2/SAGF/AEMET/MGT/PP	1.9
[AD.3]	Configuration Management Plan for NWC SAF	NWC/CDOP2/SAF/AEMET/MGT/CMP	1.4
[AD.4]	NWC SAF Product Requirements Document	NWC/CDOP2/SAF/AEMET/MGT/PRD	1.9
[AD.5]	Interface Control Document for Internal and External Interfaces of the NWC/GEO	NWC/CDOP2/AEMET/SW/ICD/1	1.1
[AD.6]	Data Output Format for the NWC/GEO	NWC/CDOP2/AEMET/SW/DOF	1.1
[AD.7]	System Version Document for the NWC/GEO	NWC/CDOP2/AEMET/SW/SCVD	1.1

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 Clear Air Product Processor of the NWC/GEO	NWC/CDOP2/GEO/AEMET/SCI/VR/ClearAir	1.0	15/10/16
[RD.2]	User Manual for the Clear Air Product Processors of the NWC/GEO: Science Part	NWC/CDOP2/GEO/AEMET/SCI/UM/ClearAir	1.0	15/10/16

Table 2: List of Referenced Documents

	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 13/47</p>
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2. GEO-ISHAI PRODUCT ALGORITHM

GEO-iSHAI algorithm version 3.0 is responsible for the physical retrieval of the atmospheric temperature and moisture profiles as well as surface skin temperature for one clear sky SEVIRI pixel, or a Field-Of-View (FOR) with contains $M \times M$ pixels. This product has been developed within the NWC SAF context, aiming to support nowcasting applications. Also TOZ can be optionally calculated using nonlinear regression.

The main outputs of GEO-iSHAI product are:

1. Total Precipitable Water (TPW)
2. Layer Precipitable Water (LPW). Corresponding to the precipitable water in three layers:
 - a. BL: Precipitable water in low layer [surface pressure - 850 hPa]
 - b. ML: Precipitable water in middle layer [850 - 500 hPa]
 - c. HL: Precipitable water in high layer [500 - 0 hPa]
3. Stability indices: they are calculated from the retrieved profiles of temperature and humidity. The calculated indices are:
 - a. Lifted Index (LI)
 - b. Showalter Index (SHW)
 - c. K-index (KI)
4. Skin Temperature (SKT)
5. Total Ozone (TOZ). This parameter is optional, must be activated by the users and the NWP GRIB files must contains ozone fields.
6. Besides the main outputs, the differences between the above parameters calculated from the retrieved profiles of temperature and humidity (and ozone profile if activated) with the parameters calculated from the spatial, temporal and vertical interpolated profiles from background NWP are written as other outputs (following 2007 Madrid Workshop recommendation). Thus the parameters diffTPW, diffBL, diffML, diffHL, diffLI, diffSHW, diffKI, diffSKT and diffTOZ are also written in the netCDF output file.

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

The main inputs of the product are SEVIRI IR brightness temperatures and NWP forecast model GRIB files. SEVIRI provides one full resolution image (3 x 3 km) every 15 minutes (or 5 minute from Rapid Scan service), at the satellite nadir for every IR channel. Thus, these products are useful in the prediction of severe weather due to their ability to measure with high temporal and spatial resolution variations of atmospheric stability and moisture. A time sequence of the images is the best way to monitor drying and moistening tendencies and stability tendencies; as example, NWC SAF GEO-iSHAI animations are available at the NWC SAF MSG web page (<http://www.nwcsaf.org/>) generated with NWC/GEO reference system at AEMET.

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

	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 14/47
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Once the outbreak of convection occurs, TPW, LPWs, LI, SHW, KI, SKT and TOZ values provided by GEO-iSHAI in clear air pixels surrounding the convective system may help the forecasters to foresee the evolution of convection. GEO-iSHAI outputs cannot predict by themselves whether storms will occur. They provide forecasters a localization and evolution of some of the ingredients and the convective forcing before thunderstorms develop. Region with unstable values on the stability indices combined with high precipitable water values indicate that the troposphere is near saturation and convection could be triggered. Convection can be produced with stable values in stability indices due to other ingredients, not correlated with the stability indices, which can also be responsible (elevated convection, dynamic forcing without thermodynamic forcing and isentropic lifting). Therefore, these NWC SAF products must be used in conjunction with other data sources (NWP profiles, radio-sounding, satellite data, Radar data, lightning strokes detectors, etc.) in order to alert the forecasters about the possibility of occurrence of mesoscale events.

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

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

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

2.1 GEO-iSHAI PROCESSING OUTLINE

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

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

The main input values are the BTs from five SEVIRI infrared channels (centred at 6.2, 7.3, 9.7, 10.8, 12.0 and 13.4 μm) and forecasted NWP fields which are used as background information. GEO-iSHAI also uses elevation dataset as static input information to determine the pixels where the land emissivity maps, pre-computed for each IR SEVIRI channel and for every month of the year, are used.

If user activates it, also TOZ is calculated using only First-Guess non-linear regressions. In this case IR9.7 SEVIRI BTs are used also as input to the First-Guess non-linear regressions together with the background ozone profile.

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

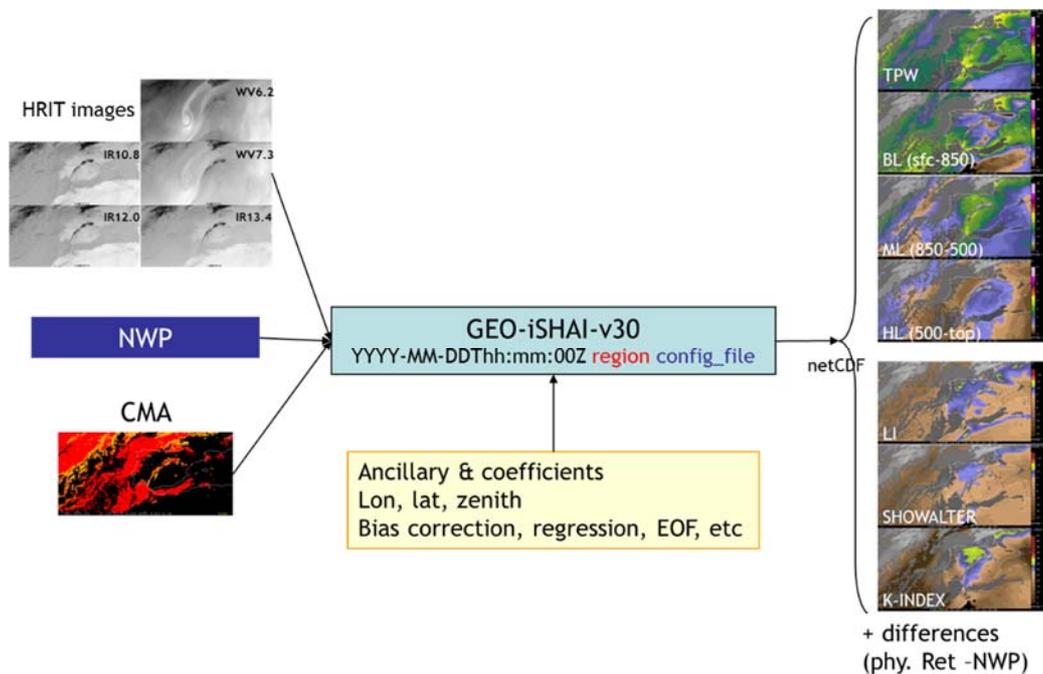


Figure 1: GEO-iSHAI inputs and outputs scheme.

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

1. Pre-processing:

- Initialisation: reading of processing options from the configuration file, reading of all coefficient file names, initialisation of RTTOV-11.2, getting calibrated SEVIRI BT, associated geographical ancillary data, IR emissivity maps and CMA for the region to process.
- Optional thinning of SEVIRI BT to process on FOR of M x N pixels (M and N are configurable parameters in the configuration file). Two methods are allowed to calculate BTs of the FOR: 1) mean value of clear pixels BTs on FOR or 2) BTs of the warmest clear pixel at IR10.8 (See section 2.2.1)

 	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 16/47</p>
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- Get collocated NWP forecast temperature and moisture profiles. 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,Ozone) profile.

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 (see section 2.2.2).

In the case of HYB mode: all the NWP process is made inside the GEO-iSHAI code. GEO-iSHAI opens directly the previous and next (relative to the time of the MSG image) ECMWF GRIB files on hybrid levels, makes the vertical interpolation on ECMWF position to the 54 RTTOV-11.2 pressure levels, makes the temporal interpolation to the date of the image and finally makes the spatial interpolation just over the clear air processed FOR.

- Bias adjustment of SEVIRI BTs. The bias correction regression coefficients are read from the common NWC/GEO datasets and BT bias correction is made (see section 2.2.3).
- Execution of non linear-regressions to calculate the first guess profiles of temperature and specific humidity using as main inputs: a) bias corrected SEVIRI BTs and b) the background NWP temperature and specific humidity profiles spatially, temporally and vertically interpolated (see section 2.2.4) at FOR.

2. Processing:

- Iterative execution of Physical Retrieval Module up to the maximum number of times established, executed if the differences between calculated RTTOV BTs from first guess profile and SEVIRI BTs are greater than a predefined threshold. (see sections 2.2.5 and 2.2.6)
- If activated by the user, calculation of ozone profile using FG non-linear regression. It is an estimated ozone profile using as main inputs: a) bias corrected SEVIRI BTs using also the IR9.7 channel and b) the background NWP temperature and ozone profiles spatially, temporally and vertically interpolated to FOR.
- To perform direct calculation of TPW, LPWs, LI, SHW and KI parameters at FOR from the retrieved profiles of T and q.
- Calculation of TOZ if activated from the estimated ozone profile.
- Compute the differences between the products (TPW, LPWs, LI, SHW and KI) calculated from retrieved profiles of T and q and the ones calculated from the background NWP profiles of T and q. Calculate the difference between SKT and the background NWP SKT.
- If activated, TOZ calculation, to compute the differences between TOZ calculated from retrieved profiles of ozone and the ones collocated from the background NWP profiles of ozone.
 - Optional writing of the intermediate T, q, and ozone profiles at the different algorithm steps. Also other parameters as surface pressure, skin temperature, SEVIRI BTs, ancillary data, etc are written.

 	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 17/47
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3. Post-processing:

- Quality control: Several quality flags have been added to the output product (see section 2.2.7).
- Filling clear pixels inside the FOR: the default method is to copy the same FOR value to all clear pixels. Another configurable option is to write the output only at the clear FOR positions (see section 2.2.8.1).
- Over cloudy pixels, one IR BT channel degraded to 7 bits (range [0 – 127]) values is stored as other field. This will be later used to generate adequate images in which cloudy pixels are grey scaled and clear pixels are colour scaled (see section 2.2.8.2). The number of the IR BT channel is a configurable parameter in the configuration file; by default it is the IR10.8 channel.
- The outputs are written in a netCDF format file (see section 2.2.8.2).

2.2 GEO-ISHA1 ALGORITHM DESCRIPTION

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

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

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

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

SEVIRI has 7 IR channels in the range [6.2 – 13.4] microns. Two channels contain strong water vapour absorption, one has strong ozone absorption and one has CO₂ absorption. The other SEVIRI infrared channels are window channels that provides information of the surface skin temperature, surface emissivity and low level moisture information. The IR 13.4 channel is located at the CO₂ absorption band and the radiances contain temperature information; while the WV6.2 and WV7.3 channels are located at the strong water vapour absorption band and the radiances contain both temperature and water vapour concentration information. For the physical retrieval mode [WV6.2, WV7.3, IR10.8, IR12.0, IR13.4] SEVIRI BTs are used in the current version of the software for T and q profiles retrieval; also SKT is retrieved in this process.

The IR9.7 channel is optionally used (user must activate it) to estimate the ozone profile using non-linear regressions similar to the non-linear regressions used to calculate the T/q profiles at First-Guess step. The estimated ozone profile is used to calculate TOZ and the difference between GEO-ISHA1 TOZ and background NWP TOZ.

	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 18/47</p>
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Concerning the non linear regression module, the current version of the software does not use of IR8.7 BTs. The decision to not use the IR8.7 channel in release 2016 is due to the uncertainties in the performance over the Sahara desert (caused by the lower IR8.7 emissivity on desert pixels) and the low improvement of the performance when IR8.7 is used on sea pixels. This decision is based in tests made using the techniques described in the validation report.

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

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

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

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

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

2.2.1 Use of Field of Regards (FOR)

The GEO-iSHAI execution on FOR (window of M x M pixels) basis was recommend, instead of pixel by pixel basis, in Jun Li’s 2008 VSA. This has been considered in order to speed up the processing and because the processing in FOR could reduce noise. A window of 3x3 pixels has been considered as adequate as the default width of the FOR. The width of the FOR (M x N pixels) is an adjustable parameter in the configuration file. This allows adjusting M or N parameters depending on the size of the region to process and the computer resources of the user.

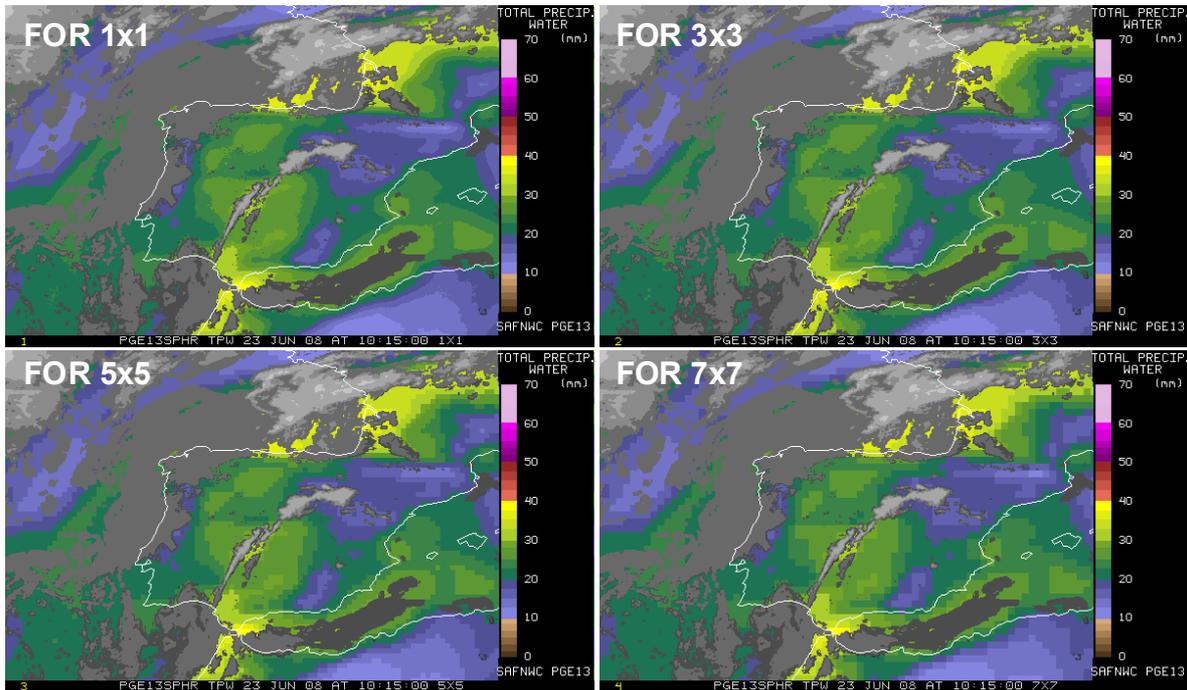


Figure 2: Examples of PGE13 SPhR TPW at 10:15UTC on 23 June 2008 calculated with different size of FOR. FOR 1x1 (top left), FOR 3x3 (top right), FOR 5x5 (bottom left) FOR 7x7 (bottom right)

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

- (1) Mean BTs of all clear pixels within the FOR.
- (2) The BTs at the IR10.8 warmest clear pixel within the FOR.

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

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

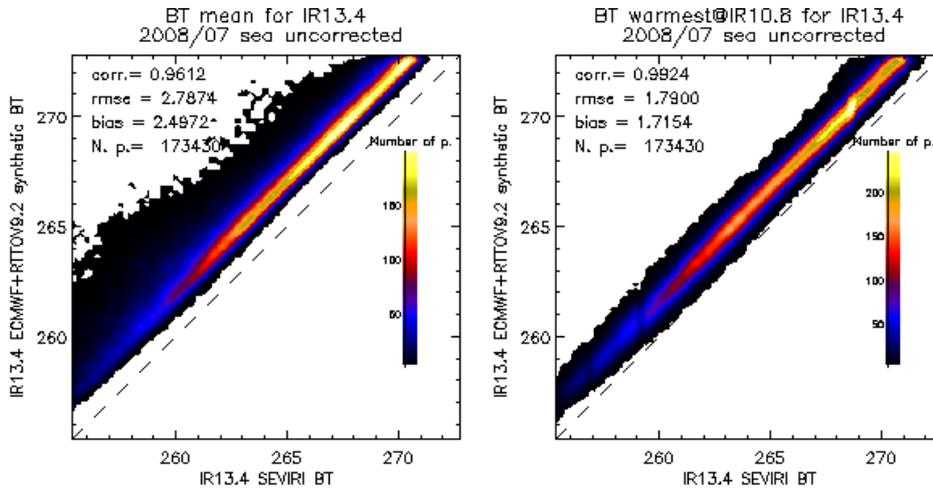


Figure 3: Scatter plots of IR13.4 SEVIRI BT versus ECMWF+RTTOV synthetic BT. On the left, mean of SEVIRI BT clear pixels in $0.5^\circ \times 0.5^\circ$ box. On the right, SEVIRI BT at IR10.8 warmest clear pixel in $0.5^\circ \times 0.5^\circ$ box for MSG-N region.

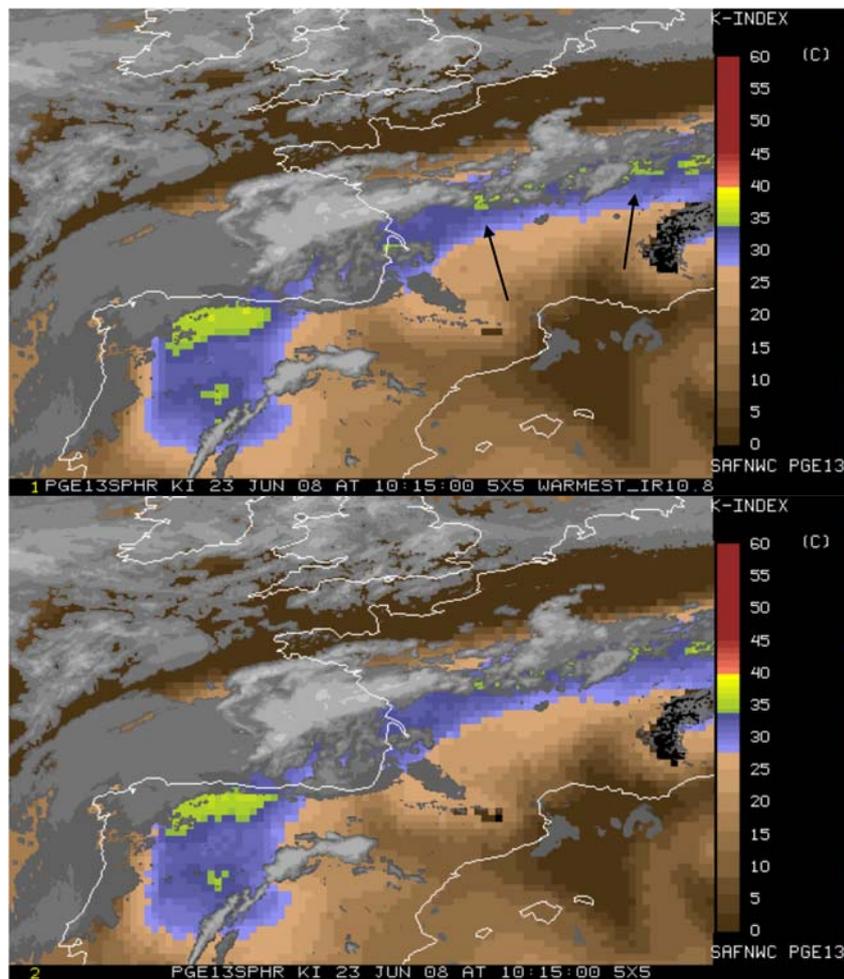


Figure 4: Top: K-Index processed with options FOR 5x5 and BTs from IR10.8 warmest clear pixel
Bottom: K-Index processed with options FOR 5x5 and BTs mean of BTs clear pixel.

	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 21/47
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2.2.2 NWP data Interpolation to 54 RTTOV-11.2 levels of NWP profiles.

As explained before, it is convenient to use as background profile NWP forecast in the $[t+00, t+24]$ hours range. The NWC/GEO library provides software which should be able to work with any NWP model and it should accept the set of fixed pressure levels available on the NWP files provided by the users to the NWC/GEO package. The same fixed pressure levels NWP GRIB files that are actually used with NWC/GEO release 2016 to generate other products can be used. Hence, any user that is running NWCSAF/GEO 2016 package should be able to run GEO-iSHAI.

In the case of GEO-iSHAI release 2016, ECMWF GRIB files on hybrid levels could be also used as inputs. As one advance for full future support 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 file the codes of section 1 of GRIB header to identify T, q, O₃, SKT and P_{sfic} fields (see details in User Manual [RD.2]). But, always GRIB files on fixed pressure levels are also needed in order to execute CMA before execution of GEO-iSHAI code.

Since it is not adequate to provide specific error matrices, EOFs, regression coefficients, etc for the great number of combinations in user pressure levels, the interpolation of different NWP model levels to 54 RTTOV-11.2 pressure levels is performed.

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

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

Vertical interpolations are made inside GEO-iSHAI. For vertical interpolation, an "ad hoc" function has been added to GEO-iSHAI. The solution adopted has been the development of a function that interpolates the temperature and humidity profiles from any set of pressure levels to the 54 RTTOV-11.2 pressure levels calling the RTTOV function "rttov_intavg_prof". This RTTOV function interpolates linearly, in the logarithm of the pressure, the NWP forecast temperature and humidity fields available on user-defined vertical pressure levels to the 54 RTTOV pressure levels. This RTTOV function copies the value of the lowest user pressure level profile to all RTTOV pressure levels with value greater than the lowest user pressure level. Since the lowest RTTOV-11.2 pressure levels have values greater than normal lowest fixed pressure levels, it has been implemented in GEO-iSHAI one extrapolation process based in the one made by ECMWF and described in section 1.3 of IFS DOCUMENTATION – Cy40r1 Operational implementation 22 November 2013. First, the extrapolation of T profile using the process described is made, and then the extrapolation of the q profile maintaining the relative humidity value at the lowest fixed pressure level is made.

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

In the case of executing GEO-iSHAI in HYB mode: the whole NWP management is made inside the GEO-iSHAI code. GEO-iSHAI opens directly the previous and next ECMWF GRIB files on hybrid levels, compared to the time of the satellite image, from *\$SAFNWC/import/NWP_data*; makes the vertical interpolation from ECMWF levels to the 54 RTTOV-11.2 pressure levels; makes the temporal interpolation to the date of the image and finally makes the spatial interpolation just at clear air processed FOR.

	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 22/47
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Another difference is that the specific humidity profile is read from the ECMWF GRIB files on hybrid levels and the conversion from relative humidity to specific humidity is not needed.

Since the lowest RTTOV-11.2 pressure levels have values greater than the lowest hybrid level at P_{sfc} (especially on mountains pixels) it has been implemented in GEO-iSHAI one extrapolation process based in the one made by ECMWF. The extrapolation process is the same as that explained above, but starting at P_{sfc} instead of at the lowest user fixed pressure level.

As a result of this process, time and spatial collocated, with the SEVIRI image, background NWP (T, q) profiles interpolated at the 54 RTTOV-11.2 pressure levels are obtained from the background NWP GRIB files with (T, q) profiles. If the TOZ calculation is activated, also the ozone profile is interpolated to the 54 RTTOV-11.2 pressure levels.

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

2.2.3 SEVIRI BT bias correction

Brightness temperature bias adjustment is very important for product quality. The original satellite measurements must be bias BT adjusted to account for the bias between the satellite observation and the synthetic radiative transfer model BTs. Since synthetic RTTOV BTs have been used to train the algorithm, differences between synthetic and measured clear-sky BTs must be mitigated with a SEVIRI BT bias correction. The biases are caused by both measurement problems and errors in the radiative transfer model. The bias BT correction is based on finding the differences between the observed SEVIRI BTs and those simulated from the radiative transfer model (here synthetic RTTOV-11.2 BTs) with robust regression. Usually there are two ways for brightness temperature bias estimation:

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

To calculate the BT bias correction, the use of collocated RTTOV BTs calculated from NWP analysis and SEVIRI BTs has been chosen. An issue in brightness temperature bias calculation is the emissivity estimation. Due to the emissivity uncertainty, brightness temperature bias estimation on window channels might not be reliable especially on desert pixels. For this reason, the BT bias correction using only sea observations has been done. BT bias correction for water vapour ($6.2 \mu\text{m}$ and $7.3 \mu\text{m}$) and CO₂ ($13.4 \mu\text{m}$) absorption channels should help the retrievals.

The coefficients of the bias adjustment's robust regression are read in release 2016 from the common NWC/GEO dataset files using NWCLIB library.

2.2.4 Use regression as first guess

The GEO-iSHAI algorithm uses non-linear regressions as first guess. The regressions use SEVIRI IR BTs and NWP forecast as basic predictors. The predictands include temperature, specific humidity profiles at each one of the RTTOV-11.2 pressure levels and the skin temperature. Since SEVIRI only has a few sounding IR channels, the temperature/moisture profiles from numerical weather prediction (NWP) forecast model are used as additional predictors. Here, the temperature forecast, the specific humidity forecast interpolated to the 54 RTTOV-11.2 pressure levels, the latitude and the fraction of land in pixel are included as additional predictors.

The dependence of the atmospheric attenuation on the satellite zenith angle has been taken into account in practically all algorithms that have been implemented to obtain derived products from IR satellite data. 76 regression coefficient sets are generated for each parameter. Each coefficient set corresponds to a local zenith angle ranging from 0 to 75 degree. In GEO-iSHAI the regression sets for T, q, ozone and SKT have been divided in separated files. There is a FG regression coefficients file that contains the 76 by 54 coefficients regressions for every zenith angle and every T at each one of the 54 RTTOV pressure levels using the predictors of Eq.1 There is a similar set 76x54 of FG regression coefficients for log(q) profile. In the case of SKT there are 76 regressions for every zenith angle.

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

$$Z = \sum_{j=1}^N A_j \cdot Tb_j + \sum_{j=1}^N B_j \cdot Tb_j^2 / 250 + C \cdot p_s + D \cdot latitude + E \cdot p_{land} + \sum_{l=1}^{54} F_{tl} \cdot T_l + \sum_{l=1}^{54} G_{wl} \cdot \log(q_l) + H \cdot T_{skin} + G_o \quad \text{Eq. 1}$$

Where:

- Z is one of the following parameters: temperature or specific humidity at each one of the 54 RTTOV pressure levels or Skin temperature
- **Tb** is the SEVIRI bias corrected brightness temperature; **T** and **q** are background NWP forecast temperature and specific humidity profile at the 54 RTTOV pressure levels respectively; **Ps** is the surface pressure; **P_{land}** is the fraction of land in pixel (0 : sea pixels and 1 : land pixels).
- **A, B, C, D, E, F, G, H and G_o** are regression coefficients;
- **N**, is the total number of SEVIRI IR channels used as predictors.
- **T_{skin}** is the Skin temperature from the ECMWF

In the case of ozone profile, the regressions include also as predictor the IR9.7 channel and instead of log(q) profile the log(ozone) profile is used.

$$Z = \sum_{j=1}^{N+IR9.7} A_j \cdot Tb_j + \sum_{j=1}^{N+IR9.7} B_j \cdot Tb_j^2 / 250 + C \cdot p_s + D \cdot latitude + E \cdot p_{land} + \sum_{l=1}^{54} F_{tl} \cdot T_l + \sum_{l=1}^{54} G_{wl} \cdot \log(ozone_l) + H \cdot T_{skin} + G_o \quad \text{Eq. 2}$$

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

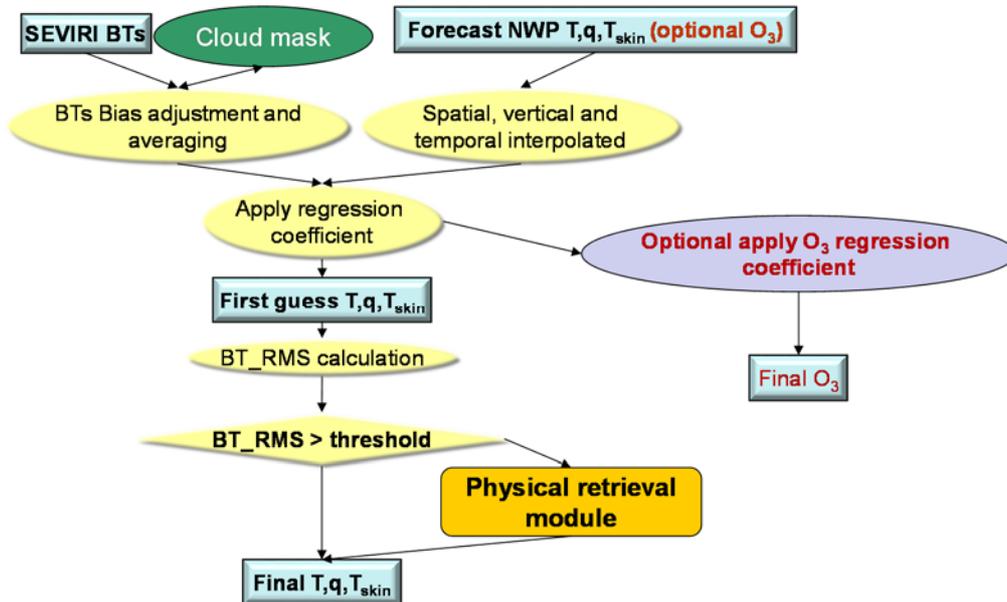


Figure 5: Regression Flowchart of the SEVIRI retrieval process

2.2.5 Mathematical Description of Physical Retrieval module

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

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

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

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

By using the Newtonian iteration

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \mathbf{J}''(\mathbf{X}_n)^{-1} \cdot \mathbf{J}'(\mathbf{X}_n) \quad \text{Eq. 4}$$

The following Quasi-Nonlinear iterative form is obtained

$$\delta \mathbf{X}_{n+1} = \left(\mathbf{F}_n'^T \cdot \mathbf{E}^{-1} \cdot \mathbf{F}_n' + \gamma \mathbf{B}^{-1} \right)^{-1} \cdot \mathbf{F}_n'^T \cdot \mathbf{E}^{-1} \cdot (\delta \mathbf{Y}_n + \mathbf{F}_n' \cdot \delta \mathbf{X}_n) \quad \text{Eq. 5}$$

Where:

\mathbf{X} is the vector of temperature and humidity profile to be solved; \mathbf{n} is the iteration step, $\mathbf{n}=0$ denotes first guess or background profile,

$$\delta \mathbf{X}_n = \mathbf{X}_n - \mathbf{X}^{FG};$$

$$\delta \mathbf{Y}^m = \mathbf{Y}^m - \mathbf{F}(\mathbf{X}_n)$$

\mathbf{F}' is the tangent linear operative (Jacobian) of forward model \mathbf{F} . The RTTOV-11.2 is used for forward model (\mathbf{F}) and Jacobian (\mathbf{F}') calculations.

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

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

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

Where $A = (\alpha_1, \alpha_2, \dots, \alpha_M)$, and $\Phi = \begin{bmatrix} \Phi_T & 0 & 0 \\ 0 & \Phi_q & 0 \\ 0 & 0 & \Phi_{Ts} \end{bmatrix}$

Φ_T is the matrix of the first \tilde{N}_T empirical orthogonal functions (EOFs) of the temperature profile; Φ_q is the matrix of the first \tilde{N}_q EOFs of the logarithm of specific humidity profiles, $\Phi_{Ts} = 1$, and $M = \tilde{N}_T + \tilde{N}_q + 1$. In GEO-iSHAI processing, 2 temperatures EOFs and 3 specific humidity EOFs are used. It is obvious that $\Phi^T \Phi = I$. Defining $\tilde{F}' = F' \cdot \Phi$, Eq. (5) becomes

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

where $A_0 = 0$, and

$$\|F(X_n) - Y^m\|^2 = \sigma^2, \quad \text{Eq. 8}$$

where σ is the observation error of SEVIRI, define $\|X\|^2 = \frac{1}{N} \sum_{i=1}^N x_i^2$, $X = (x_1, x_2, \dots, x_N)$

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

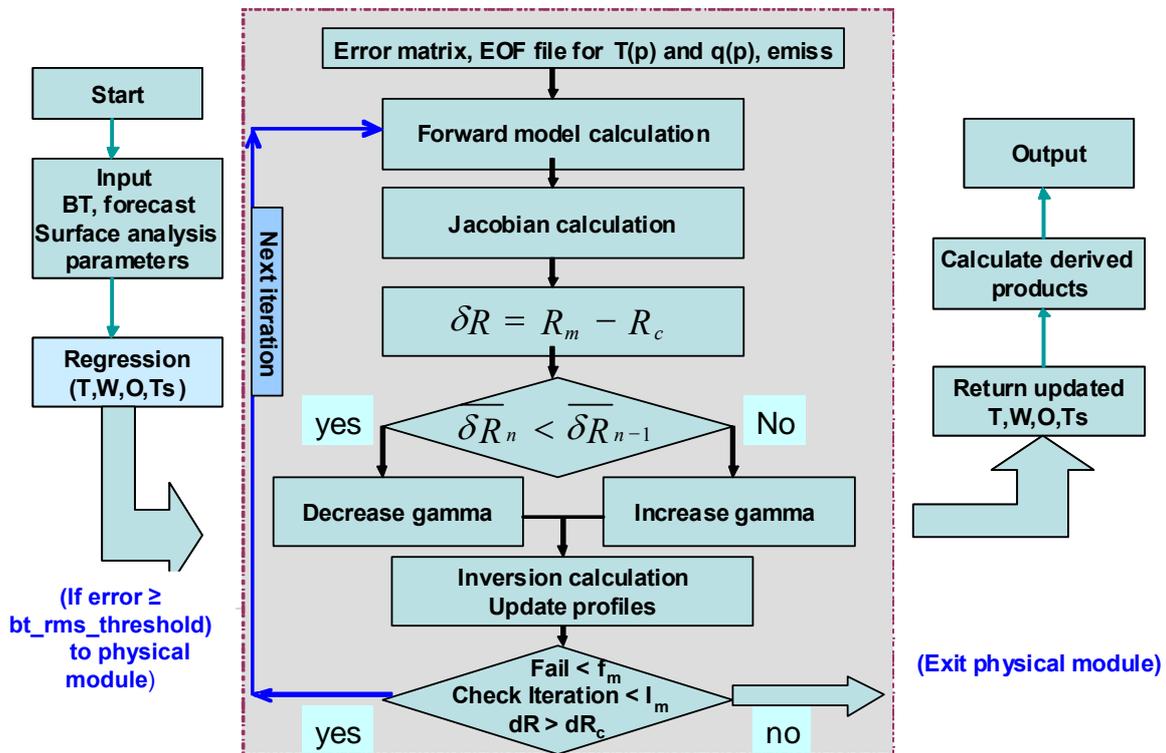


Figure 6: Variational iterative physical flowchart of the SEVIRI retrieval process

In the GEO-iSHAI retrieval, the water vapour is expressed as the logarithm of the specific humidity due to the fact that the latter is more linear to the infrared brightness temperatures than the specific humidity itself. The matrix dimensions in Eq. (5) are 109×109 where $109=2*54+1$; but matrix dimensions in Eq. (7) are *number_of_EOF* x *number_of_EOF* (by default $6 = 2$ EOF for T +3 EOF for $\log(q) + 1$ EOF for Skin temperature). This allows speeding up the process and reducing the CPU time.

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

- The threshold used to decide if the physical retrieval is executed it is fixed in the keyword `BT_RMS_THRESHOLD` (if maximum allowed difference between SEVIRI BT and RTTOV BT calculated from the first guess in the non-window channels).
- In the “check iteration” step the maximum number of iterations is fixed with the keyword `MAX_ITERATIONS`.
- In the “check iteration” step the allowed residual threshold is fixed with the keyword `MAX_RESIDUAL`.

2.2.5.1 Observed brightness temperatures (Y^m)

The bias-adjusted observed brightness temperatures vector Y^m represents the satellite measured brightness temperatures in N channels ($6.2 \mu\text{m}$, $7.3 \mu\text{m}$, $10.8 \mu\text{m}$, $12 \mu\text{m}$, and $13.4 \mu\text{m}$ are used).

2.2.5.2 RTTOV-11.2 as radiative transfer model

RTTOV version 11.2 is used in the GEO-iSHAI v3.0 algorithm implementation. Calculations are based on the atmospheric profile, surface skin temperature and surface emissivity in clear skies. RTTOV is maintained and supplied by the NWP SAF.

2.2.5.2.1 Synthetic brightness temperature (Y_n)

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

Y_n must be computed as a vector for all N IR channels.

RTTOV model is used for the radiative transfer calculations. The profile parameters are represented at L levels; it has been used $L = 54$ because it is the number of RTTOV-11.2 pressure levels. The radiation model needs the profile parameters at L prescribed pressure levels so that the first guess profile must be appropriately interpolated to these levels. Each profile is interpolated in space, time and vertically to fit the time and location of the actual satellite observation.

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

2.2.5.2.2 Weighting function (Jacobian) matrix (F')

The weighting function or Jacobian matrix F'_n (the subscript n denotes the n th iteration in the physical retrieval procedure) actually describes the change of the brightness temperature at the top of the atmosphere (TOA) with a changed atmospheric parameter:

$$F'_n = \frac{\delta Y_n(i)}{\delta X_n(j)} \quad \text{Eq. 9}$$

Where i is the channel index in the brightness temperature vector (Y) and j is the parameter index in the profile vector (X).

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

Such two-dimensional partial derivatives are also referred to as Jacobians. It is indeed the computation of these Jacobians what is a substantial factor in the computational load of the retrieval equation. Since Jacobian from RTTOV-11.2 is based on specific humidity directly, the Jacobian should be multiplied by specific humidity in order to obtain the Jacobian for natural logarithm of specific humidity.

From the Jacobian calculations, it can be seen that $13.4 \mu\text{m}$ channel provides temperature profile information; while 6.2 and $7.3 \mu\text{m}$ channels provide water vapour information. The information from forecast temperature profile along with the $13.4 \mu\text{m}$ provides temperature profile. Temperature profile is needed for water vapour retrieval in order to derive the water vapour information since these water vapour absorption channels also contain temperature information. The $12 \mu\text{m}$ and $13.4 \mu\text{m}$ channels also contain weak water vapour absorption providing useful boundary layer moisture information.

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

2.2.5.3 Discrepancy principle for regularization parameter

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

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

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

	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 28/47
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If γ is too large, more weight is given to background and the solution tends to be background or only a moderate modification of background.

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

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

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

e_k is the square root of the diagonal of \mathbf{E} or the observation error of channel k

Usually σ^2 can be estimated from the instrument noise and estimated radiative transfer model error but in version 2016 it has been calculated from the root mean square between actual SEVIRI BT after bias correction and synthetic RTTOV BT on sea pixels. In release 2016 it has been fixed to 0.333.

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

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

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

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

$$q_0 = 1.0$$

$$\text{If } \|F(X_n) - Y^m\|^2 \leq \sigma^2, \text{ then } q_n = 1.1;$$

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

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

2.2.5.4 Iteration checking and residual estimation

In the retrieval processing, several checks are made for retrieval quality control. The quantity

$Rs_n = \|F(X_n) - Y^m\|^2$ is computed to check the convergence or divergence,

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

If $Rs_{n+1} < \text{MAX_RESIDUAL}$ or $|Rs_{n+1} - Rs_n| < 0.025$ stop iteration.

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

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

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

2.2.6 Other considerations

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

$$\begin{aligned}\bar{F}'_n &= E^{-\frac{1}{2}} \cdot \tilde{F}'_n \\ \delta \bar{Y}'_n &= E^{-\frac{1}{2}} \cdot \delta Y'_n\end{aligned}\tag{Eq. 12}$$

Then Eq. (7) becomes

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

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

2.2.7 Quality control

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

- Clear air flag: Derived from the cloud mask product (CMA). This first flag allows differentiating between cloud free and cloudy pixels
- Quality flags
 - Flag to indicate if the FOR has been processed with Physical retrieval or only first guess retrieval was performed.
 - Flag to indicate the FOR where convergence have failed.
 - Residual of the profile.
 - Number of iterations done (maximum number of iteration is three).
 - BT_residual: root mean square of differences between the SEVIRI and calculated brightness temperature.

2.2.8 Post-processing

2.2.8.1 Fill clear pixels of FOR with the calculated value

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

The other option (`POST_PROC_METHOD 0`) is not to fill clear pixels and it can be used to display the pixels where physical retrieval has been calculated inside the FOR. It can be useful in cloudy regions to display where the physical retrieval has been actually calculated when SEVIRI BT at IR10.8 warmest clear pixel has been selected.

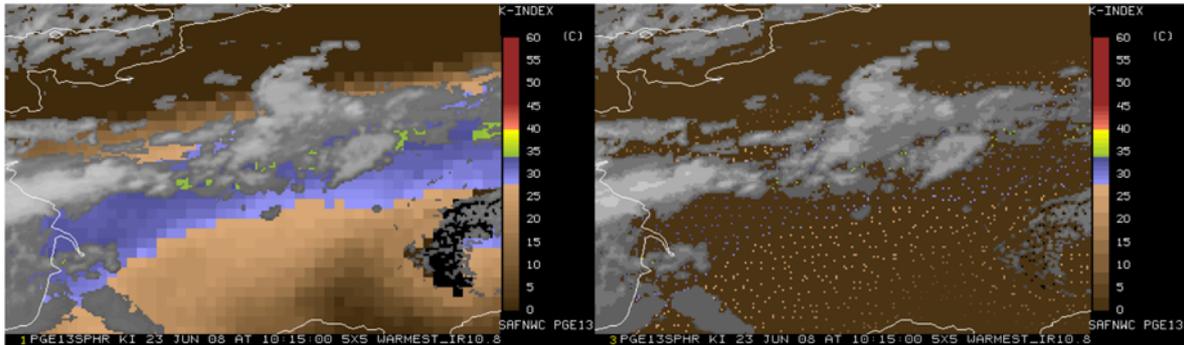


Figure 7: Zoom of K-Index processed with BT at warmest pixel in the IR10.8. The default post-processing “filling FOR” option (left) and the “not filling FOR” option (right).

2.2.8.2 Writing of outputs on netCDF file

In the NWC/GEO release 2016, the GEO-iSHAI parameter outputs at each clear air FOR are written in the netCDF as 16-bit unsigned integer after scaling and offsetting from their original float values.

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

For cloudy pixels, determined by CMA, an IR channel is also stored as a byte field degraded to 7 bits (range [0 – 127]) values for the IR channel selected in the configuration file. This IR channel is only different to missing value at cloudy pixels. It can be used to generate operational images in which cloudy pixels appear as grey scaled pixels and clear pixels appear as colour scaled pixels as in PGE13 SPhR (see section 2.4.3 for example) or CIMSS images. In GEO-iSHAI this process must be made by the user.

The quality flags are written using bits fields.

Note: In previous versions, the PGE13 SPhR parameter outputs were written in byte fields as a matrix image. At each clear air pixel the value was scaled as a byte in range [8 – 127] after scaling and offset. At each cloudy air pixels the value scaled as a byte in range [128 – 250] after scaling and offset the BT at one IR channel.

2.3 ALGORITHM INPUTS, COEFFICIENTS AND FILES

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

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

- **Inputs**
 - i) SEVIRI BT.
 - ii) Cloud Mask.
 - iii) NWP GRIB files from range $[t+00, t+24]$ hours forecasted.
- **Geographical data from NWCSAF functions**
 - a. Longitude.
 - b. Latitude.

c. Zenith angle.

- **Coefficients**

1. Bias BT corrections coefficients.
2. FG regression coefficient files.
3. Error covariance matrix of background and first guess (B^{-1}).
4. Error covariance of observation matrix (E^{-1}).
5. Empirical Orthogonal Functions coefficients.
6. RTTOV-11.2 coefficients for the MSG satellites are also needed.

- **Geographical static data files**

1. IREMIS surface IR emissivity for SEVIRI channels from University of Wisconsin baseline fit database remapped to SEVIRI projections (0° W and 9.5° E).
2. Topographic data.

- **Configuration File of GEO-iSHAI**

2.3.1 Inputs

2.3.1.1 SEVIRI BT

Several SEVIRI IR channels are the main input to GEO-iSHAI. The following SEVIRI IR BT values are needed at full IR spatial resolution:

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

Table 3: List of SEVIRI IR channels used in GEO-iSHAI version 2016.

The code is prepared to use 6 out of 8 SEVIRI IR channels for baseline predictors. The channels used for temperature, humidity and skin temperature retrieval are 6.2 μm , 7.3 μm , 10.8 μm , 12 μm , and 13.4 μm .

In this version, the BT of IR 9.7 μm is only used in to estimate the ozone profile using non-linear regressions if user activates the TOZ calculation.

Considering the diurnal changes in IR3.9 μm , this channel is not used in the GEO-iSHAI algorithm. Considering the emissivity issues and the small added value, the IR8.7 μm channel is not used in the GEO-iSHAI algorithm.

2.3.1.2 Cloud Mask (GEO-CMA)

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

 	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 32/47
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2.3.1.3 Background NWP data

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

To maintain continuity with the NWP GRIB files dataset managed by the NWCLIB software, version 3.0 of GEO-iSHAI can be executed in the default P mode. Users can use their own model and choice for the NWP supply. In real time operational mode, once the NWP GRIB files are received, the NWC/GEO software package has predefined tools (coordinated by the NWC SAF Task Manager daemon) which check every minute for new NWP data making automatically the spatial remapping to the predetermined regions to process. This avoids spending time in every call to one processor to make the remapping process. See [RD.2] for details.

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

As an attempt to get experience and the user's feedback, it is also possible to use as input other NWP models GRIB files on hybrid levels. In release 2016, the identification codes of section 1 of GRIB header for T, q, Ozone, SKT and P_{sfc} are now configurable parameters. That means that users could try to use their own NWP models with hybrid GRIB files as input to GEO-iSHAI in HYB mode. It is needed that their hybrid GRIB files must have regular longitude-latitude representation and a structure similar to the ECMWF hybrid GRIB files. The feedback of the users is expected in order to improve for future versions.

2.3.2 Geographical data from NWCSAF functions

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

2.3.3 Coefficients

2.3.3.1 BT bias correction coefficients

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

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

2.3.3.2 Regression coefficients to calculate First Guess profiles

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

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

Until PGE13 SPhR 2011 version, the error covariance matrix used was the one supplied in the framework of “VSA 2007” by Jun Li and was generated based on NCEP model and a global radiosonde base.

A specific matrix generated with ECMWF model outputs is considered more appropriate for use in the NWC/GEO as most of the users rely on this European model or many European limited area models use the ECMWF as a reference (contour conditions at initialization and validation process or cross validation with ECMWF). This matrix has been computed with the available GEO-iSHAI training and validation dataset (using 2013 year profiles from hybrid vertical GRIB files) and its inverse it’s included in the GEO-iSHAI v3.0 release 2016 version as default B^{-1} matrix.

For the calculation of B^{-1} all the profiles are at the 54 RTTOV pressure levels interpolated from the hybrid levels (91 hybrid levels till June 2013 and then 137 hybrid levels). The filename with the B^{-1} is written in the default GEO-iSHAI configuration file.

2.3.3.4 The observation error covariance matrix (E)

The errors of the observed brightness temperatures and the errors of the radiative transfer model are represented altogether by the matrix E .

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

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

In the case of GEO-iSHAI for the calculation of E^{-1} all the profiles used are at the 54 RTTOV pressure levels interpolated from 91 or 137 hybrid levels. The diagonal element is the square of observation error and it has been calculated in version 2016 using actual SEVIRI BTs after bias correction and synthetic RTTOV BTs on sea pixels of the GEO-iSHAI validation dataset for the whole 2013 year. The default observation error covariance matrix is a diagonal matrix.

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

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

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

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

- (1) to reduce the number of unknowns in the solution, which makes the solution more stable;

	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 35/47</p>
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- (2) to significantly reduce the time of computation in retrieval process; study shows that using EOF representation will not degrade the retrieval accuracy in SEVIRI profile retrieval

In the SEVIRI physical retrieval process, 2 temperature profile EOF is recommended since there is only one CO₂ absorption channel, 3 specific humidity EOFs are recommended since there are 2 water vapour absorption channels plus 12 μm weak water vapour absorption channels that provide boundary layer moisture information.

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

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

For GEO-iSHAI the process to manage the 54 RTTOV-11.2 pressure levels and to use 2013 year from hybrid ECMWF GRIB profiles in GEO-iSHAI validation dataset to calculate 2016 default EOFs has been updated. The filenames with the EOFs are written in the GEO-iSHAI configuration file.

2.3.3.6 RTTOV coefficients

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

2.3.3.7 Use of predetermined surface IR emissivity atlas

Emissivity determination for retrieval remains as a critical issue. Handling surface IR emissivity is very important since an emissivity error of 0.01 in long wave IR window region could result in approximately 0.5 K brightness temperature changes. The emissivity values from database or regression equation can be attempted.

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

- (1) Use emissivity from database:
 - a. Advantage: monthly global coverage.
 - b. Disadvantage: at MODIS channels.
- (2) Use regression based emissivity:
 - a. Advantage: dynamic emissivity, at SEVIRI channels.
 - b. Disadvantage: rely on emissivity in training data, might create false diurnal variation in SEVIRI emissivity retrievals.
- (3) Use independent retrieved emissivity with time continuity, assume skin temperature is temporally variable and emissivity is not changed because emissivity is very slowly varying:
 - a. Advantage: avoid false diurnal feature in emissivity retrievals.
 - b. Disadvantage: algorithm has not been tested, still in concept stage.
- (4) Use emissivity from LEO hyperspectral IR radiances:
 - a. Advantage: emissivity can be updated routinely and can be at any channels.
 - b. Disadvantage: none.

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

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

A realistic way is to use emissivity values from database. An emissivity database is being developed at CIMSS by combining Moderate-Resolution Imaging Spectroradiometer (MODIS) emissivity

	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 36/47</p>
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measurements and laboratory measured hyperspectral emissivity spectra. The database can be used for SEVIRI physical retrieval of profile using emissivity values spectrally, temporally and spatially interpolated. Some information about the emissivity database can be obtained from the following link: <http://cimss.ssec.wisc.edu/iremisp/>

In GEO-iSHAI release 2016, the emissivity atlases have also been changed after they have been considered as common NWCLIB datasets. After decision of NWC SAF Project Team to consider emissivity dataset as common software elements and the incorporation of management functions on the NWC/GEO NWCLIB, fixed IREMIS dataset has been selected from year 2007 following the RTTOV and Eva Borbas (U. Wisconsin) recommendations.

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

2.3.3.8 Ancillary data sets

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

In 2016 version, the elevation dataset is used to distinguish between land and sea pixels (sea pixels are those which elevation value equal to missing code). Then, in the case of land pixels the emissivity values are read from the emissivity datasets.

2.3.3.9 GEO-iSHAI Model Configuration File

GEO-iSHAI has been built as a modular and configurable by the user as possible software. GEO iSHAI model configuration file contains all the coefficients and some constant values required by GEO-iSHAI product. The model configuration file is an ASCII file and then it can be easily modified with any text editor. See the User Manual [RD.2] for details.

2.4 GEO-iSHAI OUTPUTS

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

2.4.1 Main outputs: GEO-iSHAI netCDF files description.

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

- **iSHAI_tpw**: Total precipitable water ($P_{\text{Surface}} - \text{top}$) from the retrieved specific humidity profiles in kg/m^2 .
- LPW Precipitable water in three layers from the retrieved specific humidity profiles in kg/m^2 :
 - **iSHAI_bl**: layer P_{Surface} to 850 hPa
 - **iSHAI_ml**: layer 850 to 500 hPa
 - **iSHAI_hl**: layer 500 to 0 hPa).
- **iSHAI_li**: Lifted Index from the retrieved profiles of temperature and humidity in Kelvin.
- **iSHAI_shw**: Showalter Index from the retrieved profiles of temperature and humidity in Kelvin.
- **iSHAI_ki**: K-Index from the retrieved profiles of temperature and humidity in Kelvin.
- **iSHAI_difftpw**: Difference between TPW from retrieved profile and TPW from NWP profiles in kg/m^2 .

 	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 37/47
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- **iSHAI_diffbl, iSHAI_diffml, iSHAI_diffhl**: Difference between LPWs from retrieved profile and LPWs from NWP profiles in kg/m².
- **iSHAI_diffli, iSHAI_diffki, iSHAI_diffshw**: Difference between stability indices from retrieved profile and stability indices from NWP profiles.
- **iSHAI_skt** and **iSHAI_diffskt**
- **iSHAI_toz** and **iSHAI_diffnoz**: if user activated calculation TOZ.
- Quality Flags: **iSHAI_quality, iSHAI_sflag** fields.
- 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 [AD.6]. In release 2016, 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.

2.4.2 Optional binary files outputs.

Since GEO-iSHAI is executed locally by the users, it allows to debug their local installations or create new parameters or stability indices. There are two keywords in the GEO-iSHAI configuration file to write temperature and humidity profiles on binary files at different steps of the algorithm (from the background NWP data supplied by the users to the final retrieved profiles used to calculate the main outputs).

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

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

At the present time, the generation of tools for conversion from binary to netCDF format is in progress. These tools will be generated at the best effort basis and the netCDF format will allow using application as IDV, McIDAS-V, IDL, MATLAB, etc. for one easy management of the GEO-iSHAI binary files for all kinds of visualizations. As one example of the possibilities you can see Figures 8 and 9 taken from Martinez 2013. In order to show examples of the important applications for change monitoring see the loops and animations in the presentation in last NWC SAF workshop of PGE13 SPhR. In this presentation several examples on the use for nowcasting for case studies 12th August 2011 and 20th June 2013 were presented. Also the ideas for generalization to other GEO satellites and the extension to MTG-IRS applications in nowcasting are shown in this presentation.

http://www.nwcsaf.org/WorkshopsTrainingSurveys/2015UsersWorkshop/2015UsersWSPresentations/SESSION_III/martinez_nwcsaf_workshop_madridfeb2015.pps

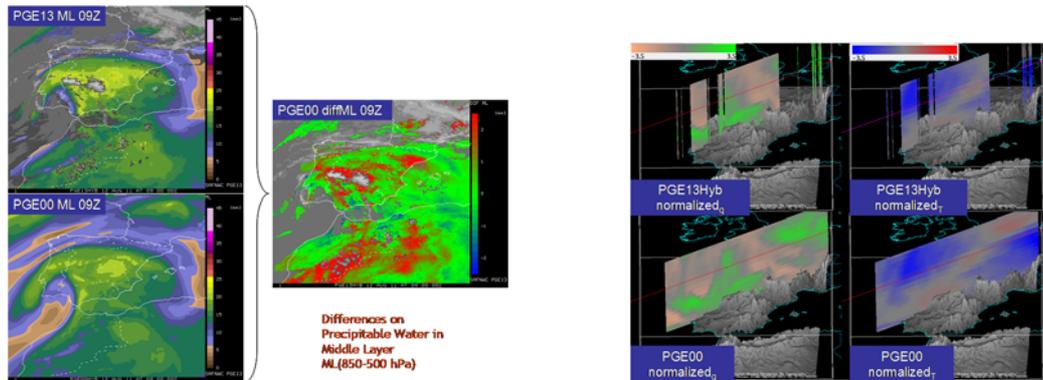


Figure 8: PGE13Hyb parameters diffML (precipitable water 850-500 hPa). Difference of precipitable water content between PGE13Hyb ML and ECMWF ML at 9 UTC on 12th August 2011. Vertical cross sections using McIDAS-V of normalized 3D arrays of T and q for 9 UTC on 12th August 2011 from PGE13Hyb and ECMWF (PGE00Hyb). To normalize them it has been subtracted the mean on every level for the t+12 ECMWF forecast in the region and divided by the standard deviation on the level for this slot.

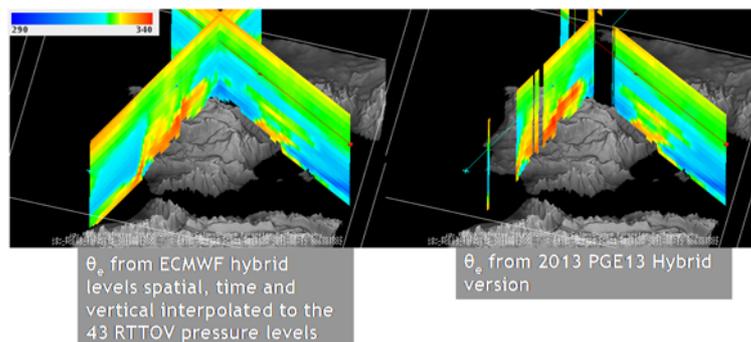


Figure 9: PGE13Hyb and ECMWF (PGE00Hyb) vertical cross sections of θ_e for 9 UTC on 12th August 2011.

2.4.3 Examples of GEO-iSHAI visualisation

Graphic displays of GEO-iSHAI product generated at the AEMET NWCSAF/MSG Reference System area will be available on real-time in the web site of the NWC SAF Help Desk (<http://www.nwcsaf.org>).

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

The best way to use GEO-iSHAI products is with adequate displays and using loops of images. In the NWC SAF web site it will be available near real time images and animations. Also images and animations from selected case studies will be provided.

The images corresponding to the 15 July 2015 at 12UTC are shown as an example in the Figures below.

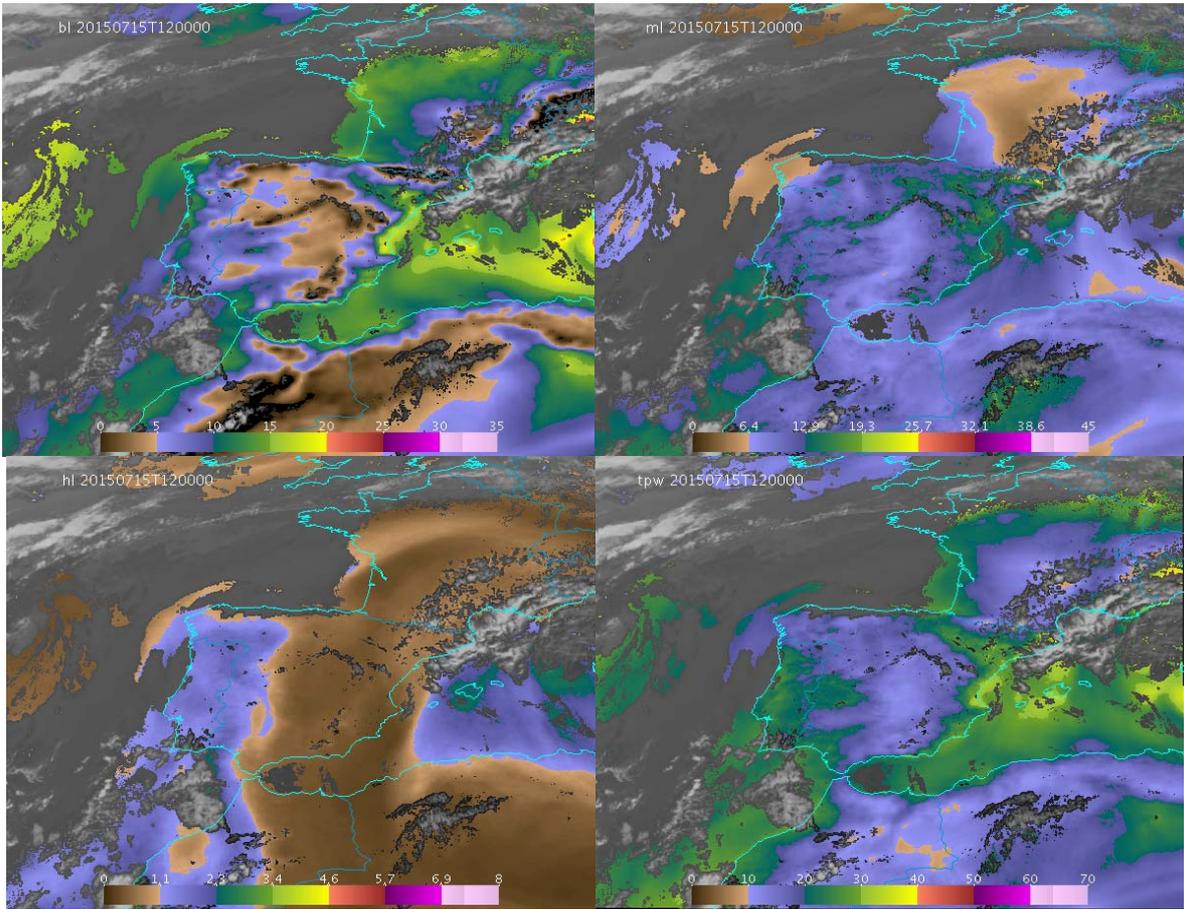


Figure 10: Example of GEO-iSHAI BL, ML, HL and TPW from 12 UTC on 15 July 2015 produced from SEVIRI on MSG-3.

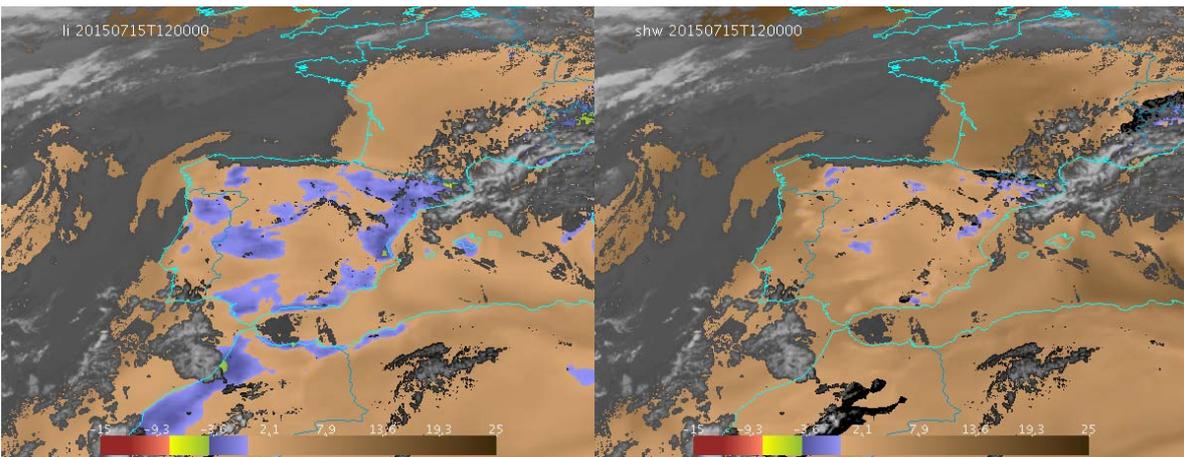


Figure 11: Example of GEO-iSHAI LI and SHW from 12 UTC on 15 July 2015 produced from SEVIRI on MSG-3.

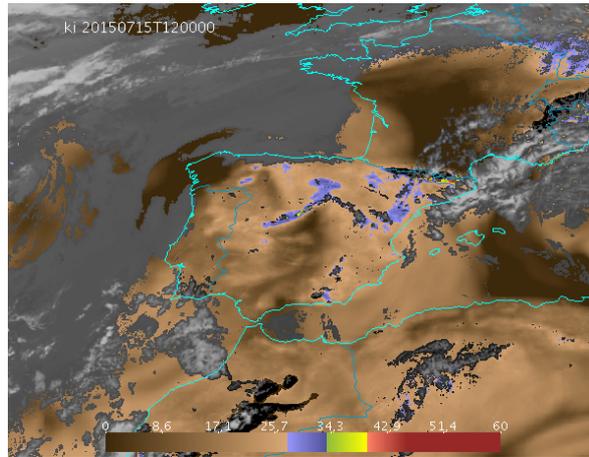


Figure 12: Example of GEO-iSHAI KI from 12 UTC on 15 July 2015 produced from SEVIRI on MSG-3.

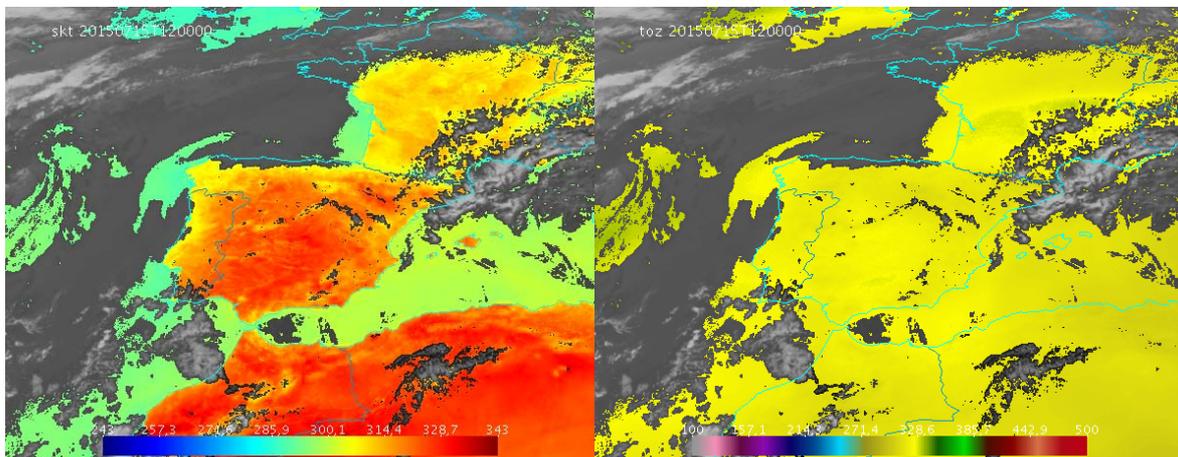


Figure 13: Example of GEO-iSHAI SKT TOZ from 12 UTC on 15 July 2015 produced from SEVIRI on MSG-3.

 	<p>Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO</p>	<p>Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 41/47</p>
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3. PRACTICAL CONSIDERATIONS

3.1 PROGRAMMING AND PROCEDURAL CONSIDERATIONS

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

In P mode, the spatial and temporal of background NWP profiles is made outside GEO-iSHAI and just the vertical interpolation/extrapolation to the 54 RTTOV-11.2 RTTOV pressure levels is made inside GEO-iSHAI code. In this case the spatial and temporal of background NWP profiles is made by the AllMappingNWP tool executed automatically by the Task manager in NRT or directly by the users on reprocessing.

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

3.2 EXCEPTION HANDLING

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

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

3.3 ASSUMPTIONS

- (1) The surface pressure used in the 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 dataset as common software elements and the incorporation of management functions on the NWC/GEO NWCLIB fixed IREMIS dataset has been selected from year 2007 following the RTTOV and Eva Borbas (U. Wisconsin) recommendations.

3.4 LIMITATIONS

- (1) iSHAI products are available over “clear” FORs only.
- (2) Since physical retrieval is an iterative process, computation is relatively expensive and an increase in the width of the FOR could be necessary when processing large regions.
- (3) The result can exhibit errors over mountain regions with large differences between the topography and the NWP topography. The same happens in desert pixels, where the difference on skin temperature between the NWP first guess and the actual 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 $0.5^\circ \times 0.5^\circ$ resolution to every 1 hour from $t+00$ to $t+24$ with $0.125^\circ \times 0.125^\circ$ resolution, have improved clearly the quality of the GEO-iSHAI outputs. 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) If possible, it is strongly recommended to the GEO-iSHAI users that use ECMWF as background NWP to make the effort to download also from the MARS the GRIB files on

 	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 42/47
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hybrid levels. 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. Fixed IREMIS monthly datasets has been selected from 2007 (Eva Borbas (U. Wisconsin) recommendation).

3.5 IMPLEMENTATION OF GEO-iSHAI

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

3.5.1.1 The GEO-iSHAI installation step

Previous condition and licences

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

Installation and building of the executable

The software installation procedure does not require special resources. It is restricted to decompress the distribution file (a gzip-compressed tar file) and to successfully build the executable GEO-iSHAI-v30 file to be stored into the *\$SAFNWC/bin* directory.

After the steps shown in [AD.7], GEO-iSHAI-v30 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 MSG satellite and for P and HYB modes. As all configuration files, it is an ASCII file, so further modification can be easily performed with a text editor. The configuration file manages all processes in the executable file.

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

3.5.1.2 The GEO-iSHAI preparation step

An output CMA netCDF file for the same slot and region is mandatory as input to GEO-iSHAI and by this reason it has to be executed *GEO-CMA-v40* before *GEO-iSHAI-v30* 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.

3.5.1.3 The GEO-iSHAI product execution step

The execution step is the real-time processing of SEVIRI images over the region. This process consists of the launch of the command *GEO-iSHAI-v30* along with the required parameters (slot, region file

 	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 43/47
---	---	--

name and model configuration file) by the Task manager after the GEO-CMA-v40 has finished. The *GEO-iSHAI-v30* is then performed following the corresponding configuration file. The use of the *GEO-iSHAI-v30* command is very easy on scripts. Here, an example of execution is provided:

```
GEO-iSHAI-v30 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 SEVIRI image

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

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

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

3.6 VALIDATION

An extensive validation for the year 2013 has been done. The applied methodology and the results are available in the Validation Report [RD.2]. Below only a brief summary of the validation with 2013 dataset is provided.

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

GEO iSHAI V3.0 summary of validation Results	Precipitable Water Low Layer – BL RMSE	Precipitable Water Medium Layer ML RMSE	Precipitable Water High Layer HL RMSE	Precipitable Water Total TPW RMSE	Showalter Index SHW RMSE
Against ECMWF Analysis – Over Sea Full Disk validation	0,688 (kg/m ²)	0,873 (kg/m ²)	0,102 (kg/m ²)	1,289 (kg/m ²)	1,134 (K)
Against ECMWF Analysis – Over Land Full Disk validation	0,438 (kg/m ²)	1,185 (kg/m ²)	0,139 (kg/m ²)	1,435 (kg/m ²)	0,726 (K)

Table 5: Summary of the GEO iSHAI statistical parameters in 2013 for odd pixels of GEO iSHAI validation dataset using as input to GEO iSHAI actual SEVIRI BTs bias corrected.

 	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 45/47
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4. SUMMARY

The availability of GEO-iSHAI allows an easy processing of SEVIRI images in an operational environment and in future for other GEO satellite images. The NWC/GEO Task Manager allows a synchronization of all tasks involved in the process (launching of events, reading of HRIT files, navigation, geographical and ancillary management, management of forecast NWP GRIB files, etc.).

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

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

The availability of PGE13 SPhR since version 2009 and GEO-iSHAI now has allowed creating a huge PGE13 and GEO-iSHAI training and validation dataset that has been very important in order to improve the operational version 2016. As the generation of training/validation dataset shows, the use of GEO-iSHAI allows generating spatially, temporally and vertically collocated dataset with NWP models, RAOB, GPS station, hyperspectral satellite, etc.

Thus, this fact will make possible to test some improvements not included in this version and it will allow testing the improvements needed for evolution of the physical retrieval algorithms in near MTG era. It will be basic for future releases of GEO-iSHAI the generalization of the process to generate training and validation dataset to other GEO satellites (Himawari, GOES-R and future MTG-FCI and MTG-IRS).

	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 46/47
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 	Algorithm Theoretical Basis Document for the Clear Air Products Processors of the NWC/GEO	Code: NWC/CDOP2/GEO/AEMET/SCI/ATBD/ClearAir Issue: 1.1 Date: 15 October 2016 File: NWC-CDOP2-GEO-AEMET-SCI-ATBD-ClearAir_v1.1.docx Page: 47/47
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