

Algorithm Theoretical Basis Document for "SEVIRI Physical Retrieval Product" (SPhR-PGE13 v2.0)

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The EUMETSAT Network of Satellite Application Facilities



Algorithm Theoretical Basis Document for "SEVIRI Physical Retrieval Product" (SPhR-PGE13 v2.0)

SAF/NWC/CDOP2/INM/SCI/ATBD/13, Issue 2, Rev.0 15 July 2013

Applicable to SAFNWC/MSG version 2013

Prepared by AEMET



REPORT SIGNATURE TABLE

Function	Name	Signature	Date
Prepared by M. A. Martinez (AEMET			15 July 2013
Reviewed by	Marcelino Manso		15 July 2013
Authorised by Pilar Fernández SAFNWC Project Manager			15 July 2013



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DOCUMENT CHANGE RECORD

Version	Date	Pages	CHANGE(S)	
0.1d	21 November 2008	50	Version prepared for PCR of PGE13 SPhR using the original ATBD provided by Jun LI (CIMSS/Wisconsin)	
0.1	24 July 2009	58	Version prepared for PGE13 SPhR v0.1 patch delivery to beta testers of NWCSAF 2009 version	
1.0d	9 April 2010	63	Submitted to DRI-2010 Review Board	
1.0	21 May 2010	54	Corrected after DRI 2010	
			Updated for version 2011.	
1.1	1 April 2011	52	New emissivity files to operate with MSG1, MSG2 and Rapid Scan mode.	
1.2	15 February 2012	49	Updated for version 2012. Update of BIAS correction coefficients for the 6 SEVIRI IR channels for MSG-1 and MSG-2. New FG non-linear regression coefficients. Computation of Empirical Orthogonal Functions (EOFs) for temperature and log(q) from ECMWF. New inverse covariance matrix computed and code update to manage inverse covariance matrix as configurable parameter.	
2.0	15 July 2013	56	Update for version 2013: regular PGE13 with update of coefficients calculated with 2102 period of PGE13 validation dataset. Update of emissivity atlases from IREMIS dataset 2012. Update for inclusion of PGE13Hyb module that allows the use of ECMWF GRIB files on hybrid levels as input	



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1. INTRODUCTION

The Eumetsat Satellite Application Facilities (SAFs) are dedicated centres of excellence for the processing of satellite data, and form an integral part of the distributed Eumetsat Application Ground Segment. SAFs are also dedicated centres for software development.

This documentation is provided by the SAF on Support to Nowcasting and Very Short Range Forecasting, NWCSAF. The main objective of the NWCSAF is to provide, develop and maintain software packages to be used with operational meteorological satellite data for nowcasting applications by National Meteorological Services and approved users. More information about the project can be found at the NWCSAF webpage, http://www.nwcsaf.org.

This document is applicable to the NWCSAF processing package for Meteosat Second Generation satellites, NWCSAF/MSG package.

1.1 PURPOSE AND SCOPE OF THE DOCUMENT

This document is the Algorithm Theoretical Basis Document (ATBD) for the PGE13 SEVIRI Physical Retrieval (SPhR) product of the NWCSAF/MSG software package. The purpose of this document is to provide a detailed description and the physical basis for the Physical Retrieval of temperature and moisture profiles with infrared (IR) brightness temperatures measured by the SEVIRI (Spinning Enhanced Visible and Infrared Imager) flown on the Meteosat second generation (MSG) meteorological satellites. 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 pixel or a Field of Regard (FOR) with M by M SEVIRI pixels.

It describes the PGE13 SPhR 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 PGE13 SPhR version v2.0, included in the NWCSAF/MSG v2013 software package delivery.



1.3 RATIONALE AND HISTORY OF PGE13 SPHR

In order to understand the reason to introduce a physical retrieval product, it must be taken into account the main objective of NWC SAF: to produce software packages for MSG and Polar satellites. In the case of NCWSAF/MSG package, the purpose of the NWC SAF algorithms is to be able to derive each parameter at pixel by pixel scale every 15 minutes over a region selected by the user (or 5 minutes in the case of Rapid Scan images).

In NWCSAF/MSG software packages prior to version 2010, the clear air parameters products were retrieved only using statistical retrievals. The core of the statistical retrieval for NWC SAF clear air products [PGE06 Total Precipitable Water (TPW), PGE07 Layer Precipitable Water (LPW) and PGE08 Stability Analysis imagery (SAI)] are neural networks for each parameter (Multi Layer Perceptron). This approach was selected at the beginning of the project in order to fulfil two important requirements stated in the User Requirement Document concerning the timeliness and the independence of NWP forecasted data.

During the 11th Meeting (February 2007), the Steering Group (SG) proposed to the AEMET Project Team to focus the work during the SAF CDOP phase on implementing a physical retrieval approach. The physical retrieval approach was not taken into account in previous phases of the NWC SAF due to constraints on computation time.

Following this decision, a Visiting Scientist Activity to make an assessment of this issue was approved. Jun Li from CIMSS at University of Wisconsin-Madison evaluated the advantages/disadvantages of two SEVIRI retrieval algorithms, MPEF and Clima (CM) SAF approaches, and analyzed the possibility of adapting to SEVIRI the new GOES-12 Sounder physical retrieval algorithm (physical iterative approach with regression as first guess) including all the improvements. In the NWC SAF Visiting Scientist Activity (VSA) report "Recommendation on Physical Retrieval Algorithm for SEVIRI Nowcasting Product", Dr. Jun Li introduced the existing physical retrieval algorithms, analysed the strength and weakness of each physical algorithm and summarized the recommendations on the physical retrieval algorithm for SEVIRI nowcasting products. As for any NWCSAF VS activity, the report is available at the official NWCSAF Web Page on: *http://www.nwcsaf.org/VSA.html#Visiting%20Scientist%20Reports*

Other activity related with the physical retrieval was the organization of the Workshop "Physical Retrieval of Clear Air Parameters from SEVIRI" in Madrid November 2007; it was organized by AEMET sponsored by EUMETSAT. The objective of this workshop was that several physical retrieval experts exchanged ideas and opinions previously to the implementation of a physical retrieval approach in the NWC SAF software package. All Workshop presentations are available on *https://www.nwcsaf.org/WorkshopsTrainingSurveys/2007PhysRetWS/Physical_Ret_Workshop_Open.html*.

Based on the Jun Li's VSA 2007 report and the recommendations of the Workshop, the Steering Group decided to develop a Physical Retrieval product on NWCSAF/MSG package. The proposed name of this new product is PGE13 SEVIRI Physical Retrieval (SPhR).

In March 2009 the Product Consolidation Review (PCR) took place in Darmstadt. The reviewers were in agreement that an initial version was distributed to selected beta users as a patch to 2009 version NWCSAF software package on summer.

In July 2009 the initial version was distributed to selected beta users (CM SAF, ZAMG and AEMET) as a patch to NWCSAF/MSG version 2009 software package. It has been internally operated at AEMET headquarters in near real time on a Linux PC since July 2009.

In May 2010 it has been approved the distribution as pre-operational product with the 2010 NWCSAF/MSG package.

In March 2011 in the CDOP 8th Steering Group meeting, the product has become operational.



In 2011 and 2012 it has been made some updates of the coefficients and all the coefficients are now calculated using the PGE13 validation dataset. Thus, all coefficients have been calculated only using MSG images and ECMWF profiles.

Summary of changes with respect to version 2012 of PGE13 SPhR

The regular PGE13 SPhR in version 2013 maintains the code of PGE13 SPhR version 2012 with the modifications of the patch made on summer 2012. Besides, the PGE13 SPhR coefficients have been updated. The PGE13 SPhR coefficients have been calculated with 2012 period of PGE13 validation dataset. Also the emissivity atlases have been updated using IREMIS datasets of 2012.

The NWC SAF/MSG package version 2013 continue with the mandatory uses of GRIB files on fixed pressure levels as background NWP input to regular PGE13, since the current version and the 2013 version of NWC SAF library only allows reading GRIB files on fixed pressure levels.

As one advance of future versions of PGE13 SPhR an optional module that allows the use of ECMWF GRIB files on hybrid levels as input to PGE13 and denoted hereafter as PGE13Hyb module has been developed and is delivered with version 2013.

Only minor changes are needed to incorporate the PGE13Hyb issues. Since the basis of the algorithm is the same the core of the ATBD is maintained. It has been considered more adequate to include paragraphs with grey background when needed for explain any PGE13Hyb module change or details.



DEFINITIONS, ACRONYMS AND ABBREVIATIONS

ABI	Advanced Baseline Imager
AEMET	Agencia Estatal de Meteorología (former INM)
AIRS	Atmospheric InfraRed Sounder
AMSR-E	Advanced Microwave Scanning Radiometer - EOS
ATBD	Algorithm Theoretical Basis Document
BL	Boundary Layer (1013hPa-850 hPa)
BT	Brightness Temperature
CDOP	Continuous Development and Operational Phase
CIMSS	Cooperative Institute for Meteorological Satellite Studies
СМа	Cloud Mask (also PGE01)
CM SAF	Climate Monitoring SAF
DEM	Digital Elevation Model
ECMWF	European Centre for Medium range Weather Forecast
EOF	Empirical Orthogonal Functions
EUMETSAT	European Meteorological Satellite Agency
FOR	Field of Regard
FOV	Field of View
GTOPO 30	Global 30 Arc Second Elevation Data - USGS - EROS Data Center
HDF	Hierarchical data Format
HL	High Layer (<500 hPa)
HRIT	High Rate Information Transmission
IASI	Infrared Atmospheric Sounding Interferometer
INM	Instituto Nacional de Meterología
IR	Infrared
KI	K-Index
LI	Lifted Index
LPW	Layer Precipitable Water
ML	Middle Layer (850hPa-500hPa)
MODIS	Moderate Resolution Imaging Spectroradiometer
MPEF	Meteorological Product Extraction Facilities
MSG	Meteosat Second Generation
NWC SAF	SAF on support NoWCasting and VSRF
NWP	Numerical Weather Prediction
PCA	Principal Component Analysis
PGE	Product Generation Element
RAOB	Radiosonde Observation
RTTOV	Rapid Transmissions for TOVs
SAF	Satellite Application Facility
SEVIRI	Spinning Enhanced Visible & Infrared Imager
SG	Steering Group
SAI	Stability Analysis Imagery
SHW	Showalter Index
SPhR	SEVIRI Physical Retrieval
SVD	Software Version Description
SW	Software To Ba Confirmed
TBC	To Be Confirmed
TBD	To Be Determined
TPW	Total Precipitable Water
URD	Users Requirement Document

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VSA Visiting Scientist Activity



REFERENCES

1.3.1 Applicable Documents

Ref.	Title	Code	Vers	Date
[AD.1]	Software User Manual for the SAFNWC/MSG Application: Software Part	SAF/NWC/CDOP2/INM/SW/SUM/2	7.0	15/12/11
[AD.2]	Product User Manual for "PGE13 SEVIRI Physical Retrieval" (SPhR– PGE13 v2.0)	SAF/NWC/CDOP2/INM/SCI/PUM/13	2.0	15/02/12
[AD.3]	Interface Control Document for the External and Internal Interfaces of the SAF NWC/MSG	SAF/NWC/CDOP2/INM/SW/ICD/1	7.0	15/12/11
[AD.4]	SAFNWC/MSG Output Products format definition	SAF/NWC/CDOP2/INM/SW/ICD/3	7.0	15/12/11
[AD.5]	Architectural Design Document for the INM related PGEs of the SAFNWC/MSG	SAF/NWC/CDOP2/INM/SW/AD/4	7.0	15/02/12
[AD.6]	Software Version Description Document for the SAFNWC/MSG Application	SAF/NWC/CDOP2/INM/SW/SVD/5	7.0	15/12/11
[AD.7]	Validation Report for "PGE13 SEVIRI Physical Retrieval" (SPhR– PGE13 v2.0)	SAF/NWC/CDOP2/INM/SCI/VR/14	1.0	15/02/12
[AD.8]	NWCSAF Product Requirements Document	SAF/NWC/CDOP2/INM/MGT/PRD	1.2	17/11/11
[AD.9]	Scientific Report: improvements in "PGE13 SEVIRI Physical Retrieval Product (SPhR)" using as input ECMWF GRIB files on hybrid levels	SAF/NWC/CDOP2/INM/SCI/RP/02	1.0	15/07/13

Table 1: List of Applicable Documents

1.3.2 Reference Documents

Ref.	Title
[RD.1]	
[RD.2]	

Table 2: List of Referenced Documents



2. PGE13 SPHR PRODUCT ALGORITHM

The PGE13 SPhR algorithm version 2.0 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-Regard (FOR) with contains M x M pixels. This product has been developed within the NWC SAF context, aiming to support nowcasting applications.

The main outputs of PGE13 SPhR product are Total Precipitable Water (TPW), Layer Precipitable Water (LPW) (corresponding to low layer water vapor [surface pressure-850 hPa], middle layer water vapor [850 hPa-500 hPa] and high layer water vapor [<500 hPa]), Lifted Index (LI), Showalter Index (SHW) and K-index (KI) calculated from the retrieved profiles of temperature and humidity.

Besides the main outputs, the differences between TPW, LPWs, LI, SHW and KI calculated with the retrieved profiles of temperature and humidity with TPW, LPWs, LI, SHW and KI calculated from the spatial, temporal and vertical interpolated profiles from background NWP are written as other outputs (following 2007 Madrid Workshop recommendation). In future versions and if any users requirement is set, other stability indices can be calculated from the retrieved temperature and humidity profiles and they could be added as outputs of PGE13 SPhR.

The main inputs of the PGE13 SPhR product are SEVIRI IR brightness temperature (BT) and numerical weather prediction (NWP) forecast model GRIB files. SEVIRI provides one full resolution image (3 x 3 km) every 15 minutes, 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 high resolution temporal and spatial 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 PGE13 SPhR animations will be available at the NWC SAF MSG web page (http://www.nwcsaf.org/) generated with NWC SAF reference system at AEMET.

NWC SAF PGE13 (SPhR) is only generated in clear sky pixels. As cloud mask is a mandatory input to PGE13 SPhR, NWC SAF PGE01 Cloud Mask (CMa) must be executed before PGE13 SPhR. That is made by the SAFNWC/MSG 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 (NWC SAF PGE01).

Once the outbreak of convection occurs, the TPW, LPWs, LI, SHW and KI values provided by PGE13 SPhR in clear air pixels surrounding the convective system may help the forecasters to foresee the evolution of convection. The PGE13 SPhR outputs cannot predict by themselves whether storms will occur. They provide to forecasters a general idea of some of the ingredients and the convective forcing if thunderstorms do develop. Region with unstable values on the stability indices combined with high precipitable water values indicate that the troposphere is near saturation and has instability. Precipitation 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 Field-of-Regard (FOR) basis. A FOR consists of M x M SEVIRI pixels of infrared bands. The default FOR size for SEVIRI process is 3 x 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 PGE13 SPhR 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: regression and the iterative physical retrieval. The cloud mask processing

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sometimes identifies cloud contaminated pixels as clear, and therefore an 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 is also available and it 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 SEVIRI BTs and the synthetic BTs calculated from the profiles and takes into account the limited number of channels and the spectral information of the SEVIRI instrument, the PGE13 SPhR can only slightly improve the humidity profiles beyond of the background NWP in middle-high levels and can only improve the spatial distribution of the retrieved fields. Thus, what PGE13 SPhR provides is a good spatial and temporal variation monitoring of the precipitable water and stability indices fields. This fact must be taken in account by the users when the PGE13 SPhR outputs are used on nowcasting.

In the section 2.1 the outline of the PGE13 SPhR 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 PGE13 SPhR outputs are described briefly.

2.1 PGE13 SPHR PROCESSING OUTLINE

As a whole, PGE13 SPhR code is designed in a modular way, so that it can be easily handled and modified it.

For the selected region, the initialization gives access to SEVIRI BTs, PGE01 Cloud Mask (CMa), satellite zenith angle and ancillary data (topographic data, land-sea mask, longitude, latitude). Only if the pixel or the FOR (in case of MxM pixels processing) is labelled as clear air and the satellite zenith angle of this pixel or FOR is below the configurable maximum zenith threshold, the Physical Retrieval module is applied and the PGE13 TPW, LPWs, LI, SHW and KI 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, 10.8, 12.0 and 13.4 μ m) and forecasted NWP fields which are used as background information. PGE13 SPhR 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.

Cloud Mask (CMa) computed by PGE01 is used as mandatory input to PGE13 SPhR and the process is only performed for pixels, or FOR (in case of MxM pixels processing), labelled as clear air.



Figure 1: PGE13 SPhR inputs and outputs scheme.

Bellow, the main steps in the algorithm and the sections where the physical bases are provided are described; in [AD.2] there is a similar description where the configurable parameters at each step in the actual version of the algorithm 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, get IR emissivity maps for region, initialisation of RTTOV-9.3, getting calibrated SEVIRI BTs and associated geographical ancillary data for region to process and reading of PGE01 CMa for region.
 - Optional thinning of SEVIRI BT to process on FOR of M x M pixels (M is a configurable parameter 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)
 - To get collocated NWP forecast temperature and moisture profiles. NWP fields of temperature and humidity (T+0 to T+24 hours range forecast) are spatially, temporally and vertically interpolated. Conversion from relative to specific humidity is also made at this step. The spatial (horizontal) interpolation to the FOR position is calculated outside of PGE13 SPhR with common functions of NWCSAF library. The interpolation in the vertical is made assuming the 43 pressure levels of RTTOV as fixed levels (See section 2.2.2)

PGE13Hyb note:

In the case of PGE13Hyb module all the NWP process is made inside the PGE13Hyb code. The PGE13Hyb open the previous and next ECMWF GRIB files on hybrid levels to the time of the image, makes the vertical interpolation on ECMWF position to the 43 RTTOV-9.3 pressure levels, makes the temporal



interpolation to the date of the image and finally makes the spatial interpolation just over clear air processed FOR.

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

- Bias adjustment of SEVIRI BTs. The bias correction regression coefficients are read from the configuration file and BT bias correction is made (See section 2.2.3).
- Execution of non linear regression 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).
- 2. Processing:
 - Iterative execution of Physical Retrieval Module up to the maximum number of times established 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)
 - To check if the retrieved profiles of temperature and specific humidity are between limits and they are physically meaningful.
 - To perform direct calculation of TPW, LPWs, LI, SHW and KI parameters at FOR from the retrieved profiles of T and q.
 - To 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.
 - Optional writing of the intermediate T and q profiles at the different algorithm steps.
- 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, the IR BT degraded to 7 bits (range [128 255]) values for the channel included in the configuration file is stored. 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 output is coded as images in HDF5 format file (See section 2.2.8.2).

2.2 PGE13 SPHR 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

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wave channels are sensitive to temperature and water vapour conditions and allow a retrieval of precipitable water parameters and the instability indices.

The problem to be solved here is to retrieve, with enough accuracy, profiles of temperature and humidity from few some 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 processing 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 bands in the range [6.2 - 13.4] microns, within which two bands contain strong water vapour absorption, one has strong ozone absorption and one has CO₂ absorption. The other SEVIRI infrared bands are window bands that contain the surface skin temperature, surface emissivity and low level moisture information. The IR 13.4 band contains the CO₂ absorption and the radiance contains the temperature information; while the WV6.2 and WV7.3 bands contain strong water vapour absorption and the radiances contain both temperature and water vapour concentration information. For the physical retrieval module [WV6.2, WV7.3, IR10.8, IR12.0, IR13.4] SEVIRI BTs are used in the current version of the software, and the use of IR8.7 over ocean is pending of further studies. Concerning the non linear regression module, the current version of the software also allows for the use of IR8.7 BT, but this possibility is not used for the time being. The decision not to use the IR8.7 channel in version 2010 was due to the uncertainties in the performance over Sahara desert caused by the lower IR8.7 channel there are no lower performances over Sahara pixels; but a test to include IR8.7 channel and to make the validation is foreseen for future versions.

The PGE13 SPhR algorithm tries to infer an actual temperature and humidity profile from the satellite observed brightness temperatures in a given set of spectral bands. 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.

In addition to the background, a first guess which is the starting point in the iteration procedure is used. The first guess is important, for example, if it contains structure similar to the real atmosphere, as the final solution will be good. A typical first guess field is a short-term forecast. However, it was found that a regression is usually better than the forecast since the regression uses combined forecast and SEVIRI brightness temperatures as predictors, so the regression will be used as the first guess (See section 2.2.4).

The air mass parameters are then derived from the retrieved profile. From clear sky brightness temperatures within 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) and instability indices: Lifted Index (LI), Showalter Index (SHW) and K-Index (KI).

Major limitations of the optimal estimation are the high computational effort and the fact that the retrieved profiles tend to retain features of the first guess due to the low spectral resolution and the use of a few spectral bands.

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In order to assure that the IR brightness temperatures are not contaminated by clouds, dust or snow/sea ice, the NWC SAF CMA product must be previously run. Thus, the PGE13 SPhR will be processed and calculated only over clear pixels determined by PGE01 CMa,.

2.2.1 Use of Field of Regards (FOR)

The PGE13 SPhR execution on FOR (window of M x M pixels) basis has been evaluated, instead of pixel by pixel basis, in Jun Li's 2008 VSA. This has been done 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 for the width of the FOR. The width of the FOR (M x M pixels) is an adjustable parameter in the configuration file. This allows adjusting M depending on the size of the region to process and the machine characteristics of the user. In some papers, the Field-of-View (FOV) is used instead to use the word pixel.



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 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° 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.



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.



2.2.2 NWP data Interpolation to 43 RTTOV levels of NWP profiles.

As explained before, it is convenient to use as background profile [t+00, t+24] hours range forecast NWP output from a model. The NWCSAF library provides software which should be able to work with any NWP model and it should accept the set of levels available on the NWP files provided by the users to the NWC SAF. The same NWP GRIB files that are actually used with NWCSAF 2013 to run PGE01 to PGE12 can be used. Hence, any user that is running NWCSAF/MSG 2013 package should be able to run PGE13.

PGE13Hyb note:

In the case of PGE13Hyb module ECMWF GRIB files on hybrid levels are used as input. But, ECMWF GRIB files on pressure levels are also needed in order to execute PGE01 CMa before execution of PGE13Hyb code.

Since it is not adequate to provide specific error matrices, EOFs, regression coefficients, etc for the great number of combination in user pressure levels, it is necessary to perform the interpolation of different NWP model to 43 RTTOV pressure levels. The NWCSAF/MSG package provides the functions and tools to manage NWP GRIB files and to make the spatial, temporal and vertical interpolation in order to get a collocated background profile of temperature and humidity at the FOR position.

The spatial interpolation, in the horizontal, is made outside the PGE13 SPhR code with the tools existing since previous version of NWCSAF/MSG package. On real time, the NWC SAF's Task Manager makes it upon the arrival of new NWP data as a predefined task. See [AD.2] for details.

Temporal and vertical interpolations are made inside PGE13. 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 NWCSAF library.

For vertical interpolation, an "ad hoc" function has been added to PGE13 SPhR. The solution adopted has been the development of a function that interpolates the temperature and humidity profiles from any set of pressure levels to 43 RTTOV pressure levels calling the RTTOV function "rttov_intavg_prof". This RTTOV function interpolates linearly in logarithm of the pressure the NWP forecast temperature and humidity fields available on user-defined vertical pressure levels to the 43 RTTOV pressure levels. In order to maintain the same NWP GRIB files as in NWCSAF 2009 version, which uses relative humidity as input, the conversion from relative humidity to specific humidity is done within PGE13 SPhR code by using the same routines used within Meteo-France PGE03.

PGE13Hyb note:

In the case of PGE13Hyb module the whole NWP process is made inside the PGE13Hyb code. The PGE13Hyb open the previous and next ECMWF GRIB files on hybrid levels to the time of the image, makes the vertical interpolation on ECMWF position to the 43 RTTOV-9.3 pressure levels, makes the temporal interpolation to the date of the image and finally makes the spatial interpolation just over clear air processed FOR.

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



Figure 5: Example conversion of Relative humidity profile at 15 pressure levels (left) to specific humidity and vertical interpolation to 43 RTTOV pressure levels (right).

As result of this process, time and spatial collocated with the SEVIRI image background NWP (T, q) profiles interpolated at the 43 RTOV pressure levels are obtained from the background NWP GRIB files with (T, Relative Humidity) profiles at the user fixed pressure. This pre-processing allows NWCSAF/MSG users to be able to run PGE13 SPhR without modifying their background NWP GRIB files supply. But, as it can be concluded from the Validation Report [AD.7], the user is stronger recommended to provide as many fixed pressure levels as possible with the most uniform and widest vertical distribution from the selected NWP model to feed the NWCSAF package.

2.2.3 BT bias correction

Brightness temperature bias adjustment is very important for product quality. The original satellite measurements must be bias-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 correction is based on finding the difference between the observed SEVIRI BTs and those simulated from the radiative transfer model (here synthetic RTTOV-9.3 BTs). 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 bands might not be reliable especially on desert pixels. By this reason, the BT bias correction using only sea observations has been done. BT bias correction for water vapour ($6.2 \mu m$ and $7.3 \mu m$) and CO2 ($13.4 \mu m$) absorption bands should help the retrievals.

The coefficients of the bias adjustment's robust regression are read from the configuration file using NWCSAF library. Meteosat 8 and Meteosat 9 have slight differences. Hence, separated configuration files for MSG-1, MSG-2 and MSG-3 with the bias correction parameters will be provided. When MSG-4 will be launched, initial bias configuration will be provided. More details in section 2.3.3.1.

Users desiring to run PGE13 SPhR without SEVIRI BT bias corrections can edit the PGE13 model configuration file and set the scale keywords to "1.0" and the offset keywords to "0.0".

PGE13Hyb note:

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Since error between actual SEVIRI BTs and synthetic RTTOV BTs depends on the profiles used to calculate the synthetic RTTOV BTs, the bias correction coefficients should be recalculated with ECMWF model data from profiles on hybrid vertical levels. By this reason, SEVIRI BTs bias correction coefficients calculated with ECMWF model data from profiles on hybrid vertical levels are written in the default configuration file for PGE13Hyb module.

2.2.4 Use regression as first guess

The PGE13 SPhR algorithm uses the regression as the first guess; and the regression uses SEVIRI IR BTs and NWP forecast as basic predictors. The predictands include temperature, specific humidity profiles and the skin temperature. Since SEVIRI only has a few sounding spectral bands, the temperature/moisture profiles from numerical weather prediction (NWP) forecast model are used as additional predictors. Here, the temperature forecast between 100 and 1013 hPa (27 levels), the specific humidity forecast between 286.6 and 1013 hPa (20 levels), the latitude and the fraction of land in pixel are included as additional predictors.

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

$$Z = \sum_{j=1}^{N} A_{j} \cdot Tb_{j} + \sum_{j=1}^{N} B_{j} \cdot Tb_{j}^{2} / 250 + C \cdot p_{s} + D \cdot latitude + E \cdot p_{land} + \sum_{l=1}^{ntemp} F_{ll} \cdot T_{l} + \sum_{l=1}^{nq} G_{wl} \cdot \log(q_{l}) + H_{0} \quad Eq. 1$$

Where:

- Z is one of the following parameters: temperature or specific humidity at the 43 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 43 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 and H are regression coefficients; N, *ntemp* and *nq* are total number of SEVIRI IR spectral bands, number of temperatures and number of specific humidity used as predictors.

PGE13Hyb note

The regression equation has the following format for every one of the 76 fixed zenith angles in the case of PGE13Hyb module:

$$Z = \sum_{j=1}^{N} A_{j} \cdot Tb_{j} + \sum_{j=1}^{N} B_{j} \cdot Tb_{j}^{2} / 250 + C \cdot p_{s} + D \cdot latitude + E \cdot p_{land} + \sum_{l=1}^{43} F_{ll} \cdot T_{l} + \sum_{l=1}^{43} G_{wl} \cdot \log(q_{l}) + H \cdot T_{skin} + G_{o} \qquad Eq. \ 1(PGE13 \ Hyb)$$

Where:

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

In PGE13Hyb case all of the 43 levels (whole profile) T and q profiles are used in the regression.

By these reasons the FG regression coefficients are different to the ones for regular PGE13. Then the filename on the PGE13 configuration file for processing with PGE13Hyb must point to one file with FG regression coefficients calculated for PGE13Hyb module.



Figure 6: Regression Flowchart of the SEVIRI retrieval process

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. Each coefficient set corresponds to a local zenith angle ranging from 0 to 75 degree. A regression set has 87 predictands (43-T, 43- q and Tskin).

The code is prepared to use 6 out of 8 (6.2 μ m, 7.3 μ m, 8.7 μ m, 10.8 μ m, 12 μ m, and 13.4 μ m) SEVIRI IR bands for baseline predictors. Considering the diurnal changes in Band 5 (3.9 μ m), this spectral band is not used in the regression. BT of IR8.7 channel can be only used at this step in the code. In the version 2010 default FG regression file, the coefficients for IR8.7 BT has been fixed to 0.0 and the IR8.7 BT is not used in the algorithm.

In summary, the following combination (in Table 3) is recommended for the first guess and background options. Option 1 is recommended, and option 2 is acceptable if regression is not used.

1 Forecast Regression Forecast error covaria	Option	Background (X_b)	First guess option (X_{FG})	Background error covariance (B)
	1	Forecast	Regression	Forecast error covariance
2 Forecast Forecast Forecast error covaria	2	Forecast	Forecast	Forecast error covariance

Table 3: Options for background and first guess selection.

Note that, in practice, the background can also be from the regression since the regression is close to the background. We found that the use of regression as both background and first guess provides the best results. This practical approach is not consistent with the theory of maximum likelihood as the brightness temperatures are used twice in both regression and physical retrieval, while it is consistent with the regularization inverse theory which is more mathematically solid. Therefore, for practical purposes, the regression is recommended for both first guess and background in the physical retrieval.

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In section 2.3.3.2. a summary of the process to calculate the FG regression coefficients in version 2010 is made. The full description is provided in [AD.7].

2.2.5 Mathematical Description of Physical Retrieval module

In this section the Physical retrieval module is described. In PGE13 SPhR 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 PGE13 SPhR approach uses an optimal method of combining observations with a background (in PGE13 SPhR from the FG regression) which accounts for the assumed error characteristics of both. The variational retrieval is performed by adjusting the atmospheric profile state, X, from the First Guess, X^{FG}, to minimize a cost function (Rodger 1976; Li and Huang 1999; Li et al. 2008). The regularization parameter (also called smoothing factor) is introduced for convergence and solution stability. The cost function is defined by

$$J(X) = \begin{bmatrix} Y^{m} - F(X) \end{bmatrix}^{T} E^{-1} \begin{bmatrix} Y^{m} - F(X) \end{bmatrix} + \begin{bmatrix} X - X^{FG} \end{bmatrix}^{T} \gamma B^{-1} \begin{bmatrix} X - X^{FG} \end{bmatrix} Eq. 2$$

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

By using the Newtonian iteration

$$X_{n+1} = X_n + J^{"}(X_n)^{-1} \cdot J^{'}(X_n)$$
 Eq. 3

The following Quasi-Nonlinear iterative form is obtained

$$\delta X_{n+1} = \left(F_n^{T} \cdot E^{-1} \cdot F_n^{T} + \gamma B^{-1} \right)^{-1} \cdot F_n^{T} \cdot E^{-1} \cdot \left(\delta Y_n + F_n^{T} \cdot \delta X_n \right) \qquad Eq. \ 4$$

Where:

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

$$\delta X_{n} = X_{n} - X^{FG};$$

$$\delta Y^{m} = Y^{m} - F(X_{n})$$

F' is the tangent linear operative (Jacobian) of forward model **F**. The RTTOV-9.3 is used for forward model (**F**) and Jacobian (**F'**) calculations.

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

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

$$X - X^{FG} = \Phi A , \qquad Eq. 5$$



Where
$$A = (\alpha_1, \alpha_2, ..., \alpha_M)$$
, and $\Phi = \begin{vmatrix} \Phi_T & 0 & 0 \\ 0 & \Phi_q & 0 \\ 0 & 0 & \Phi_{T_s} \end{vmatrix}$

 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 specific humidity profiles, $\Phi_{Ts} = 1$, and $M = \tilde{N}_T + \tilde{N}_q + 1$. In PGE13 SPhR 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. (4) becomes

$$A_{n+1} = (\tilde{F}_{n}^{T} \cdot E^{-1} \cdot \tilde{F}_{n} + \gamma B^{-1})^{-1} \cdot \tilde{F}_{n}^{T} \cdot E^{-1} \cdot (\delta Y_{n} + \tilde{F}_{n} \cdot A_{n})$$
 Eq. 6

where $A_0 = 0$, and

$$\left\|F(X_n) - Y^m\right\|^2 = \sigma^2, \qquad Eq. 7$$

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

Eq.(5) and Eq.(6) are applied to derive the solution from SEVIRI brightness temperatures.



Figure 7: Variational iterative physical flowchart of the SEVIRI retrieval process

In the PGE13 SPhR 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. (4) are 87 x 87; but matrix dimensions

in Eq. (6) 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 [AD.2] it is described how the user can configure several parameters of the PGE13 SPhR 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 $\mathbf{Y}^{\mathbf{m}}$ represents the satellite measured brightness temperatures in N spectral bands (6.2 µm, and 7.3 µm, 10.8 µm, 12 µm, and 13.4 µm are used).

2.2.5.2 <u>Use RTTOV-9.3 as radiative transfer model and use its linear tangent model for</u> <u>Jacobian calculation</u>

RTTOV version 9.3 is used in the PGE13 SPhR v2.0 algorithm implementation. Calculations are based on the atmospheric profile, surface skin temperature and surface emissivity in clear skies. The RTTOV is maintained and supplied by the NWP SAF.

2.2.5.2.1 Calculated brightness temperature (Y_n)

The calculated 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 spectral bands.

Since the RTTOV radiation model is used for the radiative transfer calculations, the profile parameters are represented at a maximum of L levels. (L = 43). 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 nth 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:

$$F_n' = \frac{\delta Y_n(i)}{\delta X_n(j)} \qquad \qquad Eq. 8$$

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Where i is the spectral band 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 spectral bands 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.



Figure 8: SEVIRI (dash line) and ABI (solid lines) Jacobian calculations for temperature (left panel) and water vapour mixing ratio (right panel) with U.S. standard atmosphere and a local zenith angle of zero. The units of x-axis are dBT/dp when one increment is made in T profile (left) and one increment is made in log(q) profile (right) at this level.

Figure 8 shows the temperature (left panel) and water vapour mixing ratio (right panel) Jacobian calculations for some SEVIRI (dash lines) and ABI (solid line) IR spectral bands from U.S. standard atmosphere with a local zenith angle of zero.

Since Jacobian from RTTOV-9.3 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 μ m band provides temperature profile information; while 6.2 and 7.3 μ m spectral bands provide water vapour information. The information from forecast temperature profile along with the 13.4 μ 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 bands also contain temperature information. The 12 μ m and 13.4 μ m bands 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 are fixed to 0.0 and the type of surface is fixed to sea, then RTTOV internally calculates emissivity values for the sea pixels. The names of the files with these emissivity maps values are read from the PGE13 SPhR model configuration file of the product (see [AD.2]).

2.2.5.3 Discrepancy principle for regularization parameter

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

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

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

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

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

Objective selection of γ is very important for accurate and stable solution. The discrepancy principal is used to select this regularization parameter (Li and Huang 1999) which is reflected by Eq. (7), where

$$\sigma^2 = \sum_{k=1}^{N} e_k^2 \qquad \qquad Eq. 9$$

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

Usually σ^2 can be estimated from the instrument noise and estimated radiative transfer model error but in version 2013 it has been calculated from the root mean square between actual SEVIRI BT after bias correction and synthetic RTTOV BT on sea pixels.

For simplicity, a numerical approach (Li et al. 2000) is adopted for solving Eq. (7); γ is changed in each iteration according to

$$\gamma_{n+1} = q_n \gamma_n, \qquad \qquad Eq. \ 10$$

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

Based on Eq. (10), q is obtained in each iteration by satisfying the following conditions:

$$q_{0} = 1.0$$

If $||F(X_{n}) - Y^{m}||^{2} < \sigma^{2}$, then $q_{n} = 1.1$;
If $||F(X_{n}) - Y^{m}||^{2} = \sigma^{2}$, then the iteration stops;
If $||F(X_{n}) - Y^{m}||^{2} > \sigma^{2}$, then $q_{n} = 0.9$;

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



2.2.5.4 Iteration checking and residual estimation

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

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

If $\delta^2 < Rs_{n+1} < Rs_n$, iteration is convergent, continue to next iteration.

If $Rs_{n+1} < sd$ or $|Rs - \delta^2| < 0.05$ 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 sd parameters are configurable by the user just by changing the values in the PGE13 SPhR configuration file. (Keywords: MAX_ITERATIONS and MAX_RESIDUAL).

2.2.6 Other considerations

For computation efficiency, the following transform can be performed for Eq. (6):

$$\overline{F_n} = E^{-\frac{1}{2}} \cdot \widetilde{F_n}$$

$$\delta \overline{Y_n} = E^{-\frac{1}{2}} \cdot \delta Y_n$$
Eq. 11

Then Eq. (6) becomes

$$A_{n+1} = \left(\overline{F_n}^{T} \cdot \overline{F_n} + \gamma B^{-1}\right)^{-1} \cdot \overline{F_n}^{T} \cdot \left(\delta \overline{Y_n} + \overline{F_n} \cdot A_n\right) \qquad Eq. 12$$

Using Eq. (12) instead of Eq. (6) will avoid some matrix multiplication and reduce computation time. The software has been codified using Eq. (12).

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 (PGE01). 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_RMS: root mean square of differences between the SEVIRI and calculated brightness temperature.
 - Convergence error: number of iterations where the convergence has failed.



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 clear air pixels inside the FOR. The selection of the post-processing method is made in PGE13 SPhR 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.

In future versions, bilinear interpolations with FOR neighbours could be implemented.



Figure 9 : Zoom of K-Index processed with BT at warmest pixel in the IR10.8. The default postprocessing "filling FOR" option (left) and the "not filling FOR" option (right).

2.2.8.2 Writing of outputs on HDF-5 file

The units of precipitable water (TPW and LPW) parameters are kg/m^2 while the units of instability 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.

Each clear air parameter output is written as an integer (range [8 - 127]) after scaling and offset. The quality flags are written using bits fields.

For cloudy pixels, determined by PGE01 (CMa), the configurable IR band is stored as another field degraded to 7 bits (range [128 - 255]) values for the channel included in the configuration file. This will later be used to generate adequate images in which cloudy pixels appear as grey scaled pixels and clear pixels appear as colour scaled pixels.

2.3 ALGORITHM INPUTS, COEFFICIENTS AND FILES

This section describes briefly the inputs and coefficients files needed to process the PGE 13 SPhR and it provides a guide on how they have been obtained. These files are available in the NWC SAF software package and they are needed by the PGE13 SPhR software. In [AD.2] and [AD.3] 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) PGE01 Cloud Mask.
- iii) NWP GRIB files from range [t+0, t+24] hours forecasted.

Geographical data from NWCSAF functions

- a. Longitude.
- b. Latitude.
- c. Zenith angle.

• Coefficients

- 1. Bias corrections coefficients.
- 2. Regression coefficient file.
- 3. Error covariance matrix of background and first guess (B).
- 4. Error covariance of observation matrix (E).
- 5. Empirical Orthogonal Functions coefficients.
- 6. RTTOV-9.3 coefficients for the MSG satellites are also needed.

• Geographical static data files

- 1. IREMIS surface IR emissivity for SEVIRI bands from University of Wisconsin baseline fit database remapped to SEVIRI projections (0° W and 9.5° E).
- 2. Topographic data.
- Configuration File of PGE13 SPhR

2.3.1 Inputs

2.3.1.1 SEVIRI BT

Several SEVIRI IR channels are the main input to PGE13 SPhR. The following SEVIRI IR BT values are needed at full IR spatial resolution:

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

Table 4: List of SEVIRI IR channels used in PGE13 SPhR version 2013.

The code is prepared to use 6 out of 8 (6.2 μ m, 7.3 μ m, 8.7 μ m, 10.8 μ m, 12 μ m, and 13.4 μ m) SEVIRI IR bands for baseline predictors. Considering the diurnal changes in IR3.9 μ m, this spectral band is not used in the PGE13 SPhR algorithm. Considering the absorption by ozone in IR9.7 μ m, this spectral band is not used in the PGE13 SPhR algorithm.

In this version, the IR 8.7 BT can only be used in the First-Guess non linear regression step. The use of IR8.7 BT over ocean on physical retrieval should be studied (the 8.7 μ m has good boundary layer moisture information but might be affected by dust aerosol) for future versions.

BT of IR8.7 channel can be only used at FG regression step in the code. In the version 2013 default FG regression file, the coefficients for IR8.7 BT has been fixed to 0.0 and the IR8.7 BT is not used in the algorithm. In case of using Jun Li's First-guess regression coefficients file, the IR8.7 BT is only used at FG non linear regression step.



2.3.1.2 PGE01 Cloud Mask (CMa)

NWC SAF PGE13 (SPhR) is only generated in clear sky pixels. As the PGE01 Cloud Mask is a mandatory input to PGE13 SPhR, NWC SAF PGE01 Cloud Mask (CMa) must be executed before PGE13 SPhR. SAFNWC/MSG 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 (NWC SAF PGE01).

2.3.1.3 Background NWP data

Background numerical weather profiles from t+00 to t+24 hour forecast are needed as mandatory input to PGE13 SPhR. These NWP data need to be spatially, temporally and vertically interpolated to get NWP data collocated with SEVIRI data. To maintain continuity with the NWP GRIB files dataset used by PGE01-12 and to avoid changes in NWCLIB software, version 2.0 of PGE13 SPhR uses relative humidity parameter as input instead of the specific humidity internally used by the software and information at fixed pressure levels instead of the hybrid levels that provide higher quality.

PGE13Hyb note:

In the case of PGE13Hyb module ECMWF GRIB files on hybrid levels from t+00 to t+24 hour forecast are used as input. See PGE13Hyb notes in [AD.2].

The spatial, temporal and vertical interpolation to get NWP data collocated with SEVIRI data is full made inside the PGE13Hyb module.

In PGE13Hyb case humidity profile parameter from ECMWF MARS is q and it is not needed the conversion from relative humidity.

But, ECMWF GRIB files on pressure levels are also needed in order to execute PGE01 CMa before execution of PGE13Hyb code.

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 SAF 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 PGE to make the remapping process. See [AD.2] for details.

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 NWCSAF library.

2.3.3 Coefficients

2.3.3.1 BT bias correction coefficients

In PGE13 SPhR such BT bias correction has been assessed in an independent step, e.g. by comparing the clear sky SEVIRI BTs with the calculated RTTOV BTs using the same radiative transfer model and collocated forecast/analysis atmospheric profiles that will be used in the PGE13 code. This is the process followed to calculate the SEVIRI BT bias correction for 2013 version of PGE13 SPhR using the PGE13 validation and training dataset. Full details of the process are described in [AD.7] or Martinez 2011 and only a summary is made bellow.

To generate the SEVIRI BT files, the beta version of PGE13 code that writes on \$SAFNWC/tmp the binary files calibrated in BTs has been used. Thus, the same radiative transfer model RTTOV-

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9.3 and the same kind of background NWP data that will be used on real time operation are used in the bias estimation (ECMWF GRIB files with 15 fixed pressure levels).

Here, the bias estimation dataset has been built with synthetic RTTOV BTs (00 and 12 UTC ECMWF analysis GRIB files with 15 fixed pressure levels temperature and relative humidity profiles with a grid step of 0.5° x 0.5° and using RTTOV-9.3) and with SEVIRI BTs for a period of 6 months (from April 2011 to September 2011). In this bias correction dataset, inside the 3400x3400 Full-Disk region only pixels over ocean have been considered. The SEVIRI BTs at the IR10.8 warmest clear pixel have been obtained in 25x25 FOR. After outliers filtering, a robust regression using LADFIT IDL function is applied to the dataset.



Figure 10: Scatter plots of SEVIRI BT versus ECMWF+RTTOV synthetic BT of 3400 x 3400 IR pixels region, for IR13.4 SEVIRI BT at IR10.8 warmest clear pixel in 25 x 25 pixels FOR. On the left before BT bias correction, on the right after robust BT bias correction.

The reason to use only ocean collocated BTs for bias estimation is that spread over ocean is lower than over land or desert boxes. This lower adjustment on land boxes could be due to: skin temperature field of background NWP data is not able to simulate very hot or very cold pixels that SEVIRI observes and the emissivity issue.

The scatter plots of SEVIRI BT at the IR10.8 warmest clear pixel versus synthetic BT, before and after BT bias correction, for several channels, are shown in Figure 10.

Once the scale and the offset parameters for each SEVIRI IR channel are obtained, the values are written in the PGE13 SPhR configuration file (see [AD.2] for details). The users that doesn't want to apply the SEVIRI BT bias correction can edit the model configuration file and fix to 1.0 the scale keywords and to 0.0 the offset keywords (see [AD.2] for details).

PGE13Hyb note:

Since error between actual SEVIRI BTs and synthetic RTTOV BTs depends on the profiles used to calculate the synthetic RTTOV BTs, the bias correction coefficients calculated with ECMWF model data from profiles on hybrid vertical levels are written in the default configuration file for PGE13Hyb module.

2.3.3.2 <u>Regression coefficients to calculate First Guess profiles</u>

In the PGE13 SPhR 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 between [t+00, t+24] range background NWP data is used as First Guess. Since forecast profile is used together

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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 a file by the PGE13 SPhR. To train the FG regressions several options are available. In the Jun Li's VSA, to generate the FG regression coefficient, a global radiosonde dataset with surface skin temperature and surface IR emissivities physically assigned (Seemann et al. 2003; 2007) was used.

For version 2013 a new FG regression coefficients file is available using the PGE13 SPhR training and validation dataset. To generate the new 2013 FG regression coefficients, a training dataset has been built using the beta version PGE13 SPhR software executed only over a network of 13001 points distributed over the SEVIRI full disk with the ECMWF model for 2012. The synthetic RTTOV BTs for ECMWF analysis and temperature and specific humidity profiles t+12 ECMWF forecast from previous 12 hour ECMWF run have been used as independent variables (see Eq. 1). Full details about the process to generate the 2012 FG regression coefficients file are described in [AD.7] or in Martinez 2011. Similar approach has been made for version 2013 calculation. The structure of the FG regression coefficients file is described on [AD.3].

The FG regression coefficient file can be changed editing the name of the regression coefficient file on the PGE13 SPhR configuration file.

PGE13Hyb note:

In the case of PGE13Hyb module for the FG regression coefficients the equation 1(PGE13Hyb) has been used and all profiles used in the calculation of the FG regression coefficients are from profiles at the 43 RTTOV pressure levels interpolated from 91 hybrid levels. In the PGE13Hyb default configuration file, the filename of the FG regression coefficients should point to one hybrid FG regression coefficients file.

2.3.3.3 The error covariance matrix of background and first guess (B)

Error covariance matrices of background have been calculated using match up files with the errors of collocated forecast and analysis or radiosondes. The assumption of no correlation existing between temperature and moisture in the error covariance matrix has been made.

The statistical error of the background is represented by the matrix B (see Table 4).

L pressure levels will be used to represent temperature and moisture profiles. In our case, as RTTOV uses 43 predefined pressure levels, L is equals to 43.

This (2*L+1) by (2*L+1) element matrix represents the correlation of the background error between a parameter and the same parameter in another level. The pairs of errors for temperature, humidity and skin temperature are assumed to be uncorrelated. The levels correspond to the RTTOV pressure levels.

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





Table 5: The background error covariance matrix

The water vapour should be expressed as logarithm of specific humidity when calculating the background error covariance matrix.

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 Nowcasting SAF as most of the users rely on this European model. This matrix has been computed with the available PGE13 SPhR training and validation dataset (using 2012 year profiles with latitude greater than 36° N) and it's included in the current PGE13 SPhR 2013 version.

PGE13Hyb note:

In the case of PGE13Hyb module for the calculation of B^{-1} all the profiles used are at the 43 RTTOV pressure levels interpolated from 91 hybrid levels. The filename with the B^{-1} is written in the PGE13Hyb default 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 by the matrix \mathbf{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 spectral bands is not known, this matrix has only diagonal elements.

The (assumed) error of the radiation model was merely added to these diagonal elements.

The observation error covariance matrix is defined as diagonal matrix. The diagonal element is the square of observation error and it has been calculated in version 2013 using actual SEVIRI BTs after bias correction and synthetic RTTOV BTs on sea pixels of the PGE13 validation dataset for the whole 2012 year.


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	$\left(e_{1}^{2} \right)$	0	0		0)
	0	e_2^2	0	 	0
E =	0	0	e_3^2		0
	0	0	0	0	e_N^2

In previous versions it was calculated using the SEVIRI instrument noise and the forward model error for each SEVIRI spectral IR band.

PGE13Hyb note:

In the case of PGE13Hyb module for the calculation of E^{-1} all the profiles used are at the 43 RTTOV pressure levels interpolated from 91 hybrid levels.

2.3.3.5 <u>Empirical orthogonal Functions (EOF) representation for temperature and</u> <u>moisture profiles</u>

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 number of independent structure functions (EOFs) can be obtained from a set of global atmospheric profile samples.

See Eq. (5) for the EOF representation of a profile.

Using EOF representation is necessary because of limited SEVIRI infrared spectral bands used.

The advantages of using EOF representation for a profile are:

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

Figure 11 shows the first 5 temperature EOFs (left panel) and first 5 water vapour mixing ratio (logarithm) EOFs calculated from a global training data set (NOAA 88 global Radiosounding).





Figure 11: The first 5 temperature EOFs (left panel) and first 5 water vapour mixing ratio EOFs derived from a global training data set. The water vapour is expressed as the logarithm of mixing ratio in EOF calculations.

EV	Cumulative Var for T	Cumulative Var for InQ	Cumulative Var for InO ₃
1	68.0 %	39.3 %	80.0 %
2	81.5 %	76.7 %	87.6 %
3	87.4 %	85.7 %	92.1 %
4	90.5 %	90.6 %	94.4 %
5	92.8 %	93.2 %	96.1 %

Table 6: The cumulative variances for T, ln(q) and $ln(O_3)$ for the first 5 EOFs.

Table 6 lists the cumulative variances for the first 5 EOFs for temperature profile (T), logarithm of water vapour mixing ratio profile and ozone mixing ratio profile (lnO_3) .

In the SEVIRI physical retrieval process, 2 temperature profile EOF is recommended since there is only one CO_2 absorption band, 3 specific humidity EOFs are recommended since there are 2 water vapour absorption bands plus 12 μ m and 13.4 μ m weak water vapour absorption bands that provide boundary layer moisture information. In the table they are enhanced in red.

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 EOF using ECMWF model PGE13 SPhR training and validation dataset have been successful and these new EOFs are now included in the current PGE13 SPhR 2013 version (using 2012 year profiles in PGE13 validation dataset with latitude greater than 36° N).

PGE13Hyb note:

In the case of PGE13Hyb module for the calculation of EOFs all the profiles used are at the 43 RTTOV pressure levels interpolated from 91 hybrid levels.

The filenames with the EOFs are written in the PGE13Hyb default configuration file.

2.3.3.6 <u>RTTOV-9.3 coefficients</u>

In addition, a clear sky fast and accurate radiative transfer model is needed in the retrieval process. In PGE13 SPhR RTTOV-9.3 radiative transfer model provided by NWP SAF is used (Eyre, 1991; Saunders and Matricardi, 2008). In early tests RTTOV-8.7 was used and currently the code has been updated to RTTOV-9.3.

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. Further study is needed on handling surface IR emissivity, for example, the use of time continuity information to derive emissivity for profile retrieval.

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

- (1) Use emissivity from database:
 - a. Advantage: monthly global coverage.
 - b. Disadvantage: at MODIS spectral bands.

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- (2) Use regression based emissivity:
 - a. Advantage: dynamic emissivity, at SEVIRI bands.
 - 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 spectral bands.
 - 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.

The concept of using time continuity is novel, for example, by assuming that the emissivity is temporally invariable while surface skin temperature is temporally variable, SEVIRI brightness temperatures from multiple time steps can be used to retrieve invariable emissivity and variable surface skin temperatures. The derived emissivity and skin temperature then can be applied to physical retrieval process. However, this method needs some risk reduction study and it will be studied for future versions. The availability of operational software of PGE13 SPhR will allow testing this on an operational environment.



Figure 12: The emissivity map derived from AIRS radiances at 8.21 µm channel (upper panel), and the emissivity spectra (lower panel) for a small region indicated by black box.

The ideal way is to use the emissivity values derived from the hyperspectral IR radiances from polar orbiting satellites. Algorithm has been developed (Li et al. 2007) for retrieving the surface emissivity spectrum from hyperspectral IR radiances retrieval, for example, to use the emissivity

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values from IASI (Infrared Atmospheric Sounding Interferometer) onboard Metop-A and AIRS (Atmospheric InfraRed Sounder) onboard EOS (Earth Observing System) Aqua platform. Global hyperspectral IR emissivity map from AIRS has been developed (Li et al. 2008). Figure 12 shows the emissivity map derived from AIRS radiances at 8.21 μ m channel (upper panel), and the emissivity spectra (lower panel) for a small region indicated by black box. Emissivity spectra are derived from 8-day composite. This will be studied for future versions.

For handling emissivity in SEVIRI product process, the first suggestion is to use emissivity values from IASI. If IASI emissivity values are not available, emissivity values from a database can be used. If neither is available, emissivity values from regression can be used; but the surface skin temperature might be negatively impacted by using regression based surface IR emissivity in physical retrieval process.

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 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: <u>http://cimss.ssec.wisc.edu/iremis/</u>. Figure 14 shows a global emissivity image of 8.3 μ m, operational MODIS emissivity product is used.



Emissivity, Version A, filled by Adjacent Month: MVD11C3.A2006091, 8.3µm

Figure 13: MODIS emissivity at 8.3 µm (Figure from the above webpage).

The generation emissivity atlas in the SEVIRI projection and channels from a database for each month has been considered as most adequate for 2013 version. A global database of monthly infrared land surface emissivity derived using input from MODIS operational land surface emissivity product (MOD11) is available. Emissivity is available globally at ten wavelengths (3.6, 4.3, 5.0, 5.8, 7.6, 8.3, 9.3, 10.8, 12.1, and 14.3 microns) with 0.05 degree spatial resolution (Seemann et al. 2007). Monthly emissivity atlases have been integrated over the SEVIRI spectral

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response functions to match the SEVIRI bands. In previous versions of PGE13 the 2006 datasets of IREMIS database has been used; in PGE13 version 2013 the emissivity atlases have been updated with 2012 IREMIS datasets. They have been remapped to SEVIRI projection at 0.0° W and 9.5°E. In the reprojection, the following process is made for each pixel in the SEVIRI projection matrix: a) the (longitude, latitude) for each one of the 3712 x 3712 matrix is read, b) the position in the IREMIS matrix is calculated for land pixels (elevation different that missing code) c) if in the IREMIS dataset the calculated position is surrounded by four neighbours with value not equal to IREMIS missing code then bilinear interpolation is made , d) in the case that in the IREMIS missing code then just the nearest neighbour is copied. Thus, for 2013 version fixed emissivity atlas for each month interpolated to the SEVIRI projection and channels from 2012 IREMIS database are the used in PGE13 SPhR. See in [AD.2] and in [AD.3] documents for details about emissivity atlas files naming and format.





Figure 14: MODIS emissivity at SEVIRI IR8.7 µm interpolated from 8.3 and 9.3 and remapped to SEVIRI 0 ° W projections. On top, full disk image. On bottom, zoom over Europe. (colour palettes are not the same)

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 SAF software package. In 2013 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.

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2.3.3.9 PGE13 SPhR Model Configuration File

PGE13 SPhR has been built as much modular and configurable by the user as possible. The PGE13 SPhR model configuration file contains all the coefficients and some constant values required by PGE13 SPhR product. The model configuration file is an ASCII file and then it can be easily modified with any text editor. See section 4.3.1 in [AD.2] for details.

2.4 PGE13 SPHR OUTPUTS

Together with the main clear air parameters (TPW, LPW and stability indices) 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: PGE13 SPhR HDF-5 files description.

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

- 1. **SPhR_TPW**: Total precipitable water ($P_{Surface}$ top) from the retrieved profiles of temperature and humidity in kg/m².
- Precipitable water in three layers LPW (SPhR_BL: P_{Surface} 850 hPa, SPhR_ML: 850 500, SPhR_HL: 500 TOP) from the retrieved profiles of temperature and humidity in kg/m².
- 3. **SPhR_LI**: Lifted Index from the retrieved profiles of temperature and humidity in Kelvin.
- 4. **SPhR_SHW**: Showalter Index from the retrieved profiles of temperature and humidity in Kelvin.
- 5. **SPhR_KI**: K-Index from the retrieved profiles of temperature and humidity in Kelvin.
- 6. **SPhR_DIFFTPW:** Difference between TPW from retrieved profile and TPW from NWP profiles in kg/m².
- 7. **SPhR_DIFFBL, SPhR_DIFFML, SPhR_DIFFHL**: Difference between LPWs from retrieved profile and LPWs from NWP profiles in kg/m².
- 8. **SPhR_DIFFLI, SPhR_DIFFKI, SPhR_DIFFSHW**: Difference between instability indices from retrieved profile and instability indices from NWP profiles.
- 9. Quality Flags: SPhR_QUALITY, SPhR_SFLAG fields.
- 10. Configurable IR channel BT degraded to 7 bits only in cloudy pixels.

It is important to highlight that, as PGE13 SPhR retrieves the complete profiles of temperature and humidity, it is possible in future versions to implement new thermal 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 HDF-5. The fields are later scaled in order to store it in 7 pixels after scaling and the values are in the range [8-127].

2.4.2 Optional binary files outputs.

Since PGE13 SPhR is executed locally by the users, it allows them to debug their local installations or create new parameters or instability indices. There are two keywords in the PGE13

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SPhR 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 PGE13 SPhR model configuration file. The main advantage of these binary files is that all temperature and humidity profiles are spatially, temporally and vertically collocated. See [AD.2] for details on how to manage the keywords. The format of the binary files is described on [AD.4].

Thus, debugging activities, vertical cross sections, 3D visualizations, and generation of validation dataset are only a few of the applications where they can be used. As example, the PGE13 validation and training dataset described in [AD.7] has been built using these binary files. At the time being, 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 to use application as IDV, McIDAS-V, IDL, MATLAB, etc. for one easy management of the PGE13 binary files



Figure 15: IDV visualization of retrieved q profiles with netCDF for 25th May 2009 at 12 UTC.

2.4.3 Examples of PGE13 SPhR visualisation

Graphic displays of PGE13 SPhR 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 (<u>http://www.nwcsaf.org</u>).

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 images corresponding to the 23 July 2009 at 12UTC are shown as an example in the Figures bellow.





Figure 16: Example of PGE13 SPhR_BL from 12 UTC on 23 July 2009 produced from SEVIRI on MSG2.



Figure 17: Example of PGE13 SPhR_ML from 12 UTC on 23 July 2009 produced from SEVIRI on MSG2.



Figure 18: Example of PGE13 SPhR_HL from 12 UTC on 23 July 2009 produced from SEVIRI on MSG2.





Figure 19: Example of PGE13 SPhR_TPW from 12 UTC on 23 July 2009 produced from SEVIRI on MSG2.



Figure 20: Example of PGE13 SPhR_LI from 12 UTC on 23 July 2009 produced from SEVIRI on MSG2.



Figure 21: Example of PGE13 SPhR_SHW from 12 UTC on 23 July 2009 produced from SEVIRI on MSG2.





Figure 22: Example of PGE13 SPhR_KI from 12 UTC on 23 July 2009 produced from SEVIRI on MSG2.



3. PRACTICAL CONSIDERATIONS

3.1 PROGRAMMING AND PROCEDURAL CONSIDERATIONS

The PGE13 SPhR requires knowledge of cloud mask information within each FOR. The PGE13 SPhR is implemented sequentially (pre-process, regression followed by iterative physical approach). The PGE13 SPhR is purely a FOR by FOR algorithm. Then it could be parallelised in future version for processing with several CPUs. The only task that is not made inside PGE13 code is the spatial interpolation of NWP before retrieval process upon the arrival of new NWP data to avoid repeating the process every slot.

PGE13Hyb note:

The spatial, temporal and vertical interpolation to get NWP data collocated with SEVIRI data is full made inside the PGE13Hyb module.

3.2 EXCEPTION HANDLING

Algorithm can not be run if any of the mandatory IR channels data or PGE01 Cloud Mask is bad or missing.

The PGE13 SPhR does check for conditions where the PGE13 SPhR can not be performed.

3.3 ASSUMPTIONS

- (1) The surface pressure used in the SPhR 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. Fixed IREMIS dataset has been selected from year 2012.

3.4 LIMITATIONS

- (1) SPhR products are available over "clear" FORs only.
- (2) Since physical retrieval it is an iterative process, computation is relative expensive and an increase in the width of the FOR could be necessary in large region processing.
- (3) The result can exhibit large errors over mountain regions with large differences between the topography and the NWP topography. The same happens in desert pixels, where the distance on skin temperature between the NWP first guess and the 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+0 to t+24 with $0.5^{\circ}x0.5^{\circ}$ resolution to every 1 hour from t+0 to t+24 with $0.125^{\circ}x0.125^{\circ}$ resolution, have improved clearly the quality of the PGE13 SPhR outputs. It is strongly recommended to feed PGE13 with temperature and humidity profiles with much fixed pressure levels as possible. In general the more accurate is the background profile the more accurate will be the retrieval.

PGE13Hyb note:

If possible, it is strongly recommended to the PGE13 users that use ECMWF as background NWP to make the effort to download also from the MARS the GRIB files on hybrid levels. The best quality is achieved using as input to PGE13 SPhR GRIB files on hybrid levels and the execution of PGE13Hyb module.



The ECMWF GRIB files on fixed pressure levels are available only at 15 fixed pressure levels. The ECMWF GRIB files have 91 hybrid levels. It is foreseen that ECMWF increases the number of hybrid levels to 137 from June 2013.

(4) Effect of emissivity temporal variation is not handled. Fixed IREMIS monthly datasets has been selected from 2012.

3.5 IMPLEMENTATION OF PGE13 SPHR

Three main steps are identified. The user manually interacts with the PGE13 SPhR software during the installation step, and the PGE13 SPhR preparation and execution steps are automatically monitored by the Task Manager (if real-time environment is selected).

3.5.1.1 <u>The PGE13 SPhR installation step</u>

Previous condition and licences

The right to use, copy or modify this software is in accordance with EUMETSAT Policy for the SAFNWC/MSG 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 PGE13 file to be stored into the \$SAFNWC/bin directory.

After the steps shown in [AD.6], PGE13 of the SAFNWC/MSG is installed and configured in the system. The operational use of NWC SAF 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 default PGE13 SPhR model configuration file is provided with the software package. 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 PGE13 SPhR preparation step

PGE01 is mandatory and it has to be executed before PGE13 execution. Also NWP spatial preprocessing should be done by the Task Manager or with the AllMapping tool.

3.5.1.3 The PGE13 SPhR 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 PGE13 along with the required parameters (slot, region file name and model configuration file) by the Task manager after the PGE01 has finished. The PGE13 is then performed following the corresponding configuration file. The use of the PGE13 command is very easy on scripts. Here, an example of execution is provided:

PGE13 YYYYMMDDhhmm region.cfg configuration_file.cfm

Where:

YYYYMMDDhhmm is the date and hour 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 PGE13 needs.

PGE13 SPhR has been designed as much modular and configurable by the user as possible. In order to configure it, as much parameters as possible are collected in the PGE13 SPhR configuration file. In [AD.2] more details about this are provided.

PGE13Hyb note:

The PGE13 code executes PGE13Hyb module if in the PGE13 configuration file (cfm extension) the keyword NWP_EXEC_MODE is fixed to **HYB**



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3.6 VALIDATION

The physical retrieval algorithm was first validated with SEVIRI data by Dr. Jun Li for period August 2006. An extensive validation for the year 2009 has been done and the complete validation report is available in [AD.7]. Bellow only a brief summary of the validation with 2009 dataset is provided.

PGE13Hyb note:

An extensive validation of PGE13Hyb module with year 2012 has been done. The complete scientific report is available in [AD.9]. Bellow only a brief summary of the validation is provided on grey background paragraph at the end of this section.

In retrieval algorithms, satisfactory results depend on the training datasets; therefore, it has been considered an important task to build a training and validation dataset (Recommendation 4 of the Madrid Workshop). PGE13 SPhR has been trained and validated using a training and validation dataset built with data splitting a part of the dataset for training the FG regression (1 out of 2 even pixels) and the other for validation and testing purpose (odd pixels). The applied methodology and the results are available in the Validation Report [AD.7]. The validation is based on the comparison of PGE13 SPhR parameters with the calculated from ECMWF model. The design was made to create a training and validation dataset using collocated SEVIRI data, ECMWF model and radiosonde profiles (provided by the University of Wyoming). The validation has been performed over a network of 13,001 points (Grid network of 1°x1° plus RAOB Stations) as can be seen in Figure 23.



Figure 23: Points of the FG regression dataset. Grid network of 1° x 1° plus Radiosonde Stations (red crosses).

In order to build the validation dataset, PGE13 SPhR code with the binary files option activated is used to get collocated structures including SEVIRI IR BTs, ECMWF profiles (t+12 & analysis), radiosoundings and the corresponding collocated geophysical parameters. The advantage of these datasets is that they are homogeneous and cover all latitudes, longitudes and days of the year. Due to the fact that NWCSAF library is not prepared to manage hybrid files, in the validation of the regular version of PGE13 the same kind of GRIB files used operationally in the NWCSAF Reference System has been used as input to PGE13 SPhR. The ECMWF GRIB files used as background NWP have 15 fixed pressure levels.

PGE13Hyb note:

The validation of PGE13Hyb module has been done with profiles only from ECMWF GRIB files on hybrid levels.

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In order to assess the performance of SPhR algorithm with the noise added by several issues (emissivity fields, contamination with clouds, and errors in skin temperature on ECMWF analysis, mountains, etc), the statistical values obtained using synthetic RTTOV BTs as input to PGE13 version 2012 from the validation for January 2009-December 2009 are summarized in the table 7 (see [AD.7] for the whole validation report). The user must take into account that the PGE13 SPhR can provide useful spatial information but SEVIRI has limited information to improve the vertical information beyond the forecast. Due to this fact, the PGE13 SPhR main improvements to the background NWP information are located in the mid and upper levels in the humidity profile.

ML parameter shows a significant reduction in RMSE. From the figures of Table 7, a reduction in ML RMSE of 12% for FG step and 16% after physical retrieval in sea pixels can be expected over sea pixels. The reduction of ML RMSE over land pixels is lower but it represents a 10% of reduction in the ML RMSE.

In the case of HL parameter the percentage in the reduction are even higher. In case HL RMSE reduction is around 21% over sea pixels and 26% over land pixels.

The former confirms the results of the vertical analysis of the performance made in Section 4.2 of [AD.7] that showed a reduction in the RMSE and an improvement over the background NWP in the q profile at middle levels by the contributions of WV channels. The reduction of RMSE in the middle levels of the q profile is also likely the reason of reduction in the TPW RMSE.

BL sea	NWP15(T+12)	FG	Phy. Retrieval	BL land	NWP15(T+12)	FG	Phy
RMSE (kg/m ²)	0,913	0,902	0,915	RMSE (kg/m	²) 0,792	0,785	
BIAS (kg/m ²)	0,028	-0,069	-0,092	BIAS (kg/m ²)) 0,144	0,137	
ML sea	NWP15(T+12)	FG	Phy. Retrieval	ML land	NWP15(T+12)	FG	Phy
RMSE (kg/m2)	1,957	1,730	1,638	RMSE (kg/m	²) 1,596	1,576	
BIAS (kg/m2)	0,969	0,745	0,750	BIAS (kg/m2	.) 0,524	0,496	
HL sea	NWP15(T+12)	FG	Phy. Retrieval	HL land	NWP15(T+12)	FG	Phy.
RMSE (kg/m2)	0,190	0,157	0,147	RMSE (kg/m	²) 0,213	0,178	
BIAS (kg/m2)	0,039	0,035	0,035	BIAS (kg/m2	2) 0,060	0,061	
TPW sea	NWP15(T+12)	FG	Phy. Retrieval	TPW land	NWP15(T+12)	FG	Phy.
RMSE (kg/m2)	2,290	2,014	1,842	RMSE (kg/m	²) 1,883	1,853	
BIAS (kg/m2)	1,036	0,711	0,693	BIAS (kg/m2	.) 0,722	0,688	

Table 7: Summary of the PGE13 SPhR statistical parameters in period January 2009 toDecember 2009 for odd pixels dataset

PGE13Hyb note

Here a summary of the validation for PGE13Hyb module is presented. It can be seen the clear improvement to use ECMWF GRIB files on hybrid levels as input to PGE13Hyb. Full details are available in the Scientific Report [AD.9]. In this case the period used is the year 2012.

BL sea	NWPHyb(t+12)	FG	Phy. Retrieval	BL land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m ²)	0.720	0.705	0.688	RMSE (kg/m ²)	0.453	0.449	0.435

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BL sea	NWPHyb(t+12)	FG	Phy. Retrieval	BL land	NWPHyb(t+12)	FG	Phy. Retrieval
BIAS (kg/m ²)	0.119	0.109	0.119	BIAS (kg/m ²)	-0.009	-0.069	-0.073
ML sea	NWPHyb(t+12)	FG	Phy. Retrieval	ML land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m2)	1.044	0.944	0.862	RMSE (kg/m ²)	0.831	0.804	0.704
BIAS (kg/m2)	0.153	0.069	0.091	BIAS (kg/m2)	0.052	-0.079	-0.115
HL sea	NWPHyb(t+12)	FG	Phy. Retrieval	HL land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m2)	0.142	0.105	0.090	RMSE (kg/m ²)	0.176	0.116	0.099
BIAS (kg/m2)	0.005	-0.007	-0.008	BIAS (kg/m2)	0.010	-0.001	-0.013
TPW sea	NWPHyb(t+12)	FG	Phy. Retrieval	TPW land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m2)	1.492	1.362	1.252	RMSE (kg/m ²)	1.106	1.035	0.913
BIAS (kg/m2)	0.278	0.171	0.202	BIAS (kg/m2)	0.054	-0.147	-0.187

Table 8: **PGE13Hyb BT_RTTOV case:** Statistical parameters for BL, ML, HL and TPW parameters over the Full Disk validation points in year 2012 for odd pixels dataset. Left) sea pixels, right) land pixels

BL sea	NWPHyb(t+12)	FG	Phy. Retrieval	BL land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m ²)	0.720	0.739	0.743	RMSE (kg/m ²)	0.453	0.458	0.460
BIAS (kg/m ²)	0.119	0.212	0.236	BIAS (kg/m ²)	-0.009	0.011	0.001
ML sea	NWPHyb(t+12)	FG	Phy. Retrieval	ML land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m2)	1.044	0.991	0.968	RMSE (kg/m ²)	0.831	0.916	0.978
BIAS (kg/m2)	0.153	0.137	0.218	 BIAS (kg/m2)	0.052	0.018	0.053
HL sea	NWPHyb(t+12)	FG	Phy. Retrieval	HL land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m2)	0.142	0.120	0.113	RMSE (kg/m ²)	0.176	0.150	0.146
BIAS (kg/m2)	0.005	-0.015	-0.021	BIAS (kg/m2)	0.010	-0.001	-0.013
TPW sea	NWPHyb(t+12)	FG	Phy. Retrieval	TPW land	NWPHyb(t+12)	FG	Phy. Retrieval
RMSE (kg/m2)	1.492	1.449	1.424	RMSE (kg/m ²)	1.106	1.177	1.240
BIAS (kg/m2)	0.278	0.334	0.433	BIAS (kg/m2)	0.054	0.027	0.040

Table 9: **PGE13Hyb BT_SEVIRI case:** Statistical parameters for BL, ML, HL and TPW parameters over the Full Disk validation points in year 2012 for odd pixels dataset. Left) sea pixels, right) land pixels.

After comparison of the Tables 7 and 8 with the RTTOV case with regular PGE13 and PGE13Hyb performances, the values of RMSE in the case of PGE13Hyb are much lower than the ones for the PGE13 with fixed pressure levels. The reduction of RMSE on sea pixels after FG and physical retrieval steps in the BL and ML layers are similar; but the reduction of RMSE after FG and physical retrieval steps in the HL is much higher in the PGE13Hyb due to the better treatment of high levels in PGE13Hyb module.



The reduction of RMSE on land pixels after FG and physical retrieval steps is greater in all layers. That means that the quality of PGE13Hyb module is greater over land likely due to a better vertical representation of the temperature and humidity profiles that is more critical on land pixels.

In Table 9 are shown the statistical result in the case when actual SEVIRI bias corrected BTs are used as input to PGE13Hyb module; see the Scientific Report [AD.9] for more details.



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4. SUMMARY

The availability of PGE13 SPhR allows an easy processing with physical retrieval of SEVIRI images in an operational environment. The NWC SAF 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 PGE13 SPhR has been designed in order to be as much 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 a large region and with small FOR's width a small region centred in its country).

PGE13Hyb note

A PGE13Hyb module that uses ECMWF GRIB files on hybrid levels as input to PGE13Hyb is also available as one processing option in version 2013. It should be considered as one advance of future full support by NWCSAF library to all NWP models on hybrid levels. The quality of PGE13Hyb module is much better; full details are available in the Scientific Report [AD.9].

PGE13Hyb module has confirmed the recommendation to feed PGE13 SPhR 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 has allowed creating a huge PGE13 training and validation dataset that has been very important in order to improve the operational version 2012.

As the generation of PGE13 SPhR training/validation dataset shows, the use of PGE13 SPhR allows generating easily spatially, temporal 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.



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