MTG-FCI: ATBD for Global Instability Indices Product

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v1D of 17 January 2011	First published version
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v3 of 08 January 2013	Following changes: Section 3.1.2: clarification concerning the term "lower boundary condition" Section 3.2: Limitations on cloudiness for TOZ retrieval clarified Section 3.4.1: Threshold for scene types to determine clear sky and cloudy retrievals is made a configurable parameter Section 3.4.2.2: Cloud top pressure thresholds for stopping the TOZ retrieval changed to a configurable parameter Section 3.4.2.2: Meaning of "surface type of FoR" clarified Section 3.4.2.2: Meaning of "surface type of FoR" clarified Section 3.4.2.2: Added section on surface emissivity choice for the cloudy retrievals Section 3.5.1: Section added on interpolating cloudy radiances to the actual cloud pressure level, after correction for emissivity Section 3.5.2: Equation (3-5) for RMS updated, and text added to make number of channels used in equation (3-5) configurable

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1 INTRODUCTION

1.1 Purpose of this Document

This document describes the algorithm theoretical basis for the derivation of the Global Instability Indices (GII) product, as it shall be derived from the Meteosat Third Generation Flexible Combined Imager (MTG-FCI). The GII derivation also includes the derivation of the total column ozone product (TOZ), i.e. the TOZ retrieval scheme is also described in this document.

1.2 Structure of this Document

Section 2 of this document provides a short overview over the MTG imaging instrument characteristics and the derived meteorological products, which will be referenced later in the text. This is followed by a detailed description of the underlying algorithm of the GII/TOZ product – its physical basis, the required input data, and a more detailed description of the product retrieval method.

A full list of acronyms is provided in section 1.4, a glossary of the equation symbols used in this document can be found in section 4.

1.3 Applicable and Reference Documents

The following documents have been used to establish this document:

Doc ID	***Title***	***Reference***
[AD-1]	MTG End Users Requirements Document	EUM/MTG/SPE/07/0036
[AD-2]	MTG Products in the Level-2 Processing Facility	EUM/C/70/10/DOC/08
[AD-3]	MTG-FCI: ATBD for Radiative Transfer Model	EUM/MTG/DOC/10/0382
[RD-1]	The lifted index as a predictor of latent instability.	Galway, J.G., 1956, *Bull. Amer. Met. Soc.*, **37**, 528-529
[RD-2]	GOES-VAS simultaneous temperature-moisture retrieval algorithm	Hayden, C.M., 1988, *J. Appl. Meteor.*, **27**, 705-733
[RD-3]	The MSG Global Instability Indices Product and Its Use as a Nowcasting Tool	Koenig, M. and E. de Coning, *Wea. Forecasting*, **24**, 272 – 285

Doc ID	***Title***	***Reference***
[RD-4]	Severe thunderstorms over western Germany – a case-study of the weather situation on 20 August 1992	Kurz, M., 1993, *Meteorol. Mag*., **122**, 177-188
[RD-5]	A nonlinear physical retrieval algorithm – its application to the GOES-8/9 sounder	Ma, X.L., T.J. Schmit, W.L. Smith, 1999, *J. Appl. Meteor*., **38**, 501-513
[RD-6]	Diagnosing convective instability from GOES-8 radiances	Rao, P.A. and H.E. Fuelberg, 1997, *J. Appl. Meteor*., **36**, 350-364
[RD-7]	Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation.	Rodgers, C.D., 1976, *Rev. Geophys. Spac. Phys*., **14**, 609-624

1.4 Acronyms and Definitions

The following table lists definitions for all acronyms used in this document.

Acronym	***Full Name***
AER	Aerosol Product
AMV	Atmospheric Motion Vectors
ASR	All Sky Radiance
ATBD	Algorithm Theoretical Basis Document
CRM	Clear Sky Reflectance Map
ECMWF	European Centre for Medium Range Weather Forecast
FCI	Flexible Combined Imager
FCI-FDSS	FCI Full Disk Scanning Service
FCI-RSS	FCI Rapid Scanning Service
FDHSI	Full Disk High Spectral Resolution Imagery
FoR	Field of Regard
GII	Global Instability Indices
GOES	Geostationary Operational Environmental Satellite
HRFI	High Spatial Resolution Fast Imagery
HRV	High Resolution Visible Channel of SEVIRI
IR	Infrared (channel)
LPW	Layer Precipitable Water
MET`	EUMETSAT Meteorological Division
MSG	Meteosat Second Generation
MTG	Meteosat Third Generation
NIR	Near Infrared (channel)
NWP	Numerical Weather Prediction
OCA	Cloud Product (Optimal Cloud Analysis)
OLR	Outgoing Longwave Radiation

Acronym	***Full Name***
RMS	Root mean square difference
RTM	Radiative Transfer Model
RTTOV	Radiative Transfer for TOVS
SCE	Scene Identification
SAF	Satellite Application Facility
SEVIRI	Spinning Enhanced Visible and Infrared Imager
SSD	Spatial Sampling Distance
TCE	EUMETSAT Technical Computing Environment
TIROS	Television and Infrared Observation Satellite
TOVS	TIROS Operational Vertical Sounder
TOZ	Total Column Ozone
TPW	Total Precipitable Water
UTC	Coordinated Universal Time
VIS	Visible (channel)

2 OVERVIEW

2.1 Relevant Instrument Characteristics

The mission of the Meteosat Third Generation (MTG) System is to provide continuous high spatial, spectral and temporal resolution observations and geophysical parameters of the Earth / Atmosphere System derived from direct measurements of its emitted and reflected radiation using satellite based sensors from the geo-stationary orbit to continue and enhance the services offered by the Second Generation of the Meteosat System (MSG) and its main instrument SEVIRI.

The meteorological products described in this document will be extracted from the data of the Flexible Combined Imager (FCI) mission. The FCI is able to scan either the full disk in 16 channels every 10 minutes with a spatial sampling distance in the range 1 – 2 km (Full Disk High Spectral Resolution Imagery (FDHSI) in support of the Full Disk Scanning Service (FCI-FDSS)) or a quarter of the earth in 4 channels every 2.5 minutes with doubled resolution (High spatial Resolution Fast Imagery (HRFI) in support of the Rapid Scanning Service (FCI-RSS)).

FDHSI and HRFI scanning can be interleaved on a single satellite (e.g. when only one imaging satellite is operational in orbit) or conducted in parallel when 2 satellites are available in orbit. Table 1 provides an overview over the FCI spectral channels and their respective spatial resolution.

The FCI acquires the spectral channels simultaneously by scanning a detector array per spectral channel in an east/west direction to form a swath. The swaths are collected moving from south to north to form an image per spectral channel covering either the full disc coverage or the local area coverage within the respective repeat cycle duration. Radiance samples are created from the detector elements at specific spatial sample locations and are then rectified to a reference grid, before dissemination to the End Users as Level 1 datasets. Spectral channels may be sampled at more than one spatial sampling distance or radiometric resolution, where the spectral channel has to fulfil FDHSI and HRFI missions or present data over an extended radiometric measurement range for fire detection applications.

Table 1: Channel specification for the Flexible Combined Imager (FCI)

Spectral Channel	*Central Wavelength, $\lambda 0$*	*Spectral Width, $\Delta\lambda 0$*	*Spatial Sampling Distance (SSD)*
VIS0.4	0.444 µm	0.060 µm	1.0 km
VIS0.5	0.510 µm	0.040 µm	1.0 km
VIS0.6	0.640 µm	0.050 µm	1.0 km 0.5 km [#1]
VIS0.8	0.865 µm	0.050 µm	1.0 km
VIS0.9	0.914 µm	0.020 µm	1.0 km
NIR1.3	1.380 µm	0.030 µm	1.0 km
NIR1.6	1.610 µm	0.050 µm	1.0 km
NIR2.2	2.250 µm	0.050 µm	1.0 km 0.5 km [#1]
IR3.8 (TIR)	3.800 µm	0.400 µm	2.0 km 1.0 km [#1]
WV6.3	6.300 µm	1.000 µm	2.0 km
WV7.3	7.350 µm	0.500 µm	2.0 km
IR8.7 (TIR)	8.700 µm	0.400 µm	2.0 km
IR9.7 (O_3)	9.660 µm	0.300 µm	2.0 km
IR10.5 (TIR)	10.500 µm	0.700 µm	2.0 km 1.0 km [#1]
IR12.3 (TIR)	12.300 µm	0.500 µm	2.0 km
IR13.3 (CO_2)	13.300 µm	0.600 µm	2.0 km

[#1]: The spectral channels VIS 0.6, NIR 2.2, IR 3.8 and IR 10.5 are delivered in both FDHSI sampling and a HRFI sampling configurations.

2.2 Generated Products

The agreed list of MTG-FCI Level 2 products is detailed in [AD-2] and is repeated here for easy reference:

1. **SCE-CLA**:
   Scene Identification (cloudy, cloud free, dust, volcanic ash, fire) and a number of cloud products (cloud top height, phase)
2. **OCA**:
   Cloud Product (cloud top pressure and temperature, cloud top phase, cloud top effective particle size, cloud optical depth, cloud sub-pixel fraction)
3. **ASR**:
   All Sky Radiance (mean IR radiance on an n x n pixel grid, together with other statistical information, for different scenes)
4. **CRM**:
   Clear Sky Reflectance Map (VIS reflectance for all non-absorbing channels, accumulated over time)
5. **GII**:
   Global Instability Indices (a number of atmospheric instability indices and layer precipitable water contents)
6. **TOZ**:
   Total Column Ozone (technically retrieved within the GII product)
7. **AER**:
   Aerosol Product (asymmetry parameter, total column aerosol optical depth, refractive index, single scattering albedo, size distribution)
8. **AMV**:
   Atmospheric Motion Vectors (vector describing the displacement of clouds or water vapour features over three consecutive images, together with a vector height)
9. **OLR**:
   Outgoing Longwave Radiation (thermal radiation flux at the top of the atmosphere leaving the earth-atmosphere system)

The products will be derived from the spectral channel information provided by the FDHSI mission, on the resolution detailed in [AD-2].

An important tool for product extraction is a radiative transfer model (RTM), as described in [AD-3]. The IR model choice for the Level 2 product extraction is RTTOV, which is developed and maintained by the Satellite Application Facility on Numerical Weather Prediction (NWP-SAF). An RTM for solar channels is likely to be product specific and is yet to be fully determined.

This ATBD describes the algorithm of the GII and TOZ product. The retrieval process makes use of the results of the SCE product. The product will be derived over a certain processing area, defined as pixels lying within a great circle arc of pre-defined size around the subsatellite point (typically 70°).

3 ALGORITHM DESCRIPTION

3.1 Physical Basis Overview

Instability parameters are derived from vertical profiles of temperature and humidity to provide some information concerning the vertical stability of the atmosphere. Various indices are used by forecasters for different applications and regions, and these indices are defined as a difference of profile parameters in different pressure levels [RD-1], [RD-4]. Such data are usually derived from radio soundings, but a few satellite derived indices also exist (e.g. derived from the GOES satellites, [RD-2], [RD-6]. The air mass parameters can be used to issue severe weather warnings if the corresponding index exceeds a certain threshold. These thresholds are usually determined empirically and should not be regarded as fixed values – they may vary from season to season and from region to region. A skilled local forecaster is absolutely necessary for a correct interpretation of the provided indices.

The chosen GII retrieval scheme also implicitly includes the retrieval of layer precipitable water and total column ozone, which are also described in this document.

The combined GII/TOZ (for simplicity hereafter only referred to as the GII product) will comprise the following instability indices, other air mass parameters relevant to atmospheric stability and ozone values:

- Lifted Index $LI = T^{air} - T^{air,\ lifted\ from\ surface}$ at 500 hPa
- K-index $KI = (T^{air(850)} - T^{air(500)}) + TD^{(850)} - (T^{air(700)} - TD^{(700)})$
- Layer Precipitable Water, (humidity, vertically integrated over three different layers)
- Total Precipitable Water, (humidity, vertically integrated over the entire atmosphere)
- Total Column Ozone (TOZ), (ozone, vertically integrated over the entire atmosphere)

where

> T^{air} is the air temperature at the indicated pressure level (e.g. $T^{air}(850)$ is at 850 hPa), expressed in Kelvin
> TD is the dew point temperature, expressed in Kelvin, again at the indicated pressure level
> *Humidity* refers to the atmospheric water vapour content expressed as mixing ratio, expressed in kg/kg (in ppmv within the radiative transfer model)
> *Ozone* refers to the atmospheric ozone content, expressed as mixing ratio, expressed in kg/kg (in ppmv within the radiative transfer model)

The main purpose of the algorithm is to retrieve a profile of atmospheric temperature, humidity and ozone, from which the above parameters can be derived. The chosen algorithm approach is a so-called statistical-physical retrieval in that prior information and measurements are combined in a statistically optimal way, with a physical radiative transfer model used to relate atmospheric properties to measurements. Prior information is required because the information contained in the observed radiances is not sufficient to completely define the atmospheric profile. The prior profile (also known as "background profile") is obtained from short range NWP forecasts and also serves as the "first guess" profile. The solution will contain information of these forecasts and will not be completely independent of the forecast. During the retrieval, the profile is adjusted such that the statistical likelihood of the profile is maximised, or – equivalently – the solution cost is minimised. Within the GII processing, this minimisation is assumed achieved when simulated radiances match observed values to within a pre-determined threshold.

Effectively the method infers temperature, humidity and ozone profiles from observed radiances in a given set of channels and given (usually NWP forecast) atmospheric profiles. The air mass parameters are then derived from the resulting profiles. The physical retrieval is an optimal estimation using an inversion technique, i.e. tries to find an atmospheric profile which best reproduces the observations [RD-7]. In general, this is a multi-solution problem, and a “background profile” is used as a constraint. This background profile is often also referred to as “first guess”, as it is fed to the iteration scheme as an initial proposal for a solution. The original first guess is then slowly modified in a controlled manner until its radiative properties fit the satellite observations. A typical first guess field is a short-term forecast. The final profile is the profile where the simulated radiance field at the top of the atmosphere matches the satellite observations, or in practice, until its difference to the observations is minimal.

The core of the retrieval is the profile adjustment step [RD-5], [RD-7]:

$$x_{n+1} = x_0 + (\mathbf{S}_x^{-1} + \mathbf{K}_n^T \cdot \mathbf{S}_y^{-1} \cdot \mathbf{K}_n)^{-1} \times \mathbf{K}_n^T \cdot \mathbf{S}_y^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0)\right] \qquad (3\text{-}1)$$

with

x: state vector (atmospheric profile, together with a lower boundary condition)
n: iteration step, n=0 denotes background profile
T_B: observed brightness temperatures
$T_{B,n}$: simulated brightness temperatures for profile of iteration step n
$\mathbf{S}_x$: error covariance matrix of background
$\mathbf{K}_n$: Jacobian matrix at iteration step n
$\mathbf{S}_y$: error covariance matrix of observed brightness temperatures and of the radiation model

Sections 3.4 and 3.5 provide a detailed description of each term in the retrieval equation.

Equation (3-1) describes the iterative method of solution; the iteration process is stopped if the difference in observed and simulated brightness temperatures is small (for details, see section 3.5.2).

Furthermore, equation (3-1) implies that the physical retrieval needs a model for the radiative forward and Jacobian calculations, i.e. the model has to be capable to simulate brightness temperatures in the MTG-FCI channels of interest for a specific atmospheric profile and viewing geometry, and for the same case has to provide the partial derivates $\partial T_B / \partial x(i)$ (change of simulated brightness temperature due to a change in the vertical profile x at level i), i.e. the Jacobians **K** in equation (3-1). The model RTTOV provided by the EUMETSAT NWP-SAF [AD-3] has this functionality. RTTOV uses a set of M fixed pressure levels between the surface and the top of the atmosphere (e.g. 0.1 hPa), so that the profile data will in the end be available on this vertical grid.

Two versions of this retrieval will be described in this document:

3.1.1 Version I – Cloud Free Conditions, Full GII/TOZ Retrieval

This version is only applicable to clear sky conditions. In this case the full set of relevant MTG-FCI channel information will be explored, and the first guess temperature, humidity, and ozone profile may be changed within the retrieval. The relevant lower boundary condition is the surface skin temperature (which may also be changed by the retrieval).

All instability and airmass parameters and the total column ozone can be derived from the final profile information. Details are provided in section 3.5.6. Details on how to terminate the iteration process are provided in section 3.5.2.

3.1.2 Version II – Cloudy Conditions, TOZ Retrieval

Theoretical considerations concerning the information content of the MTG-FCI IR9.7 channel (the ozone channel), together with the fact that most of the atmospheric ozone is in the stratosphere, showed that a meaningful retrieval of total column ozone is possible over clouds, provided that the clouds are either low or optically thin, i.e. the clouds are radiatively insignificant for the IR9.7 channel. For this special case, the lower boundary condition of the retrieval equation needs to be changed to the cloud top pressure. With respect to the atmospheric profile, only the ozone profile is subject to changes within the retrieval.

The total column ozone can then be derived from the final profile information. Details on how to terminate the iteration process are provided in section 3.5.2.

3.2 Assumptions and Limitations

As outlined in the previous section, a meaningful full GII/TOZ processing is only possible for clear sky conditions, only the TOZ product can also be retrieved over low clouds, resp. clouds which do not have a significant radiative effect upon the ozone channel signal.

An important underlying assumption of the process is that the retrieved (assumed to be the “true”) profile is not too much different from the background profile, i.e. from the forecast. The spectral information content of the MTG-FCI IR channels is certainly not high enough to derive a forecast independent atmospheric profile, i.e. for MTG-FCI many solutions for equation ***(3-1)*** exist and could theoretically be found. Usage of the forecast as background constrains the problem to the solution which is closest to the forecast, meaning that the final solution will retain certain features of the background. Validation work, based on the MSG-SEVIRI GII product, however, has shown that this is in practice fully sufficient and acceptable [RD-3].

3.3 Algorithm Basis Overview

The core of the GII algorithm is to solve the retrieval equation ***(3-1)***. The processing is done on the level of an individual image pixel or a group of pixels, e.g. defined as a box of pixels. The basic processing element will hereafter be referred to as Field-of-Regard (FoR).

For each FoR, necessary input data need to be prepared (see section 3.4). The iterative retrieval is schematically shown in Figure 1. Specific details on all the processing steps are provided in section 3.5, also with focus on the two different versions I and II.

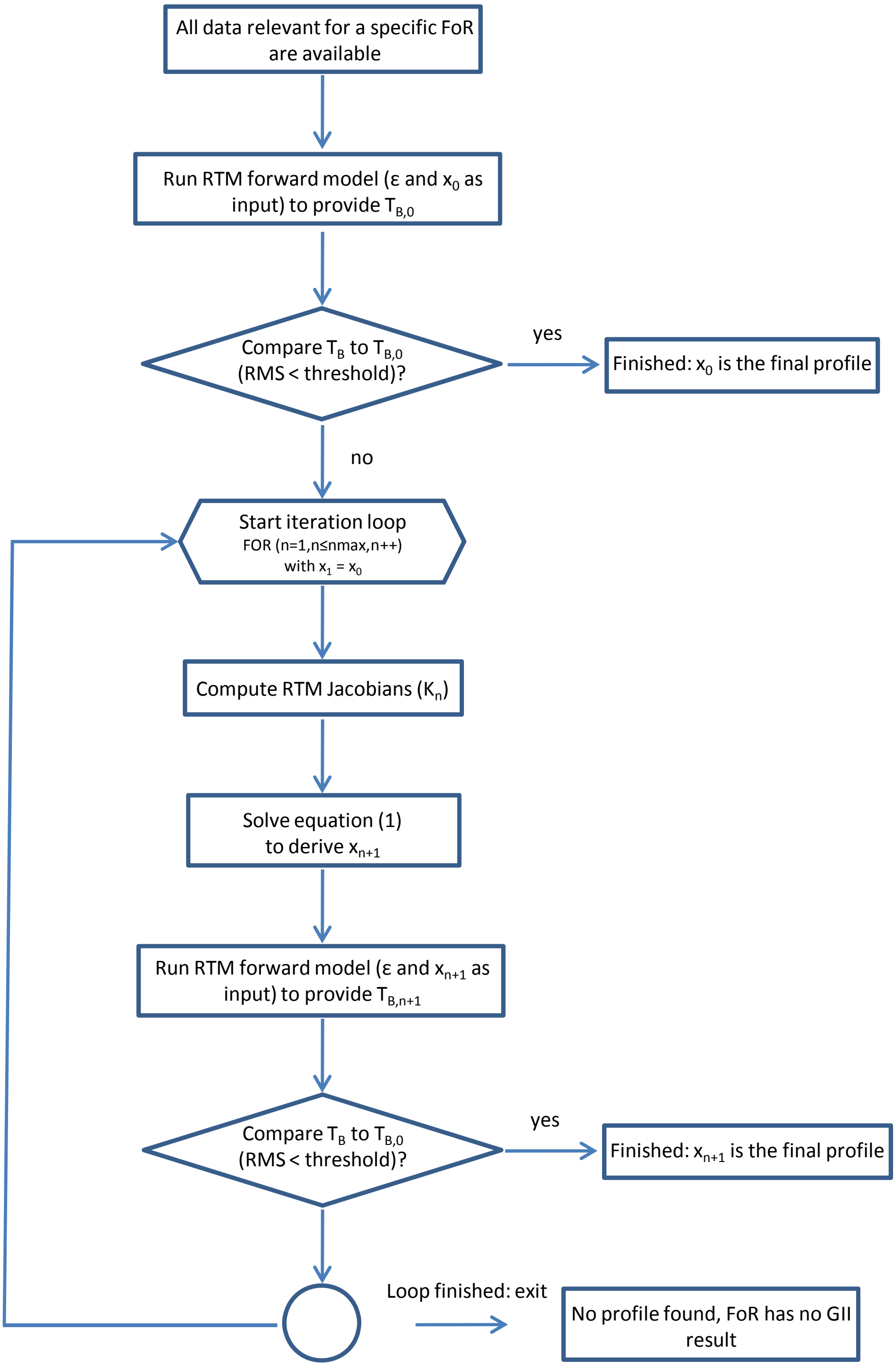

Figure 1: Schematic flow diagram for the GII/TOZ processing for a given FoR

3.4 Algorithm Input

Table 2 lists the data that needs to be available before the start of the GII processing.

Table 2: Necessary input data for the GII/TOZ processing

Parameter Description	Variable Name
Brightness Temperatures for the 7 MTG-FCI channels WV6.3, WV7.3, IR8.7, IR9.7, IR10.5, IR12.3, IR13.3, for each pixel within the processing area	$T_{B,observed}(i)$
Bias corrections for the seven MTG-FCI channels	$T_{B,bias}(i)$
Satellite viewing angles for each pixel within the processing area	ζ_{sat}
Pixel latitude and longitude	φ_{lat}, φ_{lon}
Surface emissivity information, for the seven channels, for each pixel over the processing area	$\varepsilon(i)$
ECMWF profiles of temperature, humidity, ozone, surface skin temperature for the processing area, on the m vertical levels of RTTOV, for two forecast times bracketing the image time	T(p), q(p), o3(p), T_{skin} - all combined in vector x_0
Surface type information for the ECMWF grid points within the processing area (land or sea)	SType
Results of the Cloud Mask Product, for each pixel within the processing area; underlying surface type for clear sky (land/sea)	CM
Observation and RTM error matrix	$\mathbf{S}_y$
Error Covariance Matrix of background	$\mathbf{S}_x$

3.4.1 Primary Sensor Data

For each FoR, the brightness temperatures in 7 MTG-FCI channels, as listed in Table 2, must be available. The availability of this data goes together with the Cloud Mask Product CM, which is also a pixel based product, defined on the same IR grid as the IR channels.

For the case that the FoR is larger than a single MTG-FCI IR pixel (e.g. a box of pixels), the brightness temperatures need to be averaged over this area. This averaging has to be done separately for the cloudy and cloud free pixels, as described by the CM product. This will result in average brightness temperatures for the cloud free section of the box, and in average brightness temperatures for the cloudy section of the box (obviously accounting for the fact that the entire box may be cloud free or cloud filled). The decision on which retrieval version (I or II) should be selected, is based on the number of cloud free pixels:

If more than a certain percentage of the FoR is cloud free, the Version I is selected, using the average cloud free brightness temperatures, else the cloudy retrieval is chosen, using the average cloudy brightness temperatures. This percentage shall be a setup parameter for the processing.

> Note: An absolutely correct average should use the original radiances as input, i.e. derive an average radiance, and then convert this radiance to the average temperature. However, the uncertainty introduced by averaging the brightness temperature is very small and negligible.

For the case that the FoR is just a single pixel, the decision is simply based on this pixel's cloud product: If the pixel is declared cloud free, Version I is selected, if it is cloudy, Version II shall be selected.

After having identified the correct (average) brightness temperatures for the given FoR, measurements are bias corrected. Such a correction accounts for the (possible) bias between the satellite and the radiation model and model forecasts. Such biases must be assessed in an independent step, e.g. by the bias monitoring which is routinely done at ECMWF. For all 7 channels, the bias is defined such that for each channel a fixed value is added to the original brightness temperature.

$$T_B(i) = T_{B,observed}(i) + T_{B,bias}(i) \qquad (3\text{-}2)$$

$T_{B,observed}$: observed brightness temperature for a given position
T_{bias}: bias correction term
i: index for channel

The thus defined corrected brightness temperatures are the T_B values specified in equation (3-1).

3.4.2 Ancillary Dynamic Data

3.4.2.1 Cloud Mask Product (CM)

As already described in section 3.4.1, the Cloud Mask Product CM needs to be available for the correct preparation of the FoR's brightness temperatures. This cloud mask is available on a pixel basis (of the IR channel resolution). The CM product takes the value "cloudy", "cloud free" or "unknown" – pixels with an "unknown" cloud mask shall be disregarded for the GII and TOZ processing.

3.4.2.2 Forecast Data

The other important ancillary dynamic dataset are the forecast profiles of temperature, humidity and ozone, denoted as the x_0 background profile in equation ***(3-1)***. Within the GII/TOZ processing, the x_0 background profile is also taken as the first guess, i.e. as input to the first run of the radiative forward model to derive the simulated brightness temperatures $T_{B,0}$. Since the RTTOV radiation model is used for the radiative transfer calculations, the profile parameters are represented at a maximum of m levels (m is defined within RTTOV, e.g. for RTTOV-10 m=55). The radiation model needs the profile parameters at m prescribed pressure levels so that the background profile must be appropriately interpolated to these levels (logarithmic interpolation for temperature, linear interpolation for humidity and ozone, all with respect to pressure). The level 1 is assumed to be at the top of the atmosphere, level m is at the surface.

The profile information is taken from the ECMWF forecast data, which is defined on a specific latitude/longitude grid. Each profile is interpolated both in space and time to fit the time and location of the actual satellite observation. As a surface value, the ECMWF forecasted skin temperature – also appropriately interpolated - is used in the retrieval as the temperature of the lowest layer. The observation vector thus has a length of 3m+1, i.e. m temperature values, m humidity values, m ozone values and the surface skin temperature (in this order). All temperatures are expressed in unit Kelvin, the humidity and ozone are expressed as ppmv. The pressure levels are prescribed by RTTOV and are given in hPa.

In case the actual surface pressure is smaller than the lowest RTTOV level (e.g. 1013.25 hPa), the RTTOV levels between the lowest level and the first level above the actual surface shall be simply populated with the temperature, humidity and ozone value of the lowest model level.

In the case of the special Version II processing the lower boundary condition is changed from the surface skin temperature to the cloud top pressure. The background cloud pressure (entry for x_0) is set to 882.8 hPa (or to the RTTOV prescribed pressure level in the vicinity of this value), the first guess cloud top pressure, however, is the pressure level, where

$$\left| T_B(\mathrm{channel\,IR10.5}) - T_{B,\mathrm{overcast}}(\mathrm{IR10.5}, p) \right|$$

is minimal. T_B(channel IR 10.5) is the measured and bias corrected temperature in channel IR 10.5, $T_{B,overcast}$(IR10.5,p) is the simulated brightness temperature in channel IR 10.5 for a cloud at pressure p. The $T_{B,overcast}$ results are one of the outputs of RTTOV, at each of the M pressure levels.

Note that the special Version II processing can be immediately stopped (and a default TOZ value assigned to the specific FoR) if p in the above equation is either less than a certain cloud top pressure, expressed in hPa (typically 300 or 400 hPa) or greater than the surface pressure at the location of the FoR.

Within the spatial interpolation of the ECMWF profiles, care has to be given to the actual surface type value of the forecast points compared to the (predominant) surface type of the FoR (i.e. of the pixels used for the specific retrieval). Only those ECMWF grid points, which have the same surface type (only land/sea are discriminated) shall be used for the spatial interpolation.

If, for example, a specific FoR (resp. its pixels used for the specific retrieval) has surface type “land”, but a number of the surrounding ECMWF grid points have surface type “sea” (or vice versa), these grid points shall be disregarded in the spatial interpolation. Otherwise, coastal features will be apparent in the final product. Figure 2 shows a schematic of this process.

In case, however, that all surrounding ECMWF grid points differ in their surface type from the pixel's surface type (e.g. small islands or small lakes or rivers), all four surrounding grid points have to be used.

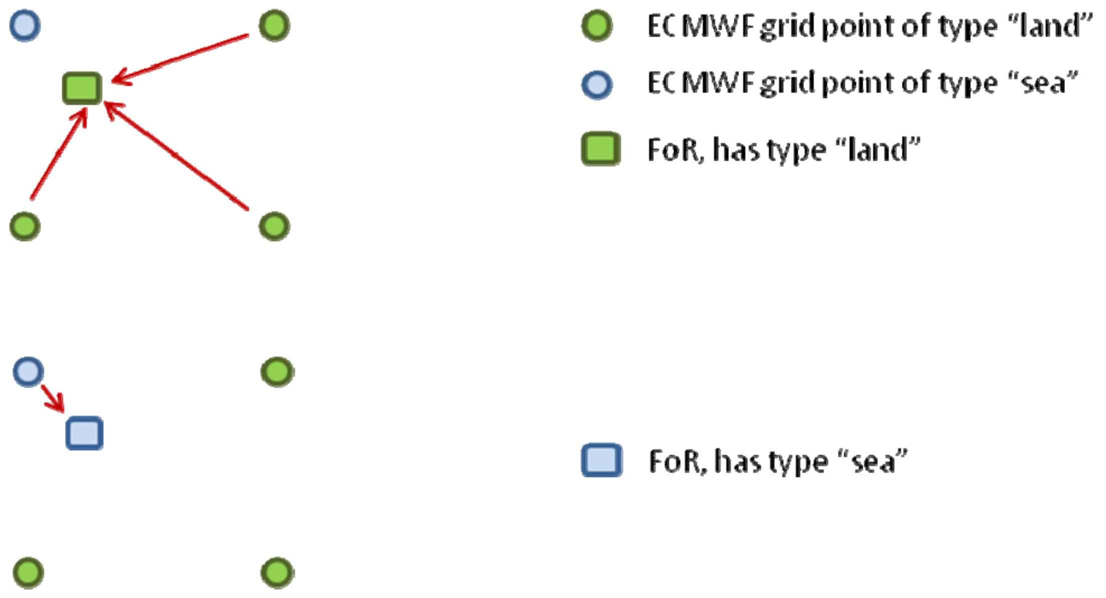

Figure 2: Schematic illustration of the use of forecast data depending on the FoR and the forecast grid surface type. Only the forecast data of the same surface type shall be used, as illustrated for the "land" case (top) and the "sea" case (bottom). The arrows denote which ECMWF grid points shall be used in these cases.

3.4.3 Ancillary Static Data

3.4.3.1 Temperature Bias Correction

For every channel the appropriate temperature bias correction terms $T_{B,bias}$ must be made available for each of the seven MTG-FCI channels. These correction terms can be taken from long-term monitoring of biases between the ECMWF model and the satellite measurements, which are e.g. available on the ECMWF web site. Although the biases may change with time, they can be assumed constant over a period of a month or longer. Temperature bias values often exhibit a diurnal cycle within the ECMWF monitoring system – this diurnal cycle shall be ignored, i.e. an average bias correction term shall be assessed from the ECMWF monitoring results.

3.4.3.2 Surface Type of ECMWF Grid Points

For each ECMWF grid point, the associated surface type (land or sea) information must be available. As it is not expected that the geographical grid information of the received ECMWF forecasts grid changes very often, this background information can be held in a static dataset.

3.4.3.3 Information on Surface and Cloud Emissivity

The RTM calculations need information on the surface emissivity for all 7 channels. The following cases are discriminated:

Processing Version I – full GII and TOZ retrieval over cloud free surface:

A-1: The FoR's predominant surface type is sea: RTTOV offers an internal calculation of the sea surface emissivity, depending on the satellite view angle. The results of these calculations shall be used (e.g. in RTTOV-10 this is the parameter CALCEMIS which has to be set to .TRUE.)

A-2: The FoR's predominant surface type is land. In this case, the available pixel-based emissivity data for all 7 channels shall be used. These data are constant over a certain period (typically a month), so the processing has to allow for a possible time dependence in this input dataset. Also, the pixel based emissivity shall be averaged over the cloud free pixels in the respective FoR.

Note: Again, the “FoR’s predominant surface type” in this context refers to the predominant surface type of the cloud free pixels

Processing Version II – TOZ retrieval over clouds:

The cloud emissivity is parameterised as follows:

$$\varepsilon(i) = a_0(i) + \frac{a_1(i)}{\cos \zeta_{sat}} + \frac{a_2(i)}{\cos^2 \zeta_{sat}} \qquad (3\text{-}3)$$

where

ε:	emissivity
i:	index for channel (1 to 7)
ζ_{sat}:	satellite viewing angle
a_0, a_1, a_2:	channel dependent, pre-calculated regression coefficients

Section 3.5.1 describes how this cloud emissivity information shall be used within the processing.

Note: For the radiation model, a surface emissivity must be assigned also for the cloudy simulations. This could be any value between 0 and 1, but for simplicity could also be taken as the average emissivity over the FoR, as explained above for the Version I processing

3.4.3.4 Covariance Matrix of Background Errors (S_x)

The statistical error of the background is represented by the matrix $\mathbf{S}_x$. This (3m+1) by (3m+1) element matrix describes the covariance of the background errors between parameters at different levels. The pairs of errors for temperature, humidity, ozone and skin temperature are assumed to be uncorrelated und thus set to 0. The levels m correspond to the RTTOV pressure levels. The matrix for Version I is schematically shown in Figure 3. Version II would have the identical matrix, with only the exception that the last (bottom right) matrix element is no longer the skin temperature covariance (which is typically 15K·15K), but is now the covariance of the cloud top pressure. A value of 200hPa·200hPa is used in this case.

Units in the covariance matrix of first guess errors have to correspond to the units of the observation vector (K^2 for temperatures, $ppmv^2$ for gases, hPa^2 for cloud height).

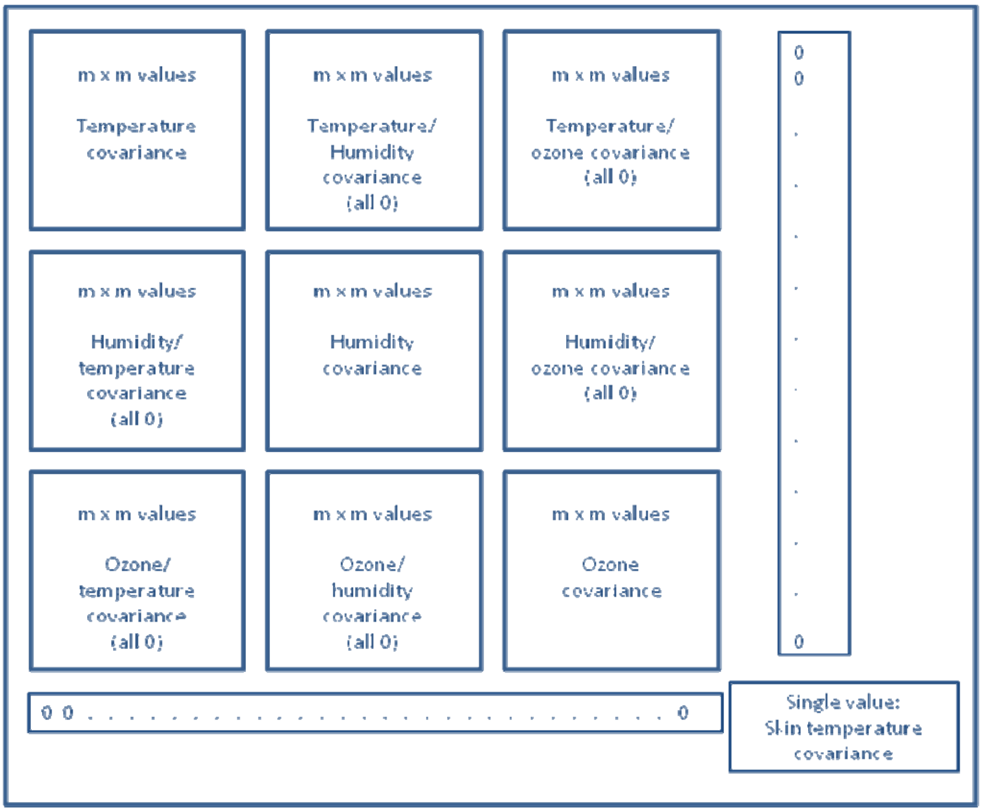

Figure 3: Schematic of the error covariance matrix S_x for Version I processing.

3.4.3.5 Observation and Radiation Model Errors (S_y)

The statistical errors of the observed brightness temperatures and the errors of the radiation model are represented by the matrix $\mathbf{S}_y$. The elements describe the covariance of the brightness temperature error of the instrument, and an assumed uncertainty of the radiation model is added to that value. As the covariance of any two channels is not known, but probably uncorrelated, they are set to 0, so the matrix has only diagonal non-zero elements, representing single channel errors. These errors are simply assumed to be the instrument noise figures for the respective channel. The (assumed) error of the radiation model (e.g. a value of typically 0.2 K) is added (in a squared sense) to these diagonal elements with the implicit assumption that instrument and model noise are uncorrelated. The matrix is of size 7 by 7, referring to the 7 MTG-FCI channels which are used in the processing. The matrix remains unchanged between the processing versions I and II.

3.5 Detailed Description

Once all input data is available and properly averaged and interpolated for a single FoR, the physical retrieval process can start, which consists of five main tasks

(a) Run the radiative transfer forward model to compute the simulated brightness temperatures for a given observation vector x_n
(b) Compare RTM temperatures to measurements to assess quality of retrieval iteration
(c) Run the radiative transfer K-model (Jacobians) to compute the matrix $\mathbf{K}_n$
(d) Solve equation (3-1)
(e) Update the observation vector x_n

3.5.1 RTM Forward Model

Version I processing – cloud free case:

The RTM forward model of RTTOV (in RTTOV-10 this is the module rttov_direct) provides the clear sky brightness temperatures for the provided temperature profile (observation vector x_0). The processing has to make sure that the corresponding variable structure in RTTOV, describing the profile, is properly populated, and has the correct units.

Note: In RTTOV-10, the structure variable is *profiles*, where

profiles % t(1:m)	are the air temperatures in K
profiles % q(1:m)	are the humidities in ppmv
profiles % o3(1:m)	are the ozone values in ppmv
profiles % skin % t	is the surface skin temperature in K
profiles % skin % p	is the surface pressure in hPa
profiles % skin % surftype =	0 (for land), = 1 (for sea)
profiles % s2m % t	is the 2m temperature (can be proxied by lowest level air temperature), in K
profiles % s2m % q	is the 2m humidity (can be proxied by the lowest level humidity), in ppmv
profiles % s2m % o	is the 2m ozone (can be proxied by the lowest level ozone), in ppmv
profiles % zenangle	satellite viewing angle in degrees
profiles % cfraction	= 0.0, cloud fraction

The results of the forward model are the brightness temperatures for the cloud free case, in RTTOV-10 these are stored in *radiance % bt_clear(1:7)* for all 7 channels, and they constitute the data for $T_{B,n}$ in equation (3-1).

Version II processing – cloudy case:

The same forward model as for the Version I processing is called, and only two parameters are changed in the input structure *profiles*:

profiles % cfraction = 1.0 – cloud fraction is set to 1 to get the cloudy case
profiles % ctp = first guess cloud pressure, in hPa
Section 3.4.2.2 describes how to obtain a first guess cloud pressure value.

The RTM output for the cloudy case has to be corrected for the actual cloud emissivity (as parameterised in section 3.4.3.3):

The radiance $L_{final}(i,k)$ at the top of the atmosphere, for channel i, and with a cloud of emissivity ε at layer k is composed of:

(a) The emission from the cloud, multiplied by the atmospheric transmission above layer k:

$$\varepsilon(i)\ L_{B,}\left[i,T(k)\right]\ \tau_a(i,k)$$

$\varepsilon(i)$: channel specific cloud emissivity for channel i
$L_{B,}[i,T(k)]$: spectral blackbody radiance for channel i at level k, which has air temperature T(k)
$\tau_a(i,k)$: atmospheric transmission in channel i above level k

(b) Downwelling radiation reflected by the cloud

$$(1-\varepsilon(i))\ L_{down}(i,k)\tau_a(i.k)$$

$1-\varepsilon(i)$: reflectivity in channel i
$L_{down}(i,k)$: downwelling radiation for channel i at level k
$\tau_a(i,k)$: atmospheric transmission in channel i above level k (as above)

(c) Contribution from the layers above the cloud, which can be inferred from

$$L_{top,overcast}(i,k) - L_B\left[i,T(k)\right]\tau_a(i,k)$$

$L_{top,overcast}(i,k)$: upwelling radiance at the top of the atmosphere, for channel i, for a cloud of ε=1 at level k,
$L_{B,}[i,T(k)]$ and $\tau_a(i,k)$ are defined as above.

The standard RTTOV output of the forward calculations provide all the necessary terms $\tau_a(i,k)$, $L_{top,overcast}(i,k)$, $L_{down}(i,k)$, while $L_{Bi}[i,T(k)]$ can be calculated from Planck's formula, summing up terms (a), (b) and (c) provides the radiance at the top of the atmosphere, if a cloud of the given emissivity is at level k.

This implies that, after the call to the RTM forward model, the resulting cloudy radiances have to be corrected according to:

$$L_{final}(i) = \varepsilon(i) L_B[i, T(k)] \tau_a(i,k) + (1-\varepsilon(i)) L_{down}(i,k) \tau_a(i,k) + L_{top.overcast}(i,k) - L_B[i, T(k)] \tau_a(i,k) \quad (3\text{-}4)$$

RTTOV provides as output (in version 10):

transmission % tau(i,k)	representing $\tau_a(i,k)$
radiance % down(i,k)	representing $L_{down}(i,k)$
radiance % overcast(i,k)	representing $L_{top,overcast}(i,k)$
radiance % surf(i,k)	representing $L_B[i,T(k)]$

The such corrected radiances $L_{final}(i)$ need to be converted to brightness temperatures T_{Bn} in equation (3-1) (for details on the radiance to brightness temperature conversion, see [AD-3]).

In the first iteration the cloud top pressure will lie at one of the defined RTM pressure levels. In the later iterations the retrieved cloud top pressure will probably lie in between the defined RTM levels. In this later case it is necessary to calculate emissivity corrected BTs at the two RTM pressure levels around the retrieved cloud top pressure. The final simulated BT will then be interpolated between these two values linearly in relation to the respective pressure levels.

3.5.2 Condition to Terminate Iterative Process

The iterative process is terminated if the simulated brightness temperatures $T_{B,n}$ are close to the observed and bias corrected temperatures T_B in the 7 channels. The actual termination criterion is the root mean square difference between the two sets of temperatures

$$RMS = \sqrt{\sum_{i=1}^{i\_final} (T_B - T_{B,n})^2} \quad (3\text{-}5)$$

For the clear sky retrievals, the RMS calculation shall be done over i_final = 7 channels, i.e. all 7 channels that are used in the retrieval. For the cloudy retrievals, the exact value of i_final and the actual channels used in the RMS calculation shall be configurable.

If RMS is lower than a certain threshold (e.g. 1 K, where thresholds can be different for the clear sky and cloudy retrievals), the atmospheric profile of the iteration step n is taken as the retrieved profile (obviously, this can also happen in step n=0, i.e. the first guess profile already well fits the satellite measurements, which is the easiest case, where the processing does not even have to solve equation (3-1)).

In the (rare) case that the RMS never meets the threshold, the iteration process has to be terminated as a retrieval failure case after a maximum number of iterations (typically 5). Also, if the RMS in iteration step (n+1) is larger than the RMS of iteration step n, this can be regarded as a failure and the retrieval can be stopped.

In summary, the iterative process is terminated if

(a) RMS meets the threshold criterion → profile of the current iteration step is the retrieval result
(b) Maximum number of allowed iteration steps is reached → failed retrieval
(c) RMS(n+1) > RMS(n) → failed retrieval

3.5.3 RTM K-Model

The K-model of RTTOV provides the Jacobian matrix $\mathbf{K}_n$ for the iteration step n (in RTTOV-10 this is the module rttov_k). This matrix describes the change of the radiation field at the top of the atmosphere with a changed atmospheric profile:

$$\mathbf{K}_n(i,k) = \frac{\partial T_{B,n}(i)}{\partial x_n(k)} \tag{3-6}$$

where i denotes a channel number and k denotes an element of the profile vector x_n. The matrix has thus 7 columns (reflecting the 7 channels) and (3m+1) rows – m for temperature, m for humidity, m for ozone, and 1 for the skin temperature resp. cloud top pressure.

In RTTOV-10, $\mathbf{K}_n$ is provided by module rttov_k, which is called with the same input as the RTM forward model rttov_direct (see section 3.5.1).

Version I processing – cloud free case:

The K-Model provides the Jacobians for air temperature (units K/K), for humidity (units K/ppmv), for ozone (units K/ppmv), for surface skin temperature (units K/K) and the structure of final $\mathbf{K}_n$ matrix is shown in Figure 4:

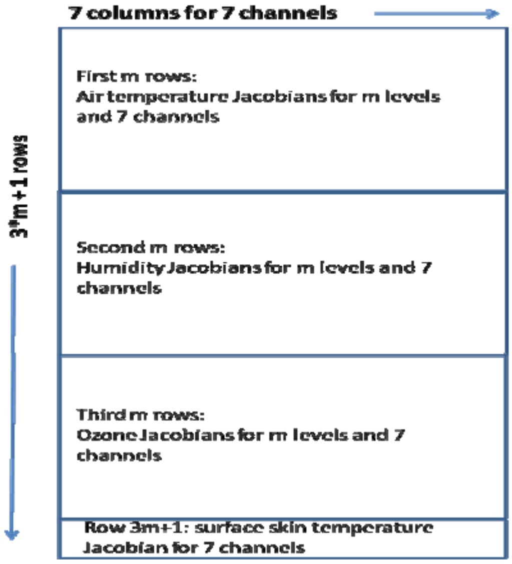

Figure 4: Structure of the final Jacobian matrix K_n for the Version I processing

Version II processing – cloudy case:

In this case, the structure of the final $\mathbf{K}_n$ matrix is (Figure 5):

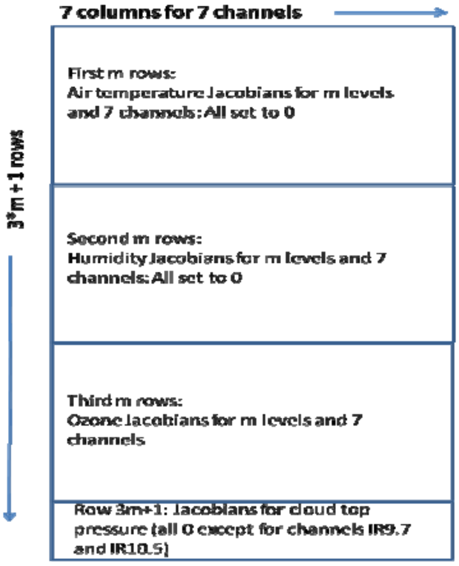

Figure 5: Structure of the final Jacobian matrix K_n for the Version II processing

The largest differences to the Version I matrix $\mathbf{K}_n$ are

(a) The Jacobians for temperature are all set to 0
(b) The Jacobians for humidity are all set to 0
(c) The last row is changed from the surface skin temperature Jacobians to cloud top pressure Jacobians (details see below), but only for channels IR9.7 and IR10.5, for all other channels these are set to 0

These settings imply that only the IR9.7 and the IR10.5 channels will be of relevance within the retrieval, i.e. only these two channels may actually contribute to a changed ozone profile together with a changed cloud top pressure (the latter only being important as a lower boundary condition, not as a product in itself). The other channels, however, may still be used in the monitoring of the minimisation success, i.e. in the computation of the RMS brightness temperature difference (section 3.5.2).

The Jacobians for the cloud top pressure (units K/hPa) are not a direct output of the RTTOV K-model, and they are calculated as follows:

(a) Get the first guess cloud level *icloud* (as described in section 3.4.2.2). *icloud* refers to a standard level as defined within RTTOV
(b) From the RTM forward model output, get the top of atmosphere radiances for clouds in level *icloud* ± a certain (small) number (e.g. 3) = *icloud1* and *icloud2*, but not lower than the surface
(c) The cloudy radiances in levels *icloud1* and *icloud2* have to be converted to brightness temperatures, for channels IR9.7 and IR10.5, yielding $T_{B,cloud}$(IR9.7) and $T_{B,cloud}$(IR10.5) for both levels

(d) The levels *icloud1* and *icloud2* are associated with pressures *p(icloud1)* and *p(icloud2)*

(e) The cloud top pressure Jacobian can then be approximated by

$$\frac{T_{B,cloud}(\text{cloud at level icloud1}) - T_{B,cloud}(\text{cloud at level icloud2})}{p(\text{level icloud1}) - p(\text{level icloud2})}$$

separately for channels IR 9.7 and IR 10.5. *icloud1* and *icloud2* are defined such that *p(icloud1) > p(icloud2)*

3.5.4 Solution of Equation (3-1)

Once all the satellite observations, atmospheric profile, error and Jacobian matrices are available, equation (3-1) can be solved for the next iteration step n+1:

$$x_{n+1} = x_0 + (\mathbf{S}_x^{-1} + \mathbf{K}_n^T \cdot \mathbf{S}_y^{-1} \cdot \mathbf{K}_n)^{-1} \times \mathbf{K}_n^T \cdot \mathbf{S}_y^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0) \right]$$

Inspection of equation (3-1) shows that it involves the inversion of a large matrix, namely

$$\mathbf{S}_x^{-1} + \mathbf{K}_n^T \cdot \mathbf{S}_y^{-1} \cdot \mathbf{K}_n$$

which is of size (3m+1) by (3m+1). Equation (3-1), however, can be rearranged to

$$x_{n+1} = x_0 + \mathbf{S}_x \cdot \mathbf{K}_n^T \cdot \left(\mathbf{K}_n \cdot \mathbf{S}_x \cdot \mathbf{K}_n^T + \mathbf{S}_y \right)^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0) \right] \qquad (3\text{-}7)$$

which only involves the inversion of a much smaller matrix

$$\mathbf{K}_n \cdot \mathbf{S}_x \cdot \mathbf{K}_n^T + \mathbf{S}_y$$

which is of size 7 by 7, 7 being the number of channels..

The aim of solving equation (3-7) is to find an expression of $x_{n+1} - x_0$, i.e. rewrite equation (3-7) to

$$x_{n+1} - x_0 = \mathbf{S}_x \cdot \mathbf{K}_n^T \cdot \left(\mathbf{K}_n \cdot \mathbf{S}_x \cdot \mathbf{K}_n^T + \mathbf{S}_y \right)^{-1} \left[T_B - T_{B,n} + \mathbf{K}_n \cdot (x_n - x_0) \right] \qquad (3\text{-}8)$$

This involves the following computational steps:

(a) Transpose matrix $\mathbf{K}_n$, yielding	$\mathbf{K}_n^T$	[size (3m+1) by (7)]
(b) Perform matrix multiplication	$\mathbf{S}_x \cdot \mathbf{K}_n^T = \mathbf{W}_1$	[size (3m+1) by (7)]
(c) Perform matrix multiplication	$\mathbf{K}_n \cdot \mathbf{W}1$	[size (7) by (7)]
(d) Add matrix $\mathbf{S}_\varepsilon$	$\mathbf{K}_n \cdot \mathbf{W}_1 + \mathbf{S}_y = \mathbf{W}_2$	[size (7) by (7)]
(e) Invert $\mathbf{W}_2$ yielding	$\mathbf{W}_2^{-1}$	[size (7) by (7)]

(f) Perform matrix multiplication $\mathbf{K}_n^T \cdot \mathbf{W}_2^{-1} = \mathbf{W}_3$ [size (3m+1) by (7)]
(g) Perform matrix multiplication $\mathbf{S}_x \cdot \mathbf{W}_3 = \mathbf{W}_4$ [size (3m+1) by (7)]
(h) Compute $\mathbf{K}_n \cdot (x_n - x_0) + T_B - T_{B,n} = v$ [size (7)]
(i) Get final result $\Delta x_{n+1} = x_{n+1} - x_0 = \mathbf{W}_4 \cdot v$ [size (3m+1)]

3.5.5 Update Observation Vector x

Once the new vector Δx_{n+1} is obtained, the observations of temperature, humidity, ozone, surface skin temperature (resp. cloud top height) can be updated according to

$$x_{n+1} = x_0 + \Delta x_{n+1} \tag{3-9}$$

i.e. the new iteration x_{n+1} is obtained by simply adding the $(x_{n+1}\text{-}x_0) = \Delta x_{n+1}$ value to the background x_0.

Version I processing – cloud free case:

Equation (3-9) provides the air temperatures $x_n(1{:}m)$ in units K, the humidities $x_n(m+1{:}2m)$ in ppmv, the ozone values $x_n(2m+1{:}3m)$ in ppmv, and the surface skin temperature $x_n(3m+1)$ in K.

Before this updated profile is used in the next iteration (starting with the RTM forward calculations), some physical constraints are applied:

(a) Relative humidity shall not exceed 100%: From the temperature and humidity, the relative humidity can be derived (for details, see section 3.5.7). For levels where this exceeds 95%, the relative humidity is set to the fixed value 95%, from which the specific humidity in ppmv is inferred. In order to have a correct value for Δx_{n+1} for the next iteration step, this is set to

$$\Delta x_{n+1} = x_{n+1}(\text{corrected for high humidity}) - x_0 \tag{3-10}$$

for the relevant levels between m+1 and 2m, x_0 being the background value, which for Version I is the first guess atmospheric profile/surface skin temperature.

(b) Humidity values should not be less than 0 ppmv: In this case the humidity values are simply set back to the first guess, and the respective Δx_{n+1} for the affected levels is set to 0.

(c) The updated ozone profile has to be within some maximum and minimum constraints (from within RTTOV, which defines minimum and maximum ozone concentrations for each RTTOV level). Ozone values below the minimum or above the maximum for the respective level are set to the minimum or maximum value, and Δx_{n+1} is changed to

$$\Delta x_{n+1} = x_{n+1}(\text{set to min/max ozone}) - x_0 \tag{3-11}$$

Note: In case the profile x_{n+1} is changed because of these physical constraints, it is important to update Δx_{n+1} as this is needed in the next iteration step!

Version II processing – cloudy case:

In this case, equation (3-9) only provides updates for the ozone values $x_{n+1}(2m+1:3m)$, as the respective Δx_{n+1} values for indices (1:2m) are all 0, because the relevant Jacobians are 0. Ozone values are updated according to the method outlined above (Version I processing), also including the same constraints as outlined in (c) above.

The updated cloud top height is also derived according to equation (3-9) (for index (3m+1), where care has to be given to the meaning of x_0 in this special case – x_0 is the cloud background pressure, not the first guess.

3.5.6 Definition of GII Indices, Precipitable Water and Total Column Ozone

3.5.6.1 Lifted Index

$$LI = T^{air} - T^{air,\ lifted\ from\ surface} \quad \text{at 500 hPa} \tag{3-12}$$

From the derived temperature profile, the air temperature at 500 hPa needs to be interpolated between the adjacent pressure levels (interpolation needs to be done logarithmically with pressure). This comprises the first T^{air} term in equation (3-12).

Concerning the second term, the characteristics of the air parcel which is to be theoretically lifted to 500 hPa, is defined as the average temperature and humidity content of the lowest 100 hPa in the atmosphere. The averaging in temperature and humidity shall be done linearly with pressure. The air parcel with such defined temperature and humidity is then lifted adiabatically from the surface to the lifting condensation level, and lifted moist adiabatically from the lifting condensation level to 500 hPa (see 3.5.7.6). The parcel temperature at 500 hPa is the second term in equation (3-12), $T^{air,\ lifted\ from\ surface}$, and the Lifted Index is simply the difference of these two terms.

In case the surface pressure is below 500 hPa, the K-Index is not defined.

3.5.6.2 K-Index

$$KI = (T^{air(850)} - T^{air(500)}) + TD^{(850)} - (T^{air(700)} - TD^{(700)}) \tag{3-13}$$

From the derived temperature profile, the air temperatures at 850, 700 and 500 hPa need to be interpolated from the adjacent respective pressure levels (interpolation needs to be done logarithmically with pressure). This defines the terms $T^{air(850)}$, $T^{air(700)}$ and $T^{air(500)}$ in equation (3-13). The dew point temperatures at 850 and 700 hPa need to be interpolated from the adjacent respective pressure levels (interpolation needs to be done logarithmically with pressure for the temperatures, linear with pressure for the humidities). This defines the terms $TD^{(850)}$ and $TD^{(700)}$ in equation (3-13). The K-Index is then computed according to equation (3-13). All temperature values in equation (3-13) are expressed in Kelvin, the K-Index, however, is commonly expressed in deg Celsius, so 273.15 needs to be subtracted from the final value of equation (3-13).

In case the surface pressure is below 850 hPa, the K-Index is not defined.

Section 3.5.7 will describe in more detail the necessary thermodynamic functions that shall be used within these calculations.

3.5.6.3 Layer Precipitable Water (LPW)

LPW shall contain the vertically integrated humidity in three layers. Layer boundaries are

(a) Surface to 850 hPa
(b) 850 to 500 hPa
(c) 500 hPa to top of atmosphere
(but the actual boundary values shall be configurable)

Humidity values (mixing ratio, expressed in kg/kg) shall first be interpolated to the layer boundaries, 850 and 500 hPa, where the interpolation is linear with pressure between the respective pressure levels.

The vertical integration shall then be done according to

$$\mathrm{LPW_i} = \frac{1}{g}\int_{p1}^{p2} q(p)\, dp \qquad (3\text{-}14)$$

where:

$\mathrm{LPW_i}$: LPW of a specific layer i
g: earth gravitational acceleration
q(p): value of water vapour mixing ratio (in kg/kg) at pressure level p
p1, p2: pressure boundaries of the layer i

LPW is expressed in $\mathrm{kg/m^2}$ (provided that pressure p is expressed in Pa).

In practice, the integration is done as a summation of the available pressure levels:

$$\mathrm{LPW_i} = \frac{1}{g}\sum \overline{q}(p)\,\Delta p \qquad (3\text{-}15)$$

$\overline{q}(p)$ is here the average humidity in the layer defined by the pressure difference Δp; the summation is done over the respective pressure levels for each LPW layer.

3.5.6.4 Total Precipitable Water (TPW)

TPW is simply the sum of the three layer precipitable water values:

$$\mathrm{TPW} = \mathrm{LPW_1} + \mathrm{LPW_2} + \mathrm{LPW_3} \qquad (3\text{-}16)$$

3.5.6.5 Total Column Ozone (TOZ)

TOZ is the vertically integrated ozone, where the vertical integration is done between the surface and the top of the atmosphere.

$$\mathrm{TOZ} = \frac{1}{g} \int_{p(\mathrm{surface})}^{p(\mathrm{top\,level})} o_3(p)\, dp \tag{3-17}$$

where:

g: earth acceleration of gravity
$o_3(p)$: value of ozone mixing ratio (in kg/kg) at pressure level p

In practice, the integration is done as a summation of the available pressure levels:

$$\mathrm{TOZ} = \frac{1}{g} \sum \overline{o}_3(p)\,\Delta p \tag{3-18}$$

$\overline{o}_3(p)$ is here the average ozone in the layer defined by the pressure difference Δp; the summation is done over all pressure levels of the vertical profile

TOZ according to equations (3-17) and (3-18) is of unit kg/m^2 (provided that pressure p is expressed in Pa).

As TOZ is commonly expressed in Dobson Units, the integral has to be divided by 21.4E-06:

$$\mathrm{TOZ(Dobson\ Units)} = \mathrm{TOZ(kg/m^2)} / 21.4\mathrm{E}\text{-}06 \tag{3-19}$$

3.5.7 Thermodynamic Formulae

A number of thermodynamic formulae are used in the GII/TOZ processing, which are described in this section.

3.5.7.1 Conversion between Units ppmv and Mixing Ratio (kg/kg)

For humidity, the conversion factors between units ppmv and mixing ratio expressed in (kg/kg) are:

Mixing ratio to ppmv:	1.60771704E+06
ppmv to mixing ratio:	1./1.60771704E+06

For ozone, the respective values are

mixing ratio to ppmv:	6.03504E+05
ppmv to mixing ratio:	1./6.03504E+05

e.g. a 0.01 kg/kg humidity mixing ratio corresponds to 0.01 * 1.60771704E+06 = 1.60771704E+05 ppmv.

3.5.7.2 Saturation Vapour Pressure for a Given Temperature T

The saturation water vapour pressure E(T) depends on air temperature only and can be expressed as

$$E(T) = 6.11 \cdot 10^{7.5 \cdot (T-273.15)/(T-273.15\ +237.3)} \tag{3-20}$$

Temperature T is expressed in units K, and the resulting vapour pressure is in units hPa.

3.5.7.3 Relative Humidity for a Given Pressure, Temperature and Mixing Ratio

For a given pressure p, a humidity mixing ratio q and a temperature T, the relative humidity RH is defined according to

$$RH = \frac{e \cdot 100}{E(T)} \tag{3-21}$$

RH is in %, v is the local vapour pressure in hPa and E(T) the saturation vapour pressure as defined in section 3.5.7.2 can be obtained via

$$e = \frac{q \cdot p}{(0.622 + 0.378\ q)} \tag{3-22}$$

The humidity mixing ratio q is expressed in kg/kg, pressure p and saturation vapour pressure in hPa, temperature in K. The resulting vapour pressure e is then also of unit hPa.

3.5.7.4 Mixing Ratio for a Given Pressure, Temperature and Relative Humidity

For a given pressure p, relative humidity RH and temperature T, the mixing ratio q is defined according to

$$q = \frac{0.622\ e}{p - 0.378\ e} \tag{3-23}$$

e is the local vapour pressure and is obtained via

$$e = \frac{E(T) \cdot RH}{100} \tag{3-24}$$

from the saturation vapour pressure E(T) and temperature T (see section 3.5.7.2). Temperature is expressed in K, pressure p in hPa, relative humidity RH in %. The resulting mixing ratio is of unit kg/kg.

3.5.7.5 Calculation of Dew Point Temperature

An empirical formula is used for the dew point calculations. For a given level with temperature T, saturation vapour pressure E(T) and relative humidity RH, the dew point TD is defined according to

$$\mathrm{TD} = \frac{243.5 \cdot \mathrm{a} - 440.8}{19.48 - \mathrm{a}} + 273.15 \qquad (3\text{-}25)$$

with

$$\mathrm{a} = \mathrm{LN}\left(\frac{\mathrm{E(T)} \cdot \mathrm{RH}}{100}\right) \qquad (3\text{-}26)$$

E(T) is given by equation (3-20).

3.5.7.6 Specific Functions Needed for the Lifted Index Calculations

For the Lifted Index, the vertical lapse rate for the (theoretically) lifted near-surface air particle is the dry adiabatic lapse rate until the lifting condensation level is reached, and the moist adiabatic lapse rate beyond this level up to 500 hPa. The near-surface air parcel is defined as the average temperature and humidity over the lowest 100hPa above the surface together with the surface pressure – these variables are in the following denoted as T_{sfc}, q_{sfc}, p_{sfc}.

The **lifting condensation level temperature** T_{lift} is obtained through the empirical formula

$$T_{lift} = \frac{1}{\dfrac{1}{T_{sfc} - 55} - \dfrac{\mathrm{LN}(RH_{sfc}/100)}{2840}} \qquad (3\text{-}27)$$

RH_{sfc} is the relative humidity of this air parcel, expressed in %, derived from T_{sfc} and p_{sfc} according to equations (3-21) and (3-22).

The **pressure of the lifting condensation level** p_{lift} is defined as the pressure, where the near-surface air parcel, having temperature T_{sfc}, reaches the lifting condensation temperature T_{lift} during a dry adiabatic process. The lifting condensation pressure can thus be obtained from the dry adiabatic formula (Poisson's equation):

$$p_{lift} = \frac{p_{sfc}}{\left(\dfrac{T_{sfc}}{T_{lift}}\right)^{R_m / c_{p,m}}} \qquad (3\text{-}28)$$

p_{lift} is given in units hPa. R_m is the gas constant for moist air, $c_{p,m}$ is the specific heat for moist air. R_m and c_p depend on the near-surface humidity q_{sfc} and are computed according to

$$\begin{aligned} R_m &= (1 + 0.608\, q_{sfc}) \cdot 287.04 \\ c_{p,m} &= (1 + 0.887\, q_{sfc}) \cdot 1005.7 \end{aligned} \qquad (3\text{-}29)$$

For the computation of the Lifted Index, two different cases now need to be distinguished:

(a) $p_{lift} \leq 500$ hPa (which in reality almost never happens)
(b) $p_{lift} > 500$ hPa

In the rare event of case (a), this implies that the temperature of the near-surface air parcel, displaced to 500 hPa, simply follows the dry adiabat, so can be easily inferred from

$$T^{\text{air, lifted from surface}} = T_{sfc} \left(\frac{500}{p_{sfc}} \right)^{R_m / c_{p,m}} \tag{3-30}$$

$T^{\text{air, lifted from surface}}$ here refers to the respective term in equation (3-12).

Usually, the lifting condensation level is well below the 500 hPa height (i.e. $p_{lift} > 500$ hPa). In this case (b), the air parcel has to follow the moist adiabat between p_{lift} and 500 hPa.

As a first step, the **equivalent potential temperature** of the near-surface air parcel, characterised by p_{sfc}, T_{sfc} and q_{sfc}, is computed:

$$\theta_e = \theta_{sfc}\, \mathrm{EXP}(b1 \cdot b2) \tag{3-31}$$

θ_{sfc} is the potential temperature of T_{sfc}, defined by

$$\theta_{sfc} = T_{sfc} \left(\frac{1000}{p_{sfc}} \right)^{R_m / c_{pm}} \tag{3-32}$$

b1 and b2 are empirical coefficients and are derived according to

$$\begin{aligned} b1 &= \frac{3.376}{T_{lift}} - 0.00254 \\ b2 &= 1000 \cdot q_{sfc} \cdot (1 + 0.81 \cdot q) \end{aligned} \tag{3-33}$$

In the next step, the **final air temperature, lifted to 500 hPa from the surface** is computed as a difference between two temperatures:

$$T^{\text{air, lifted from surface}} = T1 - T2 \tag{3-34}$$

T1 is the temperature of θ_e (equation (3-31)), if dry adiabatically displaced to 500 hPa:

$$T1 = \frac{\theta_e}{\left(\frac{1000}{500} \right)^{R_d / c_{p,d}}} \tag{3-35}$$

(obviously, 1000/500 = 2, numbers were put in for reference to Poisson's equation). R_d and $c_{p,d}$ are the gas constant and specific heat for dry air ($q = 0$ in equation (3-29))

T2 is computed using an empirical regression scheme. The following steps are involved:

(a) compute $t = T1 - 293.16$
(b) In case $t < 0$:

$$T2 = \frac{15.13}{P^4} \tag{3-36}$$

(c) In case $t \geq 0$:

$$T2 = \frac{29.93}{P^4} + 0.96 \cdot t - 14.8 \tag{3-37}$$

In both equations (3-36) and (3-37) the term P is a third order polynomial of t:

$$P = 1 + c_1\, t + c_2\, t^2 + c_3\, t^3 \tag{3-38}$$

Values of c_1, c_2, c_3 depend on the value of t:

	$t \leq 0$	$t > 0$
c_1	-8.8416605 E-03	+3.6182989 E-03
c_2	+1.4714143 E-04	-1.3603273 E-05
c_3	-9.6719890 E-07	+4.9618922 E-07

This final $T^{\text{air, lifted from surface}}$ of equation (3-34), is used in equation (3-11) for the Lifted Index.

3.6 Output Description

The output of the GII processing are:

- The Lifted Index, unit K, according to equation (3-12)
- The K-Index, unit °C, according to equation (3-13)
- Layer Precipitable Water, lower troposphere, unit kg/m^2, according to equation (3-14)
- Layer Precipitable Water, middle troposphere, unit kg/m^2, according to equation (3-14)
- Layer Precipitable Water, upper troposphere, unit kg/m^2, according to equation (3-14)
- Total Precipitable Water, unit kg/m2, according to equation (3-16)
- Total Ozone, in Dobson Units, according to equations (3-17) and (3-19)

The output is generated for each FoR. In case a FoR is more than just a single pixel, the fraction of cloud free pixels used within the FoR can be added as a quality information. This will automatically also flag the special case of Version II processing where TOZ is derived over cloudy areas (cloud free fraction = 0.0).

As the K-Index (and theoretically also the Lifted Index) can be undefined (in case of surface pressure below 850hPa or 500hPa, the final product has to allow "undefined" as output for each of the two parameters.

For the final disseminated product it must be kept in mind that the TOZ values will cover many more FoRs than the full GII output, because of the special Version II cloudy processing.

Meaningful limits for the product entries (e.g. for BUFR compression) are:

K-Index between -30 and +70 °C
Lifted Index between -20 and +40 K
TPW, LPW between 0 and 100 kg/m^2
TOZ between 0 and 700 DU

3.7 Product Performance and Examples

The retrieval of a full temperature and humidity profile within the GII processing is an ill posed problem, as the MTG-FCI infrared channels do not contain sufficient information on the vertical structure of the atmosphere, e.g. the presence of a temperature inversion cannot be inferred from the radiances measured in these channels. The GII processing thus relies heavily on the applied background (or first guess) profile and will always retain certain features of this profile.

Experience from the MSG GII product, which uses the same retrieval technique, shows that in many cases the first guess already matches the satellite observations so closely that the profile is not changed at all (i.e. the RMS, as defined by equation (3-5) is below the applied threshold). However, there are many cases where the first guess field is quite significantly changed within the retrieval, i.e. the satellite adds information, usually by changing the surface skin temperature and/or the atmospheric humidity, which obviously reflects the relevant parameters determining the MSG (and MTG-FCI) infrared radiances.

Figure 6 and Figure 7 shows an example (for the K-Index). The 12-hour ECMWF forecasted K-Index shows a zone of moderate instability over Germany, extending to the southeast over Austria and neighbouring countries (Figure 6). The retrieved K-Index (Figure 7) shows slightly higher K-values and an eastward shift of the unstable air mass, i.e. the local extremes and gradients were changed, which is a frequently observed product behaviour. In this particular case, the retrieval is supported by local radio soundings, also showing higher than forecasted K-Index values over eastern Germany and Poland.

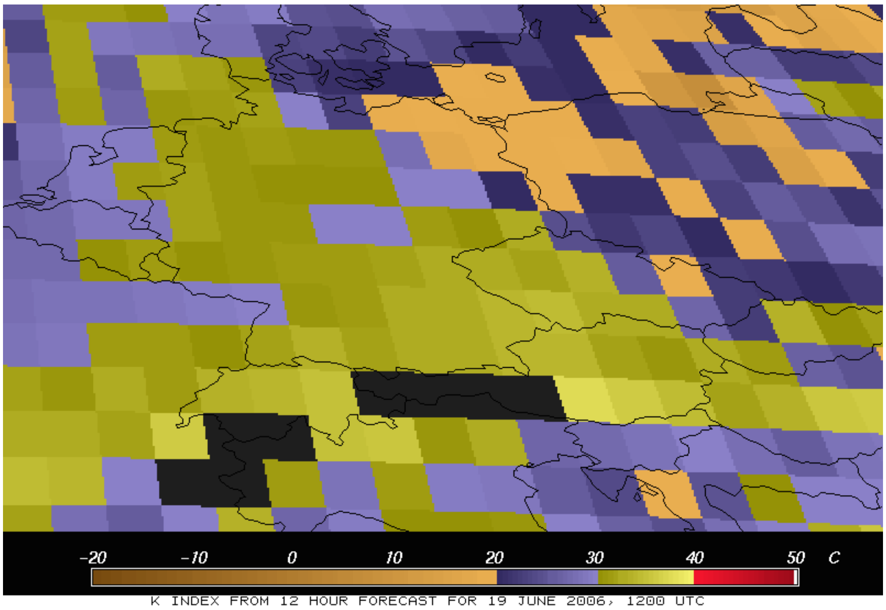

Figure 6: 12-hour forecasted K-Index, on a 1° x 1° latitude/longitude grid over central Europe, 19 June 2006, 1200 UTC

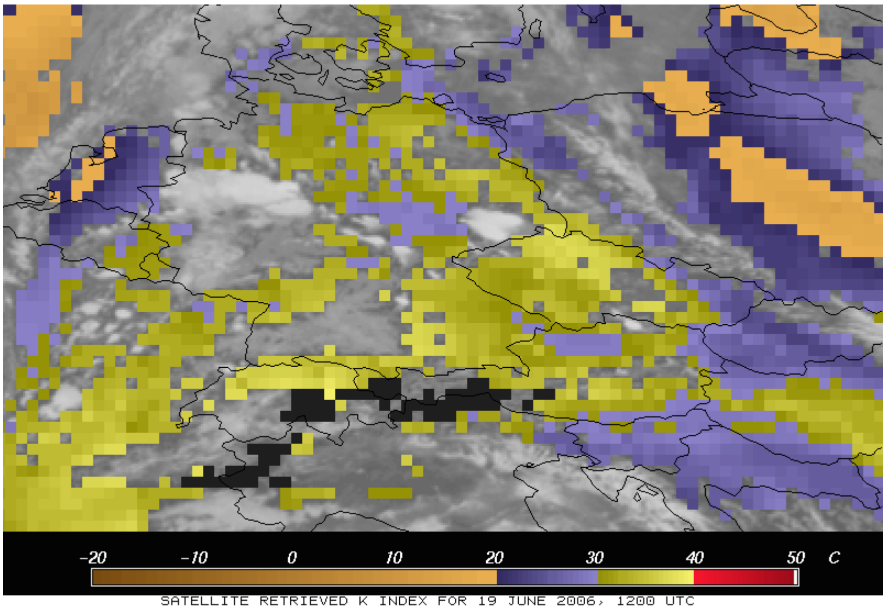

Figure 7: Retrieved K-Index, using the 12-hour forecast profiles as first guess and the MSG measurements. Clouds are shown in various shades of grey.

Figure 8 shows the number of iterations needed during the retrieval for this same case: The area of significant changes in K-Index with respect to the forecast over eastern Germany and Poland is well dominated by orange, i.e. several iterations were needed here to change the not so appropriate first guess to the final result. The Figure also illustrates that the first guess is in many cases not changed at all (green colour). Generally this happens in ~50% of the cases, where this number obviously depends on the quality of the forecast!

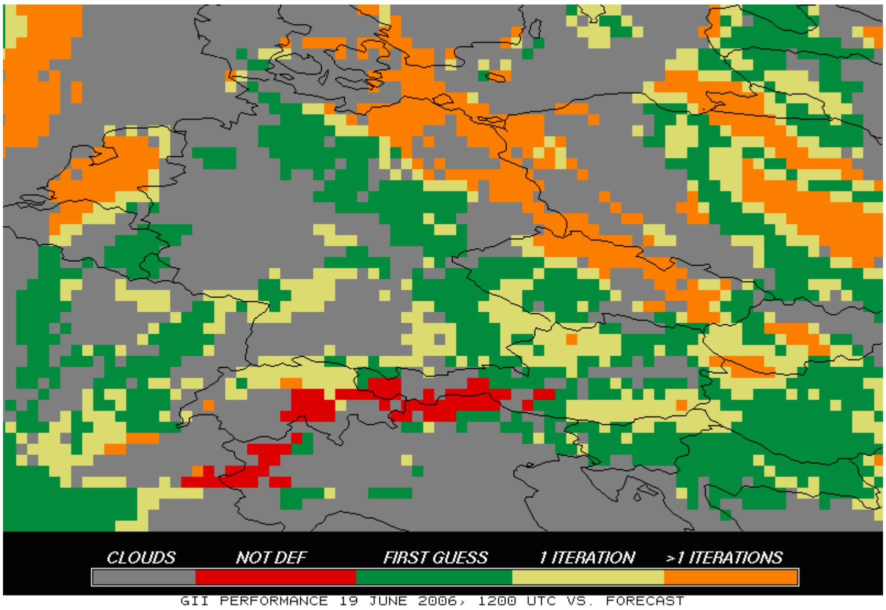

Figure 8: Internal diagnostics of the retrieval case shown in Figure 5. For the non-cloudy areas, the Figure depicts where the retrieval simply reproduced the first guess (green)m where the retrieval needed only one iteration (yellow)m and where more iterations were needed (orange). High elevation areas, where the K-Index is undefined, are indicated in red.

With respect to the retrieval of the total column ozone, theoretical considerations have shown that the most important information content of the first guess is the shape of the ozone profile and not so much the total column mass. Figure 9 and Figure 10 illustrate this, again using MSG as a proxy for MTG-FCI: Figure 7 shows the first guess TOZ field, as derived from the first guess profile together with the retrieved TOZ, where the forecasted TOZ maximum over Northwestern Africa and Western Europe is well depicted. For the retrieval shown in Figure 8, the first guess ozone field was artificially shifted eastwards by 30 deg, i.e. the retrieval was faced with a fairly wrong first guess field, but still retrieved an ozone maximum in the original position.

Figure 11 shows a “typical” ozone profile together with the MSG IR9.7 channel Jacobians, thus illustrating the actual measurement capabilities of such an IR instrument: The instrument is sensitive to ozone between ~800 hPa and 50 hPa, i.e. ozone in the very low troposphere and in the upper stratosphere cannot be detected. Any contribution to the Total Ozone value form these layers entirely come from the first guess.

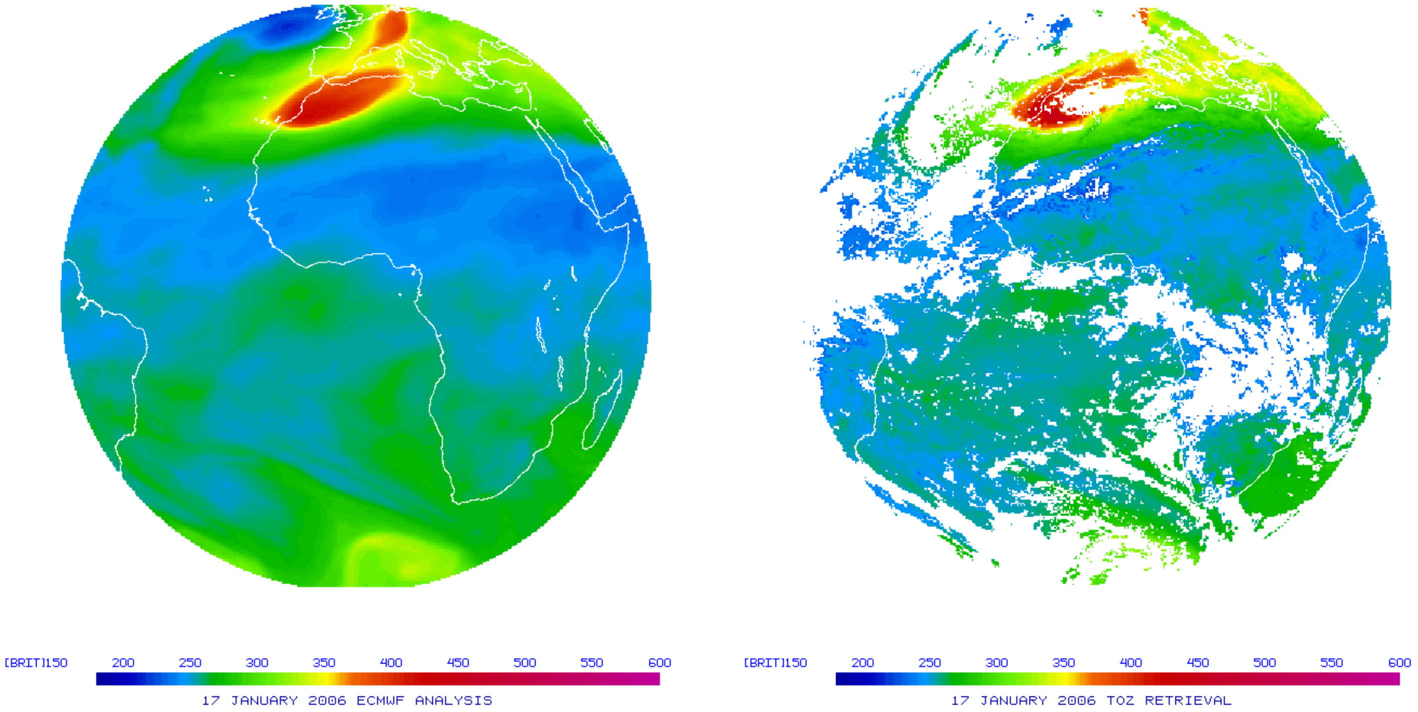

Figure 9: Example of a TOZ forecast field (left) and the retrieved TOZ field (right); clouds are shown in white. Colour scale is given in Dobson Units. In this case the retrieval well follows the first guess field.

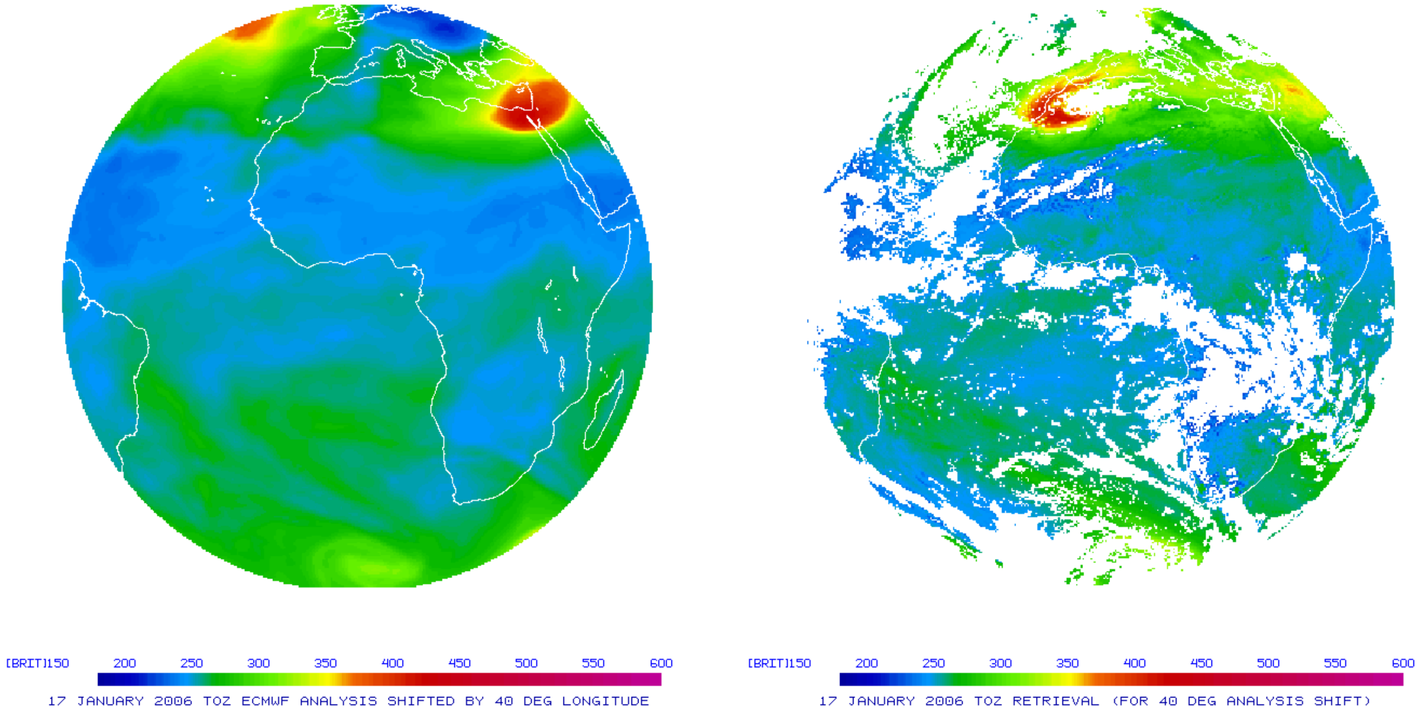

Figure 10: As Figure 7, but with a drastically changed first guess field (left: ozone field of Figure 7 were shifted by 30 deg longitude). The retrieved TOZ field (right) still correctly depicted the North African ozone maximum which was not present in the first guess.

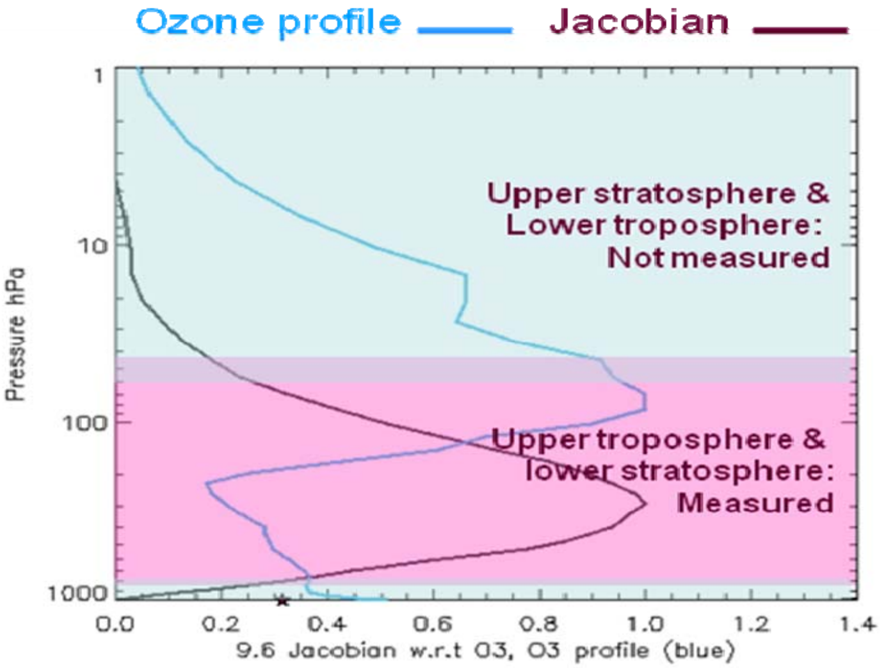

Figure 11: Simulation of the MSG IR9.7 channel Jacobians (red) for a “typical” ozone profile (blue). The Jacobians show a significant contribution to the channel between ~800 and 50 hPa, i.e. lower tropospheric and upper stratospheric ozone is not measured. Conditions for MTG-FCI will be very similar.

Typical usage of the TOZ data will focus on regional ozone maxima, as shown in Figure 9 and Figure 10. Such maxima are often associated with synoptic systems (cold air masses with a lower tropopause and hence increased ozone values in the lower stratosphere, i.e. the development, intensification and speed of such systems can be well depicted through the TOZ information, thus providing a real-time check of the performance of a numerical weather forecast.

4 GLOSSARY OF SYMBOLS

Variable Name	Meaning	Unit
a	Humidity dependent value used in equation (3-25) – dew point calculation	n/a
a_0, a_1, a_2	Regression coefficients used for cloud emissivity calculations	n/a
b_1,b_2	Empirical coefficients used in equations (3-31) and (3-33)	n/a
CM	Cloud mask (discriminates cloud free from cloudy FoR)	n/a
$c_{p,m}$	Specific heat of moist air	J/kg K
$c_{p,d}$	Specific heat of dry air	J/kg K
c_1, c_2, c_3	Regression coefficients used for the P calculations (equation (3-38))	n/a
E(T)	Saturation vapour pressure at temperature T	hPa
e	Vapour pressure	hPa
g	Earth acceleration of gravity	m/s^2
i	Index for MTG-FCI channel	n/a
icloud, icloud1, icloud2	Indices describing cloud levels	n/a
K	Matrix of Jacobians for T and T_{skin}: for q and o_3: for p_{cloud}:	K/K K/[ppmv] K/[hPa]
K	Level index (within atmospheric profile)	
KI	K Index	° C
L	Radiance (general)	mW/m^2 ster cm^{-1}
L_{down}	Downwelling radiance at surface level	mW/m^2 ster cm^{-1}
L_{final}	Cloudy radiances at top of atmosphere, corrected for cloud emissivity	mW/m^2 ster cm^{-1}
$L_{top,overcast}$	Radiance at the top of atmosphere in overcast conditions	mW/m^2 ster cm^{-1}
L_B	Blackbody radiance according to Planck's Law	mW/m^2 ster cm^{-1}
LI	Lifted Index	K
LPW, LPW_1, LPW_2, LPW_3	Layer Precipitable Water (general and in three different layers)	kg/m^2
k	Index of level element ($1 \leq k \leq M$)	n/a
m	Number of atmospheric levels in RTTOV	n/a
n	Iteration step within physical retrieval	n/a
o_3	Ozone (mixing ratio)	kg/kg or ppmv
P	Empirical coefficient used in equations (3-36) and (3-37)	n/a
p	Pressure	hPa
p^{lift}	Lifting condensation level pressure	hPa
p_{sfc}	Surface pressure	hPa