EUMETSAT

AC SAF

ATMOSPHERIC COMPOSITION MONITORING

PRODUCT USER MANUAL

Near real-time IASI Brescia SO2

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DOCUMENT STATUS SHEET

Issue	Date	Modified items/Reason for change
1.1	15/06/2017	In section 4.3 Table 1, HEIGHT: “km” has been corrected with “m”. In section 5.1 Table “2, 7, 10, 13, 16 and 25 km” has been replaced with “7000, 10000, 13000, 16000 and 25000 m” Section 5.2.2 Data filtering has been added.
1.2	14/12/2017	Page 8, line 3, ‘Metop satellite’ replaced with ‘Metop satellites’. The sentence 'In no case the different SO2 columns (...) must be added up' was replaced by ‘Under no circumstance should the different SO2 columns (...) be added up.’
1.2	12/02/2018	Page 13, section 5.2.3, some lines describing the uncertainty characterization were added.
1.2	26/03/2018	New section 5.2.4 included to describe the conversion of altitude to pressure.

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1. INTRODUCTION

1.1 Purpose and scope

This document is the Product User Manual for the Near Real Time IASI SO_2 product retrieved within the context of the Satellite Application Facility Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF) Second Continuous Development and Operations Phase (CDOP-2). This document gives a brief overview on the IASI Brescia retrieval algorithm and explains how to use and interpret the IASI Brescia SO_2 product.

1.2 Acronyms

AC SAF: Atmospheric Composition Monitoring Satellite Application Facility
CDOP-2: Second Continuous Development and Operations Phase (CDOP-2)
EUMETSAT: European Organisation for the Exploitation of Meteorological Satellites
EUMETCast: EUMETSAT multi-service data dissemination system
WMO: World Meteorological Organization
GTS: Global Telecommunication System
IASI: Infrared Atmospheric Sounding Interferometer
ULB: Université Libre de Bruxelles
LATMOS: Laboratoire Atmosphères, Milieux, Observations Spatiales

1.3 Applicable and reference documents

1.3.1 Applicable documents

[AD1] IASI Brescia SO2 Algorithm Theoretical Basis Document SAF/AC/ULB/ATBD/002 Issue 1.1, 28/07/2016
[AD2] IASI Brescia SO2 Product Specification, Requirement And Assessment SAF/AC/ULB/PSRA/002 Issue 1.2, 23/03/2017

[AD3] Product Requirements Document SAF/AC/FMI/RQ/PRD/001 Issue 1.6, 03/12/2014

1.3.2 Reference documents

[RD1] Hilton, F.; August, T.; Barnet, C.; Bouchard, A.; Camy-Peyret, C.; Clarisse, L.; Clerbaux, C.; Coheur, P.-F.; Collard, A.; Crevoisier, C.; Dufour, G.; Edwards, D.; Faijan, F.; Fourrié, N.; Gambacorta, A.; Gauguin, S.; Guidard, V.; Hurtmans, D.; Illingworth, S.; Jacquinet-Husson, N.; Kerzenmacher, T.; Klaes, D.; Lavanant, L.; Masiello, G.; Matricardi, M.; McNally, T.; Newman, S.; Pavelin, E.; Péquignot, E.; Phulpin, T.; Remedios, J.; Schlüssel, P.; Serio, C.; Strow, L.; Taylor, J.; Tobin, D.; Uspensky, A. and Zhou, D.: Hyperspectral Earth Observation with IASI. *Bull. Am. Meteorol. Soc., 93(3)*, 347-370, doi: 10.1175/BAMS-D-11-00027.1, 2012.

[RD2] Camy-Peyret, C. & Eyre, J. The IASI Science Plan. Technical report, A Report From The IASI Sounding Science Working Group, 1998.

[RD3] Clerbaux, C.; Boynard, A.; Clarisse, L.; George, M.; Hadji-Lazaro, J.; Herbin, H.; Hurtmans, D.; Pommier, M.; Razavi, A.; Turquety, S.; Wespes, C. & Coheur, P. F. Monitoring of atmospheric composition using the thermal infrared IASI/MetOp sounder. *Atmos. Chem. Phys*., 9(16):6041-6054, 2009.

[RD4] Clarisse, L., Hurtmans, D., Clerbaux, C., Hadji-Lazaro, J., Ngadi, Y. and Coheur, P. F.: Retrieval of sulphur dioxide from the infrared atmospheric sounding interferometer (IASI), Atmos. Meas. Tech., 5, 581-594, doi:10.5194/amt-5-581-2012, 2012.

[RD5] Guide to WMO Table Driven Code Forms https://www.wmo.int/pages/prog/www/WMOCodes/Guides/BUFRCREX/Layer1-2-English.pdf

[RD6] BUFR tables for the IASI SO_2 product www.eumetsat.int/website/wcm/idc/idcplg?IdcService=GET_FILE&dDocName=ZIP_IASI_SO2_BUFR_TABLES&RevisionSelectionMethod=LatestReleased&Rendition=Web

[RD7] Carn, S.A., Clarisse, L., Prata, A.J.: Multi-decadal satellite measurements of global volcanic degassing, Journal of Volcanology and Geothermal Research, 311, 99-134, http://dx.doi.org/10.1016, 2016.

[RD8] Clarisse, L., Coheur, P.-F., Theys, N., Hurtmans, D., and Clerbaux, C.: The 2011 Nabro eruption, a SO2 plume height analysis using IASI measurements, Atmos. Chem. Phys., 14, 3095-3111, doi:10.5194/acp-14-3095-2014, 2014.

[RD9] Clarisse, L., Hurtmans, D., Clerbaux, C., Hadji-Lazaro, J., Ngadi, Y. and Coheur, P.-F.: Retrieval of sulphur dioxide from the infrared atmospheric sounding interferometer (IASI), Atmos. Meas. Tech., 5, 581–594, doi:10.5194/amt-5-581-2012, 2012.

[RD10] EUMETCast Dissemination facility http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html

2. INTRODUCTION TO EUMETSAT SATELLITE APPLICATION FACILITY ON ATMOSPHERIC COMPOSITION MONITORING (AC SAF)

2.1 Background

The need for atmospheric chemistry monitoring was first realized when severe loss of stratospheric ozone was detected over the Polar Regions. At the same time, increased levels of ultraviolet radiation were observed.

Ultraviolet radiation is known to be dangerous to humans and animals (causing e.g. skin cancer, cataract, immune suppression) and having harmful effects on agriculture, forests and oceanic food chain. In addition, the global warming - besides affecting the atmospheric chemistry - also enhances the ozone depletion by cooling the stratosphere. Combined, these phenomena have immense effects on the whole planet. Therefore, monitoring the chemical composition of the atmosphere is a very important duty for EUMETSAT and the world-wide scientific community.

2.2 Objectives

The main objectives of the AC SAF is to process, archive, validate and disseminate atmospheric composition products (O_3, NO_2, SO_2, BrO, HCHO, H_2O), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 spectrometers onboard Metop-A and Metop-B satellites and some new products from the IASI mission: CO, SO_2, O_3 and HNO_3.

Another important task of the AC SAF is the research and development in radiative transfer modelling and inversion methods for obtaining long-term, high-quality atmospheric composition products from the satellite measurements.

2.3 Product categories, timeliness and dissemination

Data products are divided in two categories depending on how quickly they are available to users:

Near real-time products are available in less than three hours after measurement. These products are disseminated via EUMETCast, WMO GTS or internet.

- Near real-time trace gas columns
    - O_3, NO_2, NO_2Tropo, CO, HNO_3, SO_2
- Near real-time ozone profiles
    - coarse and high-resolution
- Near real-time absorbing aerosol indexes
    - from main science channels and polarization measurement detectors
- Near real-time UV indexes
    - clear-sky and cloud-corrected

Offline products are available in two weeks after measurement and disseminated via dedicated web services at EUMETSAT, FMI and DLR.

- Offline trace gas columns
    - O_3, NO_2, NO_2Tropo, SO_2, BrO, HCHO, H_2O

- Offline ozone profiles
    - coarse and high-resolution
- Offline absorbing aerosol indexes
    - from main science channels and polarization measurement detectors
- Offline surface UV

More information about the AC SAF project, products and services: http://acsaf.org/

AC SAF Helpdesk: helpdesk@acsaf.org

3. IASI-BRESCIA RETRIEVAL ALGORITHM

3.1 IASI instrument

IASI is an infrared Fourier transform spectrometer developed jointly by CNES (the French spatial agency) with support of the scientific community (for a review see [RD1]), and by EUMETSAT. IASI is mounted on-board the European polar-orbiting Metop satellites with the primary objective to improve numerical weather predictions, by measuring tropospheric temperature and humidity with high horizontal resolution and sampling, with 1 km vertical resolution, and with respectively 1 K and 10% accuracy [RD2]. IASI also contributes to atmospheric composition measurements for climate and chemistry applications [RD3]. To reach these two objectives, IASI measures the infrared radiation of the Earth's surface and of the atmosphere between 645 and 2760 cm^{-1} at nadir and along a 2200 km swath perpendicular to the satellite track. A total of 120 views are collected over the swath, divided as 30 arrays of 4 individual Field-of-views (FOVs) varying in size from 36 $\times\pi$ km^2 at nadir (circular 12 km diameter pixel) to 10 x 20 x π km^2 at the larger viewing angle (ellipse-shaped FOV at the end of the swath). IASI offers in this standard observing mode global coverage twice daily, with overpass times at around 9:30 and 21:30 mean local solar time. The very good spatial and temporal sampling of IASI is complemented by fairly high spectral and radiometric performances: the calibrated level 1C radiances are at 0.5 cm^{-1} apodized spectral resolution (the instrument achieves a 2 cm optical path difference), with an apodized noise that ranges below 2500 cm^{-1} between 0.1 and 0.2 K for a reference blackbody at 280 K [RD1].

3.2 Brescia overview

The Brescia algorithm calculates IASI SO_2 total columns using brightness temperature differences and look up tables assuming 5 different plumes heights (7, 10, 13, 16 and 25 km). The retrieval sequence of the Brescia SO_2 algorithm is described in the Figure 1. When the IASI L2 pressure and temperature profiles are not available, ECMWF forecasts (3h, interpolated in time and space) data are used.

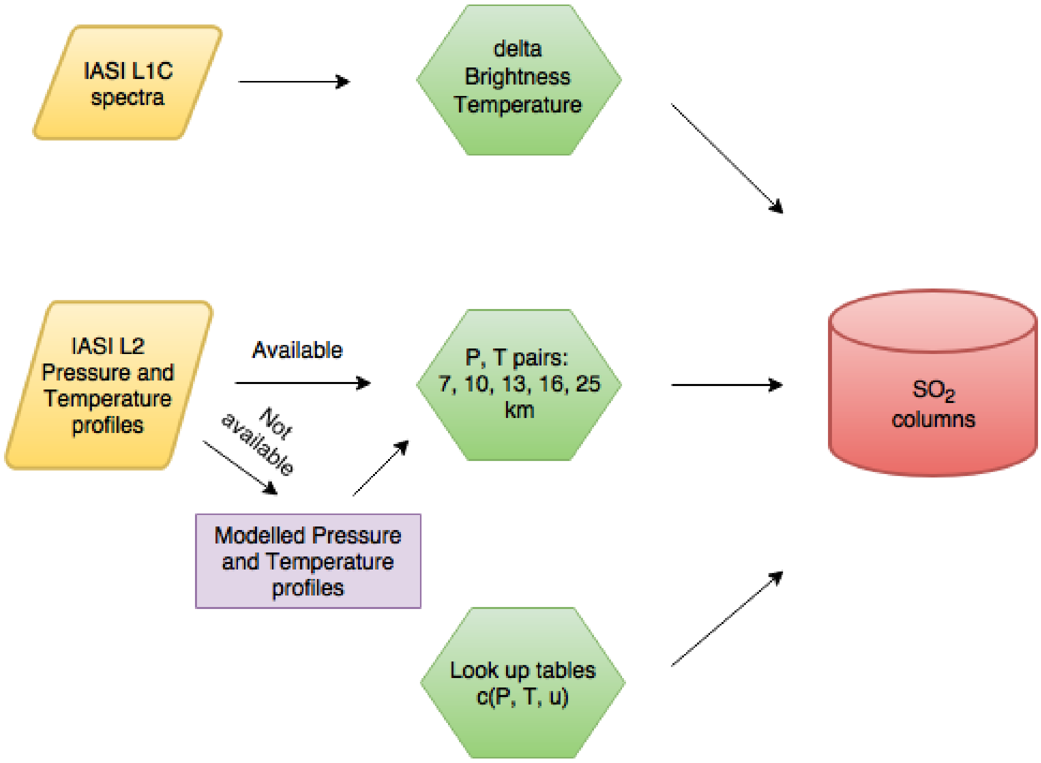

Figure 1: Graphic representation of the retrieval sequence of the Brescia SO_2 algorithm.

The algorithm description is given in the Brescia ATBD [AD1] and in [RD4].

4. IASI LEVEL 2 NRT SO2 PRODUCT

4.1 BUFR PDU file name convention

The names of the IASI Level 2 SO_2 products distributed on EUMETCast follow this example:

W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUMC_
*yyyymmdd*hhmmss_nnnnn_eps_o_so2_l2.bin

where:

yyyymmdd	the UTC year, month, day of the data start sensing time
hhmmss	the UTC hour, minute, second of the data start sensing time
nnnnn	the orbit number
*	A, B or C

4.2 BUFR file size estimate

The size of the output may vary and is on average 100 KB with a number of 480 files per day per instrument.

4.3 Content of the BUFR PDU file

The IASI Level 2 SO2 BUFR PDU file structure is the following:

001007 001031 025060 002019 002020 004001 004002 004003 004004 004005

004006 005040 201133 005041 201000 005001 006001 005043 007024 005021

007025 005022 007007 040216 007002 201130 202129 015045 201000 202000

012080 106000 031001 007007 201130 202129 015045 202000 201000

See WMO documents [RD5] for BUFR specifications. BUFR tables for the IASI SO_2 product are available in [RD6].

The descriptors are detailed below. The Brescia SO_2 product is provided in the 6 last fields (in bold).

Table 1: Data descriptors of IASI Level 2 SO_2 BUFR file

DATA DESCRIPTOR		NAME USED HEREAFTER
0-0-1007	SATELLITE IDENTIFIER	
0-0-1031	IDENTIFICATION OF ORIGINATING/GENERATING CENTRE	
0-25-060	SOFTWARE IDENTIFICATION	
0-0-2019	SATELLITE INSTRUMENTS	

0-0-2020	SATELLITE CLASSIFICATION	
0-0-4001	YEAR	
0-0-4002	MONTH	
0-0-4003	DAY	
0-0-4004	HOUR	
0-0-4005	MINUTE	
0-0-4006	SECOND	
0-0-5040	ORBIT NUMBER	
0-0-5041	SCAN LINE NUMBER	
0-0-5001	LATITUDE (HIGH ACCURACY)	
0-0-6001	LONGITUDE (HIGH ACCURACY)	
0-0-5043	FIELD OF VIEW NUMBER	
0-0-7024	SATELLITE ZENITH ANGLE	
0-0-5021	BEARING OR AZIMUTH (DEGREE TRUE)	
0-0-7025	SOLAR ZENITH ANGLE	
0-0-5022	SOLAR AZIMUTH (DEGREE TRUE)	
0-0-7007	HEIGHT (Surface altitude in meter)	
0-4-0216	**GENERAL RETRIEVAL QUALITY FLAG FOR SO2**	**SO2_QFLAG**
0-1-5045	**SO2 COL ALTITUDE** (columns at different altitudes)	**SO2_COL_AT_ALTITUDES**
0-1-2080	**BRIGHTNESS TEMPERATURE REAL PART**	**SO2_BT_DIFFERENCE**
0-3-1001	**DELAYED DESCRIPTOR REPLICATION FACTOR (**Number of SO2 Levels NLSO2)	**number of altitudes=5**
0-0-7007	**HEIGHT**	**altitudes in m of the 5 altitudes levels**
0-0-7002	**HEIGHT OR ALTITUDE**	**SO2_ALTITUDE* (altitude of the plume)**
0-1-5045	**SULFUR DIOXIDE**	**SO2_COL* (total column)**

* Placeholders for future versions

5. THE BRESCIA SO2 PRODUCT

5.1 Product description

The Brescia SO_2 product includes several variables, described in Table 1 (bold) and in Table 2. The principal product is a SO_2 total column, given at 5 estimated altitudes: 7, 10, 13, 16 and 25 km.

Table 2: Description and units of Brescia SO2 product available in the IASI L2 SO2 BUFR files

Name	Description	Units
SO2_QFLAG	General retrieval quality flag SO2_QFAG=**9** (default value) or SO2_QFAG=**11** (T/P from forecasts in the absence of IASI L2 Products)	NA
SO2_COL_AT_ALTITUDES	SO_2 column at an estimated altitude of 7000, 10000, 13000, 16000 and 25000 m	DU*
SO2_BT_DIFFERENCE	SO_2 Brightness temperature difference	K
Placeholders for future versions:		
SO2_ALTITUDE	*Retrieved plume altitude*	*km*
SO2_COL	*SO2 column at the retrieved plume altitude from an neural network approach*	*DU**

*1 DU=2.69 10^{16} molecules /cm²

5.2 Using the product

5.2.1 Quality flags

All retrieved SO_2 columns are considered best quality retrievals and can be used. The following 2 flags give the piece of information about the pressure and temperature profiles used in the retrievals:
SO2_QFLAG = 9 when the values are calculated with the IASI L2;
SO2_QFLAG=11 means that the pressure and temperature profiles are missing in the IASI L2 data and that model/forecast data have been used instead.

5.2.2 Data filtering

We recommend to only look at the retrievals in the neighbourhood of SO2_BT_DIFFERENCE>1K pixels, and not use the pixels with a SO2_BT_DIFFERENCE<0.4K (not enough SO2 to have a reliable retrieval). See Figure 2 for an example. The size of the region around SO2_BT_DIFFERENCE>1K pixels is let to the user's estimate.

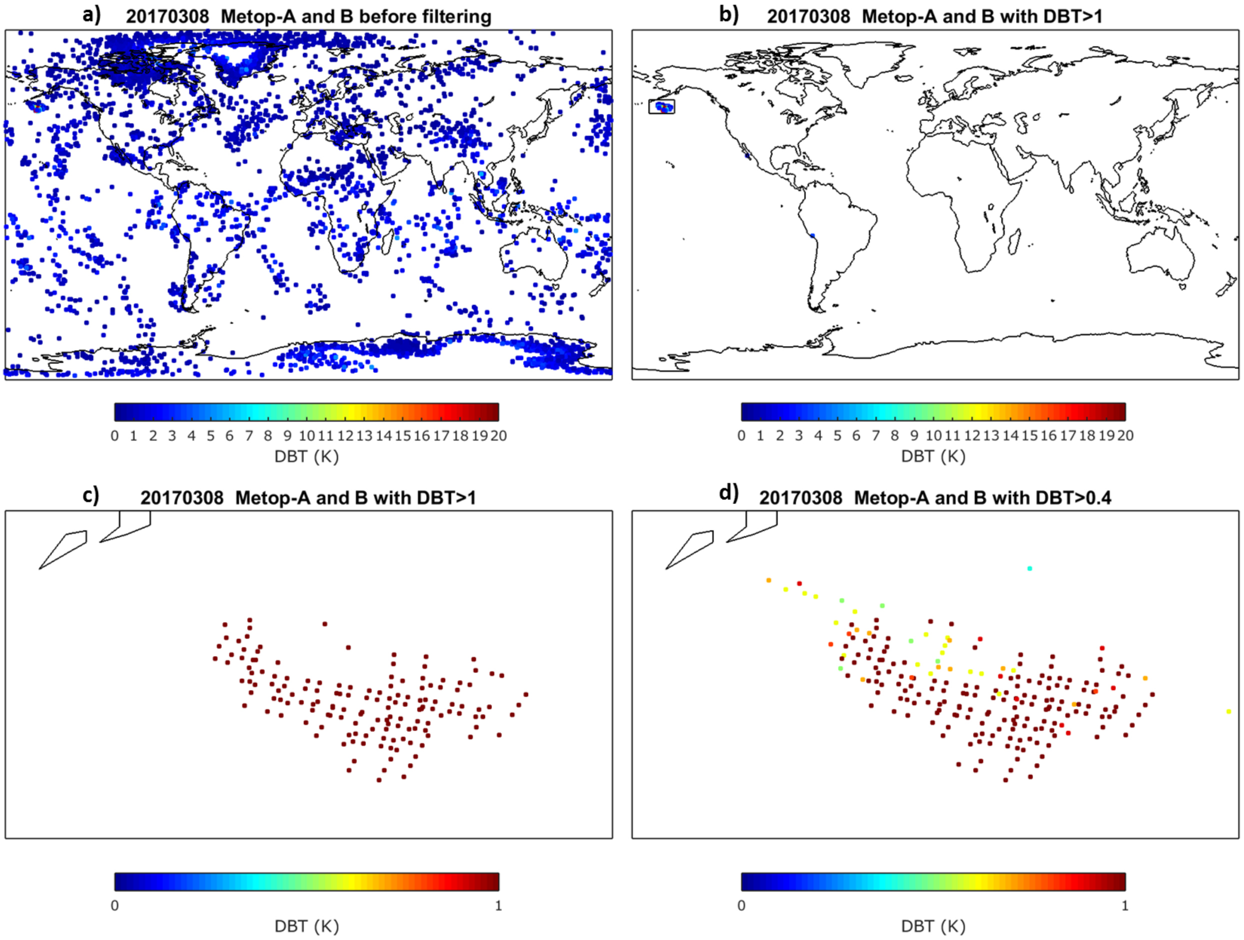

Figure 2: Filtering example using SO2_BT_DIFFERENCE (DBT) for 8 March 2017: (a) all Metop-A and B retrievals where SO_2 is detected, (b) only pixels with DBT>1, (c) zoom in the Alaska Gulf (rectangle in subplot b), (d) in the neighbourhood of pixels with DBT>1, one can consider pixels with DBT>0.4.

5.2.3 SO_2 column and uncertainty characterization

In the current version, the altitude of the SO_2 plume is not given. This field will be delivered in the next versions. The user has to assume the plume's altitude or get the information from another source, in order to pick the proper SO_2 column. Under no circumstance should the different SO_2 columns (at 7, 10, 13, 16 and 25 km) be added up. Only one SO_2 column must be used for one location. Examples of applications can be found in [RD7] and [RD8].

A characterization of how the uncertainty in the assumed altitude translates to an uncertainty in the final column can be obtained using the variance formula:

$$\sigma_{SO2} = \frac{\partial SO2}{\partial alt} \sigma_{alt} \qquad (1)$$

Here, σ_{alt} is the uncertainty on the altitude (user provided, e.g. 1 km) the derivative of the SO_2 column with respect to altitude $\left(\frac{\partial SO2}{\partial alt}\right)$ can be calculated numerically from the 5 SO_2 columns. This uncertainty can be relatively small for high altitudes (e.g. 10-20% around the tropopause, see Figure 7 in [RD9]), while for lower altitudes can reach over 100%.

5.2.4 Altitude-pressure conversion

Temperature and humidity vertical profiles extracted from **IASI L2 twt product** are given on 101 pressure levels (in Pa). The information of the temperature and humidity can be used to calculate 101 corresponding altitude levels as outlined below. After that, the pressure at a specific altitude can be obtained by interpolating (linear interpolation should be sufficient) the pressure grid at the desired altitude.

Introducing the following notation:
surface altitude = z_0 ("HEIGHT", from BUFR files)
surface pressure = p_0 ("PRESSURE (HIGH PRECISION)" from IASI L2 twt product)
surface temperature = T_o, first level of the temperature profile T (extracted from IASI L2 twt product)
surface humidity = q_o, first level of the humidity profile q (extracted from IASI L2 twt product)

The acceleration due to the gravity is function of the geographic latitude ϕ and of the altitude z_i:

$$g(z_i, \phi) = g_\phi - (3.085462 \times 10^{-6} + 2.27 \times 10^{-9} \cos(2\phi))z_i + (7.254 \times 10^{-13} + 1.0 \times 10^{-20} \cos(2\phi))\, z_i^2 - (1.517 \times 10^{-19} + 6 \times 10^{-22} \cos(2\phi)) z_i^3 \quad (2)$$

where

$$g_\phi = 9.806160(1 - 0.0026373 \cos(2\phi) + 0.0000059 \cos^2(2\phi)) \text{ ms}^{-2} \quad (3)$$

The mean virtual temperature between two pressure levels p_i and p_{i+1} (just above level i) is then:

$$\overline{Tv_{i,i+1}} = \frac{T_i(1+0.608\, q_i) + T_{i+1}(1+0.608\, q_{i+1})}{2} \quad (4)$$

with T_i and q_i, the temperature and humidity at p_i, respectively, and T_{i+1} and q_{i+1}, the temperature and humidity at p_{i+1}, respectively.

Then the altitude of the pressure level p_{i+1} can be estimated from the pressure level p_i (just below level i+1):

$$z_{i+1} = z_i + \frac{R \times \overline{Tv_{i,i+1}}}{g(z_i, \phi)} \times \ln \frac{p_i}{p_{i+1}} \quad (5)$$

with R = 287.06 $JK^{-1}kg^{-1}$, the gas constant for dry air.

Note that for the conversion of the SO_2 altitude levels to pressures, care must be taken to first add the surface altitude z_0 to the SO_2 altitude levels, as these are all defined with respect to the surface altitude.

5.3 Product requirements

The product requirements are given in terms of threshold, target and optimal values in Table 5 below. This information is taken from the Brescia SO_2 product specification, requirement and assessment document [AD2] and is also given in the Product Requirements Document [AD3].

Table 5: Brescia SO_2 product requirements.

		Error*			Spatial resolution	Spatial coverage	NRT
		Threshold	**Target**	**Optimal**			
Total column	Below 10km	200%	100%	50%	IASI pixel	Global	<3h
	Above 10 km	100%	35%	20%	IASI pixel	Global	<3h

*difference of quantity value obtained by measurement and true value of the quantity intended to be measured, as defined by CEOS/ISO:19159 (ISO/TS 19159-1:2014(en), Geographic information - Calibration and validation of remote sensing imagery sensors and data — Part 1: Optical sensors).

5.4 Product dissemination and archiving

5.4.1 Near real time Product dissemination

The IASI Level 2 products are disseminated to users in near real-time through EUMETCast [RD10] with a time lapse of two hours from sensing to delivery. The data are disseminated in WMO (BUFR) format. A description of the IASI SO_2 Level 2 BUFR content is given in Section 4.3.

5.4.2 Archive retrieval

The IASI Level 2 products available from the EUMETSAT Data Centre are archived as full orbits. The products in the EUMETSAT Data Centre are available either in EPS native, in BUFR or in NetCDF format. Visibility of EPS products to the users is 6 hours after sensing (start) time.