

**EUMETSAT****ACSAF**ATMOSPHERIC COMPOSITION
MONITORING**PRODUCT USER MANUAL****Near real-time IASI Brescia SO₂**

Prepared by: Rosa Astoreca
Daniel Hurtmans
Lieven Clarisse
Pierre Coheur
Maya George
Juliette Hadji-Lazaro
Cathy Clerbaux

Université Libre de Bruxelles, Belgium
Université Libre de Bruxelles, Belgium
Université Libre de Bruxelles, Belgium
Université Libre de Bruxelles, Belgium
LATMOS, France
LATMOS, France
LATMOS, France

DOCUMENT STATUS SHEET

| Issue | Date | Modified items/Reason for change |
|-------|------|----------------------------------|
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |

DRAFT

TABLE OF CONTENTS

| | |
|--|-----------|
| 1. INTRODUCTION | 4 |
| 1.1 Purpose and scope | 4 |
| 1.2 Acronyms | 4 |
| 1.3 Applicable and reference documents | 4 |
| 1.3.1 Applicable documents..... | 4 |
| 1.3.2 Reference documents..... | 4 |
| 2. INTRODUCTION TO EUMETSAT SATELLITE APPLICATION FACILITY ON ATMOSPHERIC COMPOSITION MONITORING (AC SAF) | 6 |
| 2.1 Background | 6 |
| 2.2 Objectives..... | 6 |
| 2.3 Product categories, timeliness and dissemination | 6 |
| 3. IASI-BRESCIA RETRIEVAL ALGORITHM | 8 |
| 3.1 IASI instrument..... | 8 |
| 3.2 Brescia overview..... | 8 |
| 4. IASI LEVEL 2 NRT SO₂ PRODUCT..... | 10 |
| 4.1 BUFR PDU file name convention..... | 10 |
| 4.2 BUFR file size estimate | 10 |
| 4.3 Content of the BUFR PDU file | 10 |
| 5. THE BRESCIA SO₂ PRODUCT..... | 12 |
| 5.1 Product description..... | 12 |
| 5.2 Using the product | 12 |
| 5.2.1 Quality Flags..... | 12 |
| 5.2.2 SO ₂ column | 12 |
| 5.3 Product requirements | 13 |
| 5.4 Product dissemination and archiving | 13 |
| 5.4.1 Near real time Product dissemination | 13 |
| 5.4.2 Archive retrieval | 13 |

1. INTRODUCTION

1.1 Purpose and scope

This document is the Product User Manual for the Near Real Time IASI SO₂ 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 SO₂ 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.; Fajjan, 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 SO₂ 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] 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_2 Tropo, 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_2 Tropo, 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

DRAFT

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 satellite 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 $10 \times 20 \times \pi$ 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.

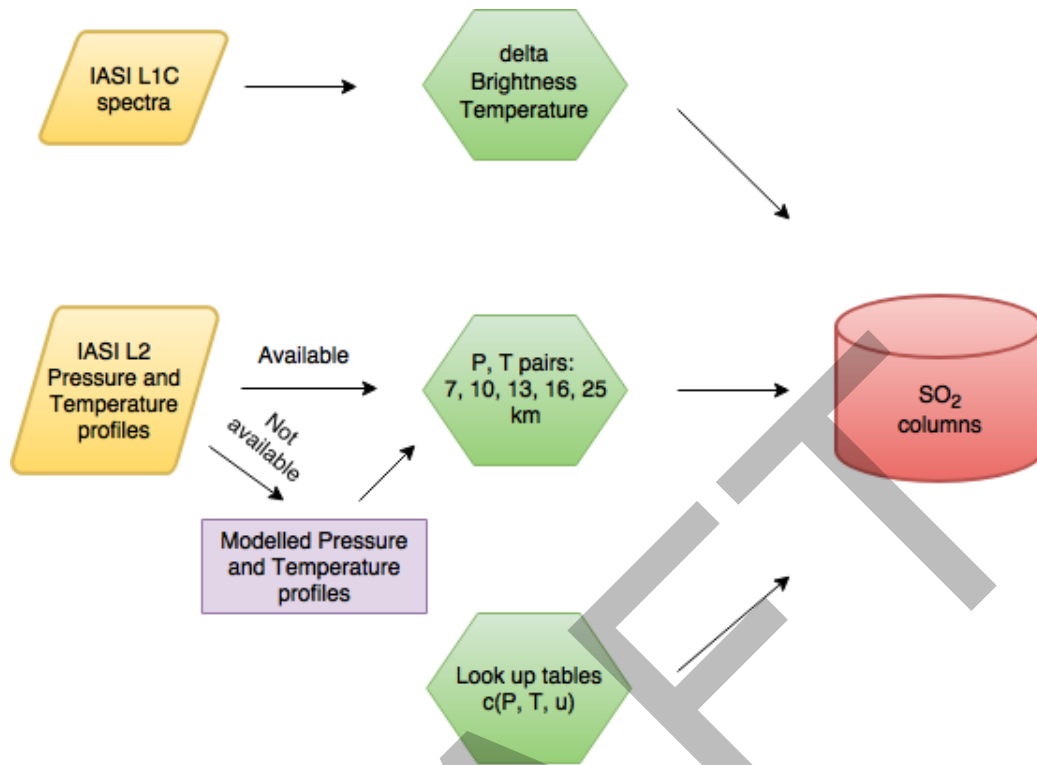


Figure 1: Graphic representation of the retrieval sequence of the Brescia SO₂ algorithm.

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 SO2 products distributed on EUMETCast follow this example:

W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUMC_ yyyymmddhhmmss_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 SO₂ product are available in [RD6].

The descriptors are detailed below. The Brescia SO₂ product is provided in the 6 last fields (in bold).

Table 1: Data descriptors of IASI Level 2 SO2 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 km 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 SO₂ product includes several variables, described in Table 1 (bold) and in Table 2. The principal product is a SO₂ 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 SO ₂ _QFLAG= 9 (default value) or SO ₂ _QFLAG= 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 7, 10, 13, 16 and 25 km | DU* |
| SO₂_BT_DIFFERENCE | SO ₂ Brightness temperature difference | K |
| Placeholders for future versions: | | |
| <i>SO₂_ALTITUDE</i> | <i>Retrieved plume altitude</i> | <i>km</i> |
| <i>SO₂_COL</i> | <i>SO₂ column at the retrieved plume altitude from an neural network approach</i> | <i>DU*</i> |

*1 DU=2.69 10¹⁶ molecules /cm²

5.2 Using the product

5.2.1 Quality Flags

All retrieved SO₂ 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 SO₂ column

In the current version, the altitude of the SO₂ 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 SO₂ column. In no case the different SO₂ columns (at 7, 10, 13, 16 and 25 km) must be added up. Only one SO₂ column must be used for one location. Examples of applications can be found in [RD7] and [RD8].

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 SO₂ product specification, requirement and assessment document [AD2] and is also given in the Product Requirements Document [AD3].

Table 5: Brescia SO₂ 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 [RD9] with a time lapse of two hours from sensing to delivery. The data are disseminated in WMO (BUFR) format. A description of the IASI SO₂ 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.