EUMETSAT AC SAF
ATMOSPHERIC COMPOSITION MONITORING

PRODUCT USER MANUAL

NRT IASI NH_3 HDF5

Prepared by:	Rosa Astoreca	Université Libre de Bruxelles, Belgium
	Daniel Hurtmans	Université Libre de Bruxelles, Belgium
	Lieven Clarisse	Université Libre de Bruxelles, Belgium
	Pierre Coheur	Université Libre de Bruxelles, Belgium
	Juliette Hadji-Lazaro	LATMOS, France
	Sarah Safieddine	LATMOS, France
	Cathy Clerbaux	LATMOS, France

DOCUMENT STATUS SHEET

Issue	Date	Modified items/Reason for change
1.0	26/06/2025	First PUM for the HDF5 NRT NH_3 product. Not reviewed.

RELATED PRODUCT LIST

Product ID	Product name	Platform
O3M-356, O3M-357	IASI NRT NH_3	Metop-B, Metop-C

TABLE OF CONTENTS

1. INTRODUCTION

1.1 Purpose and scope

This document is the Product User Manual for the IASI NRT NH_3 HDF5 product retrieved within the context of the Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF). This document gives a brief overview of the IASI NH3 retrieval algorithm and explains how to use and interpret the IASI NH_3 product.

This document has been written as CHIANTI v20210816 was running at EUMETSAT.

1.2 Acronyms

AC SAF: Atmospheric Composition Monitoring Satellite Application Facility
EUMETSAT: European Organisation for the Exploitation of Meteorological Satellites
EUMETCast: EUMETSAT multi-service data dissemination system
HDF5: Hierarchical Data Format
IASI: Infrared Atmospheric Sounding Interferometer
ULB: Université libre de Bruxelles
LATMOS: Laboratoire Atmosphères, Observations Spatiales

1.3 Applicable and reference documents

1.3.1 Applicable documents

[AD1] IASI NH_3 Algorithm Theoretical Basis Document SAF/AC/ULB/NH3_ATBD Issue 1.2, 03/03/2022

[AD2] IASI NH3 Product Specification, Requirement and Assessment SAF/AC/ULB/ NH3_PSRA Issue 1.1, 24/02/2022

[AD3] Product Requirements Document SAF/AC/FMI/RQ/PRD/001 Issue 2.2, 20/12/2023

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] Whitburn, S., Damme, M. V., Clarisse, L., Bauduin, S., Heald, C. L., Hadji-Lazaro, J., & Coheur, P.-F. A flexible and robust neural network IASI-NH3 retrieval algorithm. *J. Geophys. Res.: Atm.*, *121*. https://doi.org/10.1002/2016JD024828, 2016

[RD5] Van Damme, M., Whitburn, S., Clarisse, L., Clerbaux, C., Hurtmans, D., and Coheur, P.-F.: ***Version 2 of the IASI NH_3 neural network retrieval algorithm: near-real-time and reanalysed datasets***, Atmos. Meas. Tech., 10, 4905–4914, https://doi.org/10.5194/amt-10-4905-2017, 2017.

[RD6] Franco, B., Clarisse, L., Stavrakou, T., Muller, J. F., Van Damme, M., Whitburn, S., Hadji-Lazaro, J., Hurtmans, D., Taraborrelli, D., Clerbaux, C., & Coheur, P.-F.: ***A General Framework for Global Retrievals of Trace Gases From IASI: Application to Methanol, Formic Acid, and PAN***. Journal of Geophysical Research: Atmospheres, 123(24), 13,963-13,984. doi:10.1029/2018JD029633, 2018

[RD7] Van Damme, M., Clarisse, L., Franco, B., Sutton, M. A., Erisman, J. W., Wichink Kruit, R., van Zanten, M., Whitburn, S., Hadji-Lazaro, J., Hurtmans, D., Clerbaux, C., & Coheur, P.-F. ***Global, regional and national trends of atmospheric ammonia derived from a decadal (2008-2018) satellite record***. Environmental Research Letters, 16(5), 055017. doi:10.1088/1748-9326/abd5e0, 2021.

[RD8] EUMETCast Dissemination facility: https://user.eumetsat.int/catalogue

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

Background

The monitoring of atmospheric chemistry is essential due to several human caused changes in the atmosphere, like global warming, loss of stratospheric ozone, increasing UV radiation, and pollution. Furthermore, the monitoring is used to react to the threats caused by the natural hazards as well as follow the effects of the international protocols.

Therefore, monitoring the chemical composition and radiation of the atmosphere is a very important duty for EUMETSAT and the target is to provide information for policy makers, scientists and general public.

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, OClO, CO, NH3), 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 and IASI instruments onboard Metop satellites.

Another important task besides the near real-time (NRT) and offline data dissemination is the provision of long-term, high-quality atmospheric composition products resulting from reprocessing activities.

Product categories, timeliness and dissemination

NRT 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 (total and tropospheric O_3 and NO_2, total SO_2, total HCHO, CO) and high-resolution ozone profiles
- 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 within two weeks after measurement and disseminated via dedicated web services at EUMETSAT and AC SAF.

- Offline trace gas columns (total and tropospheric O_3 and NO_2, total SO_2, total BrO, total HCHO, total H_2O) and high-resolution ozone profiles
- Offline absorbing aerosol indexes from main science channels and polarization measurement detectors
- Offline surface UV, daily doses and daily maximum values with several weighting functions

Data records are available after reprocessing activities from the EUMETSAT Data Centre and/or the AC SAF archives.

- Data records generated in reprocessing
- Lambertian-equivalent reflectivity
- Total OClO

Users can access the AC SAF offline products and data records (free of charge) by registering at the AC SAF web site.

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

AC SAF Helpdesk: helpdesk@acsaf.org

Twitter: https://twitter.com/Atmospheric_SAF

3. IASI NH_3 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 NH_3 algorithm overview

A schematic overview of the ANNI retrieval is presented in Figure 1. The actual calculation of the columns (red boxes in Figure 1) relies on two computational steps:

1. The calculation for each IASI observation of a hyperspectral range index (HRI). This quantity is a very sensitive, broadband spectral index that quantifies the signal strength of a target absorber in a radiance spectrum.

2. The conversion of the HRI into a total column abundance via an artificial feedforward neural network (NN).

In addition to the HRI, the NN relies on a series of auxiliary parameters related to the state of the atmosphere and of the surface. Perturbations to the input data of the NN allows quantification of the uncertainties associated with single-pixel retrieved columns. Appropriate filtering of the data (before and after the retrieval) removes cloudy scenes and observations with limited or no sensitivity to the target trace gas. Finally, in general (for most species in the ANNI retrieval framework), a calibration offset is added to the retrieved columns to account for the constant, climatological background column of the target gas in the atmosphere (green box in Figure 1). However, this last step is not done for NH_3, as background concentrations are extremely low and below the detection limit of IASI.

While the retrieval itself is simple and fast, the initial setup (blue and red boxes in Figure 1) of the HRI and NN is nontrivial. In particular, both rely on weight constants that must be determined with care beforehand from a data set of real (for the HRI) and synthetic (for the NN) IASI spectra. The algorithm description is given in the NH_3 ATBD [AD1] and in [RD4, RD5, RD6, RD7].

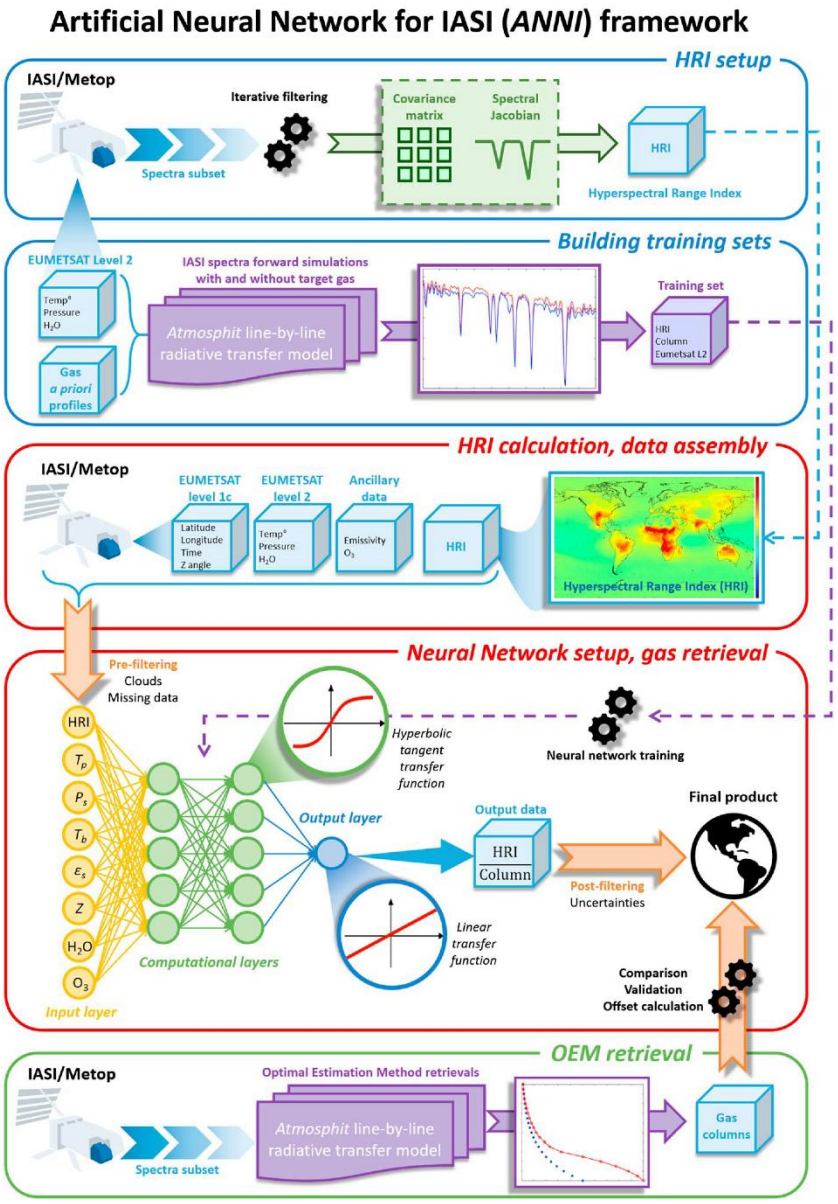

Figure 1: Conceptual flowchart of the ANNI retrieval method of trace gases.

4. IASI LEVEL 2 NRT NH_3 PRODUCT

4.1 HDF5 file name convention

The names of the IASI Level 2 NRT NH_3 products distributed on EUMETCast follow this example:

W_XX-EUMETSAT- Darmstadt,SOUNDING+SATELLITE,METOP*+IASI_C_EUMP_ *yyyymmdd*hhmmss_nnnnn_ACSAF_CHIANTI_l2.h5

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
*	B, C

4.2 HDF5 file size estimate

The size of the output may vary and is on average 22 M with a number of 480 files per day per instrument.

4.3 Content of the HDF5 file

This table describes variables included in the IASI NRT Level 2 NH_3 HDF5 files.

Table 1: Variables name and description

Variables name in HDF5 file	**Variables location**
longitude	/location/longitude
latitude	/location/latitude
time	/location/time
date	/location/date
orbit	/location/orbit
scanline	/location/scanline
general quality flag (gqf)	/fitted/diagnostics/QFLAG
BDIV	/fitted/diagnostics/BDIV
NH3 total columns	/fitted/Total Column
NH3 Error	/fitted/Error
HRI	/fitted/HRI

5. THE NH_3 PRODUCT

5.1 Product description

The NH_3 product includes several variables, described in Table 1 and in Table 2. The principal product is the NH_3 total columns and an estimated error on these columns. Also included are the HRI and the general quality flag.

Table 2: Description and units of the NH_3 product available in the IASI L2 NRT NH_3 HDF5 files

Name	Description	Units
NH3 total columns	Total columns	mol/cm^2
NH3 error	Estimated error on total columns	mol/cm^2
HRI	Index that quantifies the signal strength of a target absorber in a radiance spectrum.	unitless
general_quality_flag	General quality flag	unitless

5.2 Using the product

5.2.1 General quality flag

1. **Stringent quality assurance**

   For these observations, the following conditions are both satisfied:

   - | NH_3 column/HRI | < 15×10^{15} molec/cm^2
   - | NH_3 | > 0 molec/cm^2 or |HRI| < 1.5

2. **Weak quality assurance**

   These are observations, which do not pass the stringent quality assurance test, but satisfy the following weaker conditions:

   - | NH_3 column/HRI | < 30×10^{15} molec/cm^2
   - | NH_3 | > 0 molec/cm^2 or |HRI| < 1.5

3. **No quality assurance**

   These are all the remaining observations.

5.2.2 Data filtering

It is recommended to use data with classification 1 (stringent quality assurance). However, some data users might want to have access to more (noisy) data. Classification 2 (week quality assurance) is therefore also provided, but to be used with care.

5.3 Product requirements

The product requirements are given in terms of threshold, target and optimal values in Table 3 below. This information is taken from the NH_3 product specification, requirement and assessment document [AD2] and is also given in the Product Requirements Document [AD3].

Table 3: NH_3 product requirements.

		Error*			Spatial resolution	Spatial coverage	NRT
		Threshold	**Target**	**Optimal**			
NH_3 total column		RE < 200 % or AE < $1x10^{16}$ molec/cm²	RE < 100 % or AE < $5x10^{15}$ molec/cm²	RE < 50 % or AE < $1x10^{15}$ molec/cm²	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 NRT Product dissemination

The IASI Level 2 products are disseminated to users in near real-time through EUMETCast [RD6] with a time lapse of two hours from sensing to delivery. The data are disseminated in HDF5 format. A full description of the IASI Level 2 NRT NH_3 HDF5 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 in NetCDF format.