

Data Product Specifications, External Interfaces and Validation Means

16.12.2011

Issue 2



PROJECT:	MACC	Monitoring Atmospheric Composition and Climate
SUB-PROJECT / CLUSTER:	MAN	Management and System Engineering
WORK PACKAGE / TASK:	MAN_3	System engineering for the GMES Atmospheric Service
DELIVERABLES:	D_MAN_3.5 (b), D_MAN_3.6, D_MAN_3.7	

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EU FP7 – MACC
Data product specifications and validation

REF.: FP7-MACC-MAN-3-7
 ISSUE: 2
 REVISION: 10
 DATE: 16.12.2011
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title / titre	Data product specifications, external interfaces and validation means
editor / éditeur	Anne De Rudder (IASB-BIRA)
reference / référence	FP7-MACC-MAN-3-7
issue / édition	2
revision / révision	10
status / état	draft
date of issue / date d'édition	16.12.2011
document type / type de document	Framework/Management Document

	FUNCTION	NAME	DATE
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DOCUMENT CHANGE RECORD

Issue	Revision	Date	Modified Items / Reason for Change	
1	0	22.7.2010	Document structure set up, draft instructions written.	
		7.9.2011	Instructions, tables & structure completed; sent to subproject leaders.	
	1	27.9.2011	27.9.2011	Executive summary adapted to new portfolio (in annex). Instructions updated. Section on service line description removed. Added Section 6 (Abstract).
			28.9.2011	Sent to subproject leaders for circulation to individual product providers.
		2	12.10.2011	Integration of information on EURAD-IM.
		3	26.10.2011	Integration of information on MET.NO pollution origin graphic locator.
			28.10.2011	Reminder sent to subproject leaders.
		4	29.10.2011	Integration of information on CO ₂ flux inversions.
		5	30.10.2011	Integration of information on BASCOE.
		6	26.11.2011	Integration of information on SOLEMI, SoDa and MACC-RAD.
2	9	1.12.2011	Integration of information on RAD-UV.	
		8	9.12.2011	Integration of information on GFAS and GFED.
		10.12.2011	Issue of individual abstracts in PDF format.	
	9	16.12.2011	Ex-MACC-RAD renamed RAD-SOLAR. Errata corrected.	
	10	16.12.2011	Integration of information and issue of abstract on SYNAER.	
		16.12.2011	Update of portfolio, summary, introduction and references.	

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EXECUTIVE SUMMARY

Monitoring Atmospheric Composition and Climate (MACC) is the EU FP7 project establishing the core global and regional atmospheric environmental service of the Global Monitoring for the Environment and Security (GMES) European programme. MACC data products available to users (within and outside of the MACC community) are delivered according to three temporal modes of production:

- Near-real time and forecast;
- Delayed mode (validated recent data);
- Reanalysis mode.

Within each mode of production, data products are sorted according to the geographic scale to which they apply (global or regional) and to the nature of the physical parameters they address. The MACC product portfolio is provided as Annex 1 to this document.

This report presents the replies to a questionnaire that was circulated among MACC service providers. The aim of the enquiry was to collect information on external interfaces (Part 2 of Deliverable D_MAN_3.5), validation means (Deliverable D_MAN_3.6) and service and product specifications (Deliverable D_MAN_3.7). At the time of issue, thirteen products or services have been documented in this way.

At the occasion of the enquiry, abstracts summarising the main features of each product have also been written or derived from the information provided, in view of being published on the MACC website. The product abstracts are grouped in Annex 2.



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1 INTRODUCTION

This report presents the returns to an enquiry circulated among the MACC product providers, via the MACC subproject leaders, from the beginning of September to the beginning of December 2011. The collected information covers three MACC deliverables:

- D_MAN_3.5 (Part 2): External interfaces.
- D_MAN_3.6: Validation means.
- D_MAN_3.7: Service specifications.

The first draft of the document was divided according to the different MACC subprojects in an attempt to group MACC products into service lines. To meet a requirement from the MACC Management Board, this structure was abandoned and replaced by a classification of the MACC products by

- 1°) mode of delivery in terms of delay between data production and availability (short: NRT & forecast; medium, including further validation: “delayed”; long: “reanalysis”);
- 2°) geographic coverage extension (global versus regional);
- 3°) category of physical parameter (GHG, RG, aerosol, emissions, solar radiation).

This implied that services supplying the same product in different modes had to be either split up into several sub-services (e.g. BASCOE reanalysis and NRT analysis) or arbitrarily placed in one category (e.g. SYANER, which offers a NRT and a delayed versions; or the Met.No origin locator of pollution episodes, which works in record, delayed and forecast modes).


A version of the MACC portfolio was produced along these lines, submitted to the subproject leaders and updated according to their comments. The resulting portfolio is provided in Annex 1.

The information on every product is divided in three sections: product and service description; product generation and validation; and quality control measures in place.

Preformatted tables were proposed to the product providers to help them circumscribe the questions addressed, and to ensure some homogeneity in the nature of the collected information and in its display. Tables were provided in a Word document and, as an alternative, as Excel spreadsheets, to accommodate individual preferences. There were five tables, respectively addressing

- Product specifications;
- Service specifications;
- Intermediate and final product validation;
- Validation data;
- Quality control.

Subproject leaders were divided as to the pertinence and/or the feasibility of the enquiry on product specifications and validation means. The MACC Management Board suggested that, instead of replying to the enquiry, product providers would write a two-page description to be placed online for download by interested users. The template was hence completed by an additional section to provide room for that abstract; product providers were asked to complete the section devoted to the abstract and, optionally, the rest of the document. Surprisingly, all product providers who replied did fill in the tables, while only some of them contributed an abstract. In these last cases, missing abstracts have been derived from the

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information provided in the tables. Abstracts are grouped in Annex 2. Separate leaflets have also been edited for each documented product.

Few product providers did respond to the enquiry, either because the questionnaire was not forwarded to them by their subproject leader, or because they estimated that answering the questions was unfeasible or pointless. In total, thirteen products or services are documented in the present report, which hence provides a rather biased view of the MACC products; for example, only one member of the European-scale ensemble AQ analysis and forecast service is represented – and extremely well documented.

Finally, it must be noted that SOLEMI and SoDa are precursors of the future RAD-SOLAR solar irradiance service. All three are documented here.

External interfaces


For each product, information on external interfaces can be found in two places: as the “Upstream external information providers” in the Service Specification table and as the “Validation data provider” in the Validation data tables.

External interfaces documented in the present report include channels from the following data sources to various MACC groups:

- ECMWF : operational analyses of winds, temperature, surface pressure - feeding BASCOE NRT analysis;
- ECMWF : IFS operational forecast – feeding EURAD-IM;
- NASA/JPL : retrievals of Aura/MLS observations – feeding BASCOE NRT analysis;
- NASA – feeding GFAS and GFED;
- NASA / AERONET – used for validation by SYNAER;
- ESA / Envisat – feeding SYNAER;
- EUMETSAT LSA SAF – feeding GFAS;
- EUMETSAT / MetOP – feeding SYNAER;
- TNO : emission data – feeding EURAD-IM;
- European national environmental agencies : O₃, NO, NO₂, CO, SO₂, PM_{2.5}, PM₁₀ – used for validation by EURAD-IM;
- NILU : various chemical components from the EMEP measurement database – used for validation by the Met.No locator of the origin of pollution episodes;
- Baseline Surface Radiation Network (BSRN) : ground measurements – used for validation by SOLEMI, SoDa and RAD-SOLAR;
- Global Atmospheric Watch (GAW) : ground measurements – idem;
- International Daylight Measurement Programme (IDMP) : validation data – idem;
- World Radiation Data Center (WRDC) : validation data – idem;
- National meteorological services – idem;
- DLR – idem;
- Centre for Energy-Related, Environmental and Technological Research (CIEMAT) – idem;
- CRES – idem.

Validation means

For each product, information on validation means and on quality are to be found in the last three types of tables

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“Intermediate and final product validation”;


“Validation data”;

“Quality control”.

The first of these tables was supposed to be filled in for each intermediate product generated along the processing chain leading to the final product. However, the returns only included a validation table pertaining to the end product.

Service specifications

Finally, specifications are recorded in the two tables “Service Specifications” and “Product Specifications” under the “Product and service description” section. Several product specification tables may be associated to one described service. It has been left up to the authors to describe services and products as they understand them.

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2 NEAR-REAL TIME (NRT) AND FORECAST MODES - GLOBAL PRODUCTS

2.1 BASCOE NRT Analysis of Stratospheric Ozone

2.1.1 Product and service description

Product specifications


Product name	BASCOE NRT analysis of stratospheric ozone
Product brief description	Analyses of stratospheric ozone by the BASCOE data assimilation system using Aura/MLS-SCI level 2 (v2.2) satellite observations
Product developer(s)	BIRA-IASB, Ringlaan 3, B-1180 Brussel, Contact by e-mail: macc@aeronomie.be
Targeted applications	- Monitoring of polar stratospheric ozone depletion - Quasi-operational evaluation of the MACC integrated stratospheric ozone service
Available version number(s)	q02.05
Differences between available versions (summary)	N/A
Product display	Maps and time-series interpolated at 1, 50, 100 hPa pressure levels Maps and time-series of total columns Movies (max twice per year to illustrate current ozone hole event)
Main current user(s)	MACC
Digital format	HDF-4, PNG
Parameters	
Parameter / physical quantity	volume mixing ratio
Unit	dimensionless (mole/mole)
Generation method	Observations assimilated into a model
Platform / instrument / observational network / technique / model	BASCOE Chemical Data Assimilation System
Immediacy	NRT (4 days delayed)
Temporal coverage	2009/07/01 - now
Time resolution	3h
Geographic coverage	global
Horizontal resolution	3.75° x 2.5° (lon x lat)
Vertical extent	0.1 hPa to the surface (data should not be used in the troposphere)
Vertical resolution	37 levels, most of them lying in the stratosphere.
Other independent variables	Surface pressure (Pa) global, 3.75° x 2.5° (lon x lat) by average of ECMWF operational analyses
Typical range of values	0 - 12.0e-6
Quality indicator(s)	N/A

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Standard(s) of reference	N/A
Publication(s)	Lefever et al., 2011b [10].
Additional information	/

Service specifications

Delivery service name	MACC stratospheric ozone service
Service description / purpose	Monitoring of stratospheric ozone and the chemical substances that destroy it in real time with networks of ground-based instruments, satellites and forecasting models. Follow-up of the evolution of the ozone hole day after day, year after year, both over the Arctic and over the Antarctic. Distribution of NRT and historic data by analyses of ozone and ozone-related constituents by 4 different systems.
Service provider(s)	ECMWF, BIRA-IASB, DLR, KNMI
Service URL	http://www.gmes-stratosphere.eu
Contact details	macc@aeronomie.be
Operational stage	Partly operational The largest part of the service is operational, except for <ul style="list-style-type: none"> - the monitoring and evaluation of the non-ozone species from IFS-MOZART - the NRT evaluation against satellite and groundbased observations
Date of entry into operation	M15 (August 2010)
Upstream external information providers	<ul style="list-style-type: none"> • ECMWF operational analyses of winds, temperature, surface pressure • NASA/JPL retrievals of Aura/MLS observations (scientific product delayed by 2 days)
Delivery mode	consultation; 'pull' of the datasets described in the table above.
Delivery medium / channel	web download; ftp for the datasets described in the table above.
Update regularity / frequency	Daily: all datasets/plots are delivered/updated once per day, at different times of the day depending on the dataset.
Update delay	no delay
Delivery delay	no delay
Historical record	YES
Historical record availability	YES
Historical record time coverage	BASCOE/UARS-MLS: 1992-1999 BASCOE/MIPAS: 2002-2004 BASCOE/AURA-MLS: 2004-2010 SACADA/GOME: 1996-2003 IFS-MOZART : 2003-2010
Backup frequency	Daily
Documentation provided	<ul style="list-style-type: none"> • The web site describes the setup of the models used • For both the NRT and historical datasets of BASCOE and SACADA, documentation on metadata is available online. • There is a user guide available on the service website
Metadata standard	Datasets by IFS-MOZART, SACADA and TM3DAM are not distributed by this service Datasets by BASCOE are in HDF-4 with all necessary metadata provided as global attributes (see documentation) using locally defined metadata conventions (GDFB version 1).

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Support facilities provided	Online data visualisation, monthly averaged data for IFS-MOZART reanalysis, automatically updated comparison between different models (relative differences).
Conditions on use	N/A
Conditions of access	N/A
Standard(s) of reference	N/A
Publication(s)	Lefever et al, 2011b [10].
Additional information	/


2.1.2 Product generation and validation

Validation of intermediate and final products

Product name	BASCOE NRT analysis of stratospheric ozone
Brief product description	Analyses of stratospheric ozone by the BASCOE data assimilation system using Aura/MLS-SCI level 2 (v2.2) satellite observations
Validation method	Vertically resolved mean bias and standard deviations of differences w.r.t. independent observations for 5 latitude bands (90°S-60°S, 60°S-30°S, 30°S-30°N, 30°N-60°N, 60°N-90°N)
Validation data	ACE/FTS (see table below).
Quality indicator	N/A
Information content analysis	N/A
Assessment of product against user requirements	No
Standard(s) of reference	N/A
Publication(s)	Viscardy et al., in press [12]. Lefever et al., 2011a [9].

Validation data

Dataset name	ACE/FTS
Dataset provider / source	
Parameter / physical quantity	
Unit	
Generation method	
Platform / instrument / network / model name	
Immediacy	
Temporal coverage	
Time resolution	
Vertical extent	
Vertical resolution	
Geographic coverage	
Horizontal resolution	
Other independent variables	


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Typical range of values over the domain of definition	
Accuracy / precision	
Format	
Publication(s)	
Additional information	

2.1.3 Quality control

Quality control

Product name	BASCOE NRT analyses of stratospheric ozone and related species (i.e. this table applies to the 2 NRT products defined in Sections 2.1 and 2.2)
Version numbering	Versions are numbered following qXX.YY.ZZ where XX denotes major version changes, YY minor version changes and ZZ build numbers (i.e. which have no impact on the output). Build numbers are not written in the output filenames to ensure consistency of output names for each version.
Version documentation	Internal documentation on the wiki of the intranet, through a text file in the Subversion repository, and through log entries of the Subversion database.
Frequency of quality checks	Daily
Confidence interval monitoring	The maxima of the typical value range (see T1) are not implemented yet. Negative values are clipped automatically and result in warnings in the log files.
Provision of QI(s)	Naming and content of daily generated log files
Graphic representation of QI(s)	No
Criteria for flagging or discarding new data	N/A
Data corruption	N/A
Product degradation	N/A
False alerts / failure rate	N/A
Monitoring of delivery regularity	<ul style="list-style-type: none"> • Emails with processing status are sent daily to macc@aeronomie.be • Logfiles are listed on the web (with automatic and daily updates). Their names depend on basic processing events (no satellite data available; assimilation failed and forward modelling was used instead). Hence a quicklook on current and past processing outcome is available anytime and everywhere: see http://macc.aeronomie.be/logs/bascoe_AMLS_NRT_loglist.txt
User feedback mechanism	email to macc@aeronomie.be
Additional information	


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2.2 BASCOE NRT Analysis of Ozone-Related Species

2.2.1 Product and service description

Product specifications

Product name	BASCOE NRT analysis of ozone-related species
Product brief description	Analyses of chemical species related to stratospheric ozone (H ₂ O, HNO ₃ , HCl, N ₂ O, HOCl, NO _x) by the BASCOE data assimilation system using Aura/MLS-SCI level 2 (v2.2) satellite observations.
Product developer(s)	BIRA-IASB, Ringlaan 3, B-1180 Brussel, Contact by e-mail: macc@aeronomie.be
Targeted applications	- Monitoring of processes related to polar stratospheric ozone depletion e.g. transport, PSC formation, chlorine activation, denitrification, dehydration, etc. - Quasi-operational evaluation of the MACC integrated stratospheric ozone service
Available version number(s)	q02.05
Differences between available versions (summary)	N/A
Product display	Maps and time-series interpolated at 1, 50, 100 hPa pressure levels
Main current user(s)	MACC
Digital format	HDF-4, PNG
Parameters	
Parameter / physical quantity	volume mixing ratio
Unit	dimensionless (mole/mole)
Generation method	Observations assimilated into a model
Platform / instrument / observational network / technique / model	BASCOE Chemical Data Assimilation System
Immediacy	NRT (4 days delayed)
Temporal coverage	2009/07/01 - now
Time resolution	3h
Geographic coverage	global
Horizontal resolution	3.75° x 2.5° (lon x lat)
Vertical extent	0.1 hPa to the surface (data should not be used in the troposphere)
Vertical resolution	37 levels, most of them lying in the stratosphere.
Other independent variables	Surface pressure (Pa) global, 3.75° x 2.5° (lon x lat) by average of ECMWF operational analyses
Typical range of values	depends on species H ₂ O: 0 – 0.05 HNO ₃ : 0 – 15e-9 HCl: 0 - 6e-9 N ₂ O: 0 – 0.5e-6 NO ₂ : 0 – 0.25e-9 NO: 0 – 0.2e-9 HOCl: 0 – 20e-9 (Note: this species is not validated – see Section 2.2.2)

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Quality indicator(s)	N/A
Standard(s) of reference	N/A
Publication(s)	Lefever et al., 2011b [10].
Additional information	/

Service specifications

See Section 2.1.1.

2.2.2 Product generation and validation

Validation of intermediate and final products

Product name	BASCOE NRT analysis of ozone-related species
Brief product description	Analyses of chemical species related to stratospheric ozone (H ₂ O, HNO ₃ , HCl, N ₂ O, HOCl, NO _x) by the BASCOE data assimilation system using Aura/MLS-SCI level 2 (v2.2) satellite observations.
Validation method	N/A
Validation data	N/A
Quality indicator	N/A
Information content analysis	N/A
Assessment of product against user requirements	No
Standard(s) of reference	N/A
Publication(s)	Lahoz et al., 2011 [8]. Lefever et al., 2011a [9].

2.2.3 Quality control


See Section 2.1.3.

2.3 SYNAER Aerosol

2.3.1 Product and service description

Product specifications


Product name	SYNAER
Product brief description	aerosol optical depth and aerosol type
Product developer(s)	DLR, thomas.holzer-popp@dlr.de
Targeted applications	climate record, air quality assimilation
Available version number(s)	latest: v2.2
Differences between available versions (summary)	earlier version have larger uncertainty and should be discarded
Product display	gif daily and monthly maps

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Main current user(s)	NILU / EMEP (SLA); internal: R-EDA (assimilation)
Digital format	HDF4
Parameters	
Parameter / physical quantity	AOD at 550 nm; aerosol type number; derived parameters such as multi-spectral AOD, Angstrom coefficient, fine/coarse mode AOD, components AOD (sulfate, dust, soot, sea salt); single scattering albedo
Unit	dimensionless
Generation method	satellite retrieval from 2 sensors
Platform / instrument / observational network / technique / model	ENVISAT: radiometer AATSR + spectrometer SCIAMACHY (MetOP: radioemter AVHRR + spectrometer GOME-2)
Immediacy	NRT 24 hrs. / record
Temporal coverage	2003 - 2011
Time resolution	repeat cycle at equator 12 days
Geographic coverage	global (2008), MSG FOV (Europe, Africa, Atlantic, parts of South America and Asia)
Horizontal resolution	pixel 60x30 km ²
Vertical extent	total column
Vertical resolution	n.a.
Other independent variables	n.a.
Typical range of values	diagnostics: fit error, surface albedo, cloud fraction, absorbing geometry
Quality indicator(s)	AOD 0.5; mix number 1-40
Standard(s) of reference	bias - 0.06; rmse 0.12; envelope: for 67% of all good pixels AOD550 falls within $\pm 20\% \pm 0.1$
Publication(s)	
Additional information	

Service specifications

Delivery service name	SYNAER
Service description / purpose	aerosol satellite observations including composition
Service provider(s)	DLR
Service URL	http://www.gmes-atmosphere.eu/services/gac/aerosol_record/ ; http://wdc.dlr.de/php/indexer_r.php?dir_index=16&url=/data_products/AER_OSOLS/synaer_orbit_hdf_archive.php
Contact details	thomas.holzer-popp@dlr.de
Operational stage	operational
Date of entry into operation	NRT 6/2009, record 10/2011
Upstream external information providers	ESA / ENVISAT; EUMETSAT / MetOP
Delivery mode	push
Delivery medium / channel	ftp, web site
Update regularity / frequency	daily
Update delay	< 24 hrs.
Delivery delay	n.a.

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Historical record	archive
Historical record availability	available through web
Historical record time coverage	2003-2011
Backup frequency	monthly
Documentation provided	web site contains format and algorithm descriptions
Metadata standard	n.a.
Support facilities provided	online visualisation (gif pre-calculated)
Conditions on use	none
Conditions of access	none
Standard(s) of reference	n.a.
Publication(s)	Holzer-Popp, Schroedter and Gesell, 2002a [16] Holzer-Popp, Schroedter and Gesell, 2002b [17] Holzer-Popp et al., 2008 [18] Holzer-Popp et al., 2009 [19] Holzer-Popp, 2010 [20]
Additional information	-


2.3.2 Product generation and validation

Validation of intermediate and final products

Product name	SYNAER
Brief product description	AOD and aerosol type
Validation method	comparison to ground-based observations (± 60 min ± 50 km)
Validation data 1	AERONET
Validation data 2	future: MACC, AEROCOM, MODIS/MISR
Quality indicator 1	bias
Quality indicator 2	rmse
Quality indicator 3	envelope
Information content analysis	yes (see Holzer-Popp et al., 2008 [18]); error of reflectances and critical retrieval parameters taken into account
Assessment of product against user requirements	PROMOTE URD
Standard(s) of reference	n.a.
Publication(s)	Holzer-Popp, Schroedter and Gesell, 2002a [16] Holzer-Popp, Schroedter and Gesell, 2002b [17] Holzer-Popp et al., 2008 [18] Holzer-Popp et al., 2009 [19]
Additional information	-

Validation data

Dataset name	AERONET
Dataset provider / source	NASA
Parameter / physical quantity	multi-spectral AOD; other parameters (inversion method)


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Unit	dimensionless
Generation method	sun photometer
Platform / instrument / network / model name	CIMEL instruments
Immediacy	NRT + record
Temporal coverage	depending on stations since 1995
Time resolution	15 min
Vertical extent	total column
Vertical resolution	n.a.
Geographic coverage	n.a.
Horizontal resolution	global / ~ 200 permanent stations + campaigns
Other independent variables	stations
Typical range of values over the domain of definition	water vapour column
Accuracy / precision	AOD 0-5
Format	AOD rmse 0.01
Publication(s)	
Additional information	

2.3.3 Quality control

Quality control

Product name	SYNAER
Version numbering	after algorithm change + validation new version number is issued
Version documentation	version numbers are explained in a document on the website
Frequency of quality checks	daily depending on staff presence
Confidence interval monitoring	no
Provision of QI(s)	validation information is available on the website
Graphic representation of QI(s)	such information is contained in validation report
Criteria for flagging or discarding new data	exclusion criteria documented in report and website recommended to flag bad pixels
Data corruption	n.a.
Product degradation	n.a.
False alerts / failure rate	n.a.
Monitoring of delivery regularity	website
User feedback mechanism	e-mail
Additional information	

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2.4 Global Fire Assimilation System (GFAS)

2.4.1 Product and service description

Product specifications

Product name	Global Fire Assimilation System (GFAS)
Product brief description	global emission fluxes for 40+ species from open biomass burning based on satellite-based FRP observations
Product developer(s)	ECMWF, FZJ, KCL, VUA
Targeted applications	input for global aerosol, reactive gas and greenhouse gas models and regional air quality models of MACC
Available version number(s)	0, 1.0, 1.1
Differences between available versions (summary)	spatial resolution, FRP observation use, data assimilation, conversion factors, quality control, emission factors (see Kaiser et al., 2011 [16]). v1.1 is a higher-resolution version (0.1deg) of v1.1.
Product display	map
Main current user(s)	MACC
Digital format	gif,kml, grib, netcdf
Parameters	
Parameter / physical quantity	fire radiative power (FRP) areal density, combustion rate areal density, species emission areal density daily averages
Unit	W/m ² , kg/s/m ² , kg/s/m ²
Generation method	observational data assimilation
Platform / instrument / observational network / technique / model	MODIS aboard Terra and Aqua (LEO), SEVIRI aboard Meteosat-9 (GEO)
Immediacy	NRT
Temporal coverage	since 2003
Time resolution	1 day
Geographic coverage	global
Horizontal resolution	v0: T159, v1.0: 0.5deg, v1.1: 0.1deg
Vertical extent	N/A
Vertical resolution	N/A
Other independent variables	N/A
Typical range of values	> 0
Quality indicator(s)	effective fraction of observed area
Standard(s) of reference	N / A
Publication(s)	
Additional information	

Service specifications

Delivery service name	
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Service description / purpose	
Service provider(s)	ECMWF, FZJ
Service URL	gmes-atmosphere.eu/fire, http://macc.icg.kfa-juelich.de:50080/access?catalog=http://macc.icg.kfa-juelich.de:58080/MACC_wildfire
Contact details	j.kaiser@ecmwf.int
Operational stage	routine production
Date of entry into operation	1-Jun-09
Upstream external information providers	NASA, EUMETSAT LSA SAF
Delivery mode	"pull"
Delivery medium / channel	MARS retrieval, OGC-compliant WCS scripting, web download
Update regularity / frequency	daily
Update delay	10 minutes
Delivery delay	N / A
Historical record	yes
Historical record availability	yes
Historical record time coverage	since 2003
Backup frequency	N / A
Documentation provided	with product, online, scientific literature
Metadata standard	GRIB
Support facilities provided	online data visualisation, extraction example scripts, email list
Conditions on use	
Conditions of access	
Standard(s) of reference	N / A
Publication(s)	Kaiser et al., 2011 [16].
Additional information	

2.4.2 Product generation and validation

Validation of intermediate and final products

Product name	
Brief product description	
Validation method	see Kaiser et al., 2011 [16].
Validation data 1	
Quality indicator 1	
Information content analysis	
Assessment of product against user requirements	
Standard(s) of reference	
Publication(s)	

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2.4.3 Quality control

Quality control

Product name	Global Fire Assimilation System (GFAS)
Version numbering	yes
Version documentation	yes
Frequency of quality checks	daily
Confidence interval monitoring	yes
Provision of QI(s)	yes
Graphic representation of QI(s)	no
Criteria for flagging or discarding new data	confidence interval
Data corruption	The data assimilation automatically uses information from earlier observations as fall-back.
Product degradation	The processing is performed consistently in one resolution.
False alerts / failure rate	N / A
Monitoring of delivery regularity	yes
User feedback mechanism	email
Additional information	

2.5 RAD-UV - Monitoring and Forecasting UV Radiation


2.5.1 Product and service description

As part of the GEMS/MACC analysis and forecast project, UV-radiation has been computed in the IFS model with a dedicated UV-processor (Morcrette and Arola, 2007 [21]). Surface irradiance in 5 cm⁻¹ wide spectral intervals is computed on-line within the forecast model, and the UV-index is computed from the distribution of the spectral irradiance using a standard skin response function.

The UV-Index is available from the ECMWF MARS archive.

Product specifications


Product name	RAD-UV
Product brief description	UV-related surface parameters
Product developer(s)	ECMWF
Targeted applications	
Available version number(s)	Reference to ECMWF operational model cycle
Differences between available versions (summary)	
Product display	www.gmes-atmosphere.eu follow the links
Main current user(s)	
Digital format	MARS by default, NetCDF on request

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Parameters	
Parameter / physical quantity	UV-Index, spectral distribution of clear- and total-sky surface UV irradiance between 280 and 400 nm (by step of 5 nm)
Unit	UV-Index dimensionless, irradiance in W/m ²
Generation method	Computed as part of the MACC/ECMWF observational data assimilation and subsequent forecast
Platform / instrument / observational network / technique / model	ECMWF assimilation system
Immediacy	NRT and forecast.
Temporal coverage	
Time resolution	3-hourly
Geographic coverage	global
Horizontal resolution	~80x80 km ²
Vertical extent	N/A
Vertical resolution	N/A
Other independent variables	
Typical range of values	
Quality indicator(s)	
Standard(s) of reference	
Publication(s)	Morcrette and Arola, 2007 [21].
Additional information	

Service specifications

Delivery service name	RAD-UV
Service description / purpose	
Service provider(s)	ECMWF
Service URL	
Contact details	
Operational stage	partly operational (as the rest of the MACC products)
Date of entry into operation	
Upstream external information providers	
Delivery mode	On request
Delivery medium / channel	MARS extraction
Update regularity / frequency	daily
Update delay	Depending on requests
Delivery delay	Depending on requests
Historical record	yes
Historical record availability	yes
Historical record time coverage	
Backup frequency	

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Documentation provided	MARS extraction document
Metadata standard	MARS
Support facilities provided	Scientist contact
Conditions on use	
Conditions of access	On request
Standard(s) of reference	
Publication(s)	Morcrette and Arola, 2007 [21].
Additional information	

2.5.2 Product generation and validation


Each step of the development and improvement of the system has been accompanied by comparison against both ground-based and satellite-based UV data, as extensively as possible. During GEMS AER sub-project, prognostic aerosol model was developed for IFS, which has since been coupled with the UV processor. A re-analysis run, including the UV processor with prognostic aerosols, was launched earlier in the MACC project. FMI has carried out a validation work in RAD sub-project, comparing UV processor against ground-based UV data. The special focus has been on the aerosol effect on UV through the prognostic aerosols. Therefore satellite-UV, that does not account properly for absorbing aerosols, has not been included in these comparisons. In addition to UV comparisons, aerosol loading (AOD) and other optical properties (e.g. single scattering albedo) from the processor have been compared against measurements from the Aerosol Robotic Network (AERONET).

Validation of intermediate and final products

Product name	RAD-UV
Brief product description	UV-related surface parameters
Validation method	Comparison with ground measurements
Validation data	
Quality indicator	
Information content analysis	
Assessment of product against user requirements	
Standard(s) of reference	
Publication(s)	Morcrette and Arola, 2007 [21].

Validation data

Dataset name	
Dataset provider / source	
Parameter / physical quantity	
Unit	
Generation method	
Platform / instrument / network / model name	


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Immediacy	NRT / forecast.
Temporal coverage	
Time resolution	
Vertical extent	
Vertical resolution	N/A
Geographic coverage	global
Horizontal resolution	~80x80 km ²
Other independent variables	
Typical range of values over the domain of definition	
Accuracy / precision	
Format	MARS, NetCDF on request
Publication(s)	Morcrette and Arola, 2007 [21].
Additional information	

2.5.3 Quality control

Quality control

Product name	
Version numbering	Follows numbering of ECMWF operational cycles
Version documentation	
Frequency of quality checks	
Confidence interval monitoring	
Provision of QI(s)	
Graphic representation of QI(s)	
Criteria for flagging or discarding new data	
Data corruption	
Product degradation	
False alerts / failure rate	
Monitoring of delivery regularity	
User feedback mechanism	
Additional information	

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3 NEAR-REAL TIME (NRT) AND FORECAST MODES – REGIONAL PRODUCTS

3.1 European-Scale AQ Analysis by EURAD-IM

3.1.1 Product and service description


The comprehensive chemical data assimilation scheme EURAD-IM, developed at the Rhenish Institute of Environmental Research at the University of Cologne provides daily 72h AQ forecasts and AQ analyses for the previous day on a domain covering whole Europe with 15 km horizontal resolution using a Lambert conformal projection. Predicted hourly concentrations of O₃, NO, NO₂, CO, SO₂, total NMVOC, PM_{2.5}, PM₁₀, and concentrations of the particulate matter constituents SO₄²⁻, NO₃⁻, NH₄⁺, secondary organics, sea salt, mineral dust and primary anthropogenic material as well as analysed hourly concentrations of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ are regularly delivered in NetCDF format. Physical dimension of gas phase and aerosol phase species is ppb and µg/m³, respectively. The air pollutant concentrations are available on 23 non-equidistant terrain following layers between the surface and 100 hPa. Thickness of the near surface layer is about 35 m, 16 layers are below 3000 m.

Hourly concentrations of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ are also available in grib2 format on a latitude/longitude grid covering the region from 15° W to 35° E and 35° N to 70° N with a resolution of 0.15° x 0.125° in the near surface layer and at 500 m, 1000 m, 3000 m, and 5000 m. Physical dimension of air pollutants in grib2 format is kg/m³.

The EURAD-IM AQ forecast and analysis is used for the generation of ensemble products and for public information purposes.

Service specifications


Delivery service name	European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by EURAD-IM
Service description / purpose	European-scale regional air quality forecast, production of ensemble forecast, public information
Service provider(s)	Rheinisches Institut für Umweltforschung an der Universität zu Köln
Service URL	https://www.gmes-atmosphere.eu/services/raq/raq_nrt/
Contact details	e-mail: he@eurad.uni-koeln.de , telephon #: +49 221 4002220
Operational stage	Pre-operational
Date of entry into operation	Feb 2009
Upstream external information providers	ECMWF (IFS operational forecast), TNO (emission data), MACC sub-project G-RG (NRT forecast of global reactive gases)
Delivery mode	Push
Delivery medium / channel	FTP
Update regularity / frequency	Daily

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Update delay	1 h
Delivery delay	1 h to several days, dependent on type of request
Historical record	Available
Historical record availability	On request
Historical record time coverage	Since Feb 2009
Backup frequency	Daily
Documentation provided	For Background information see EURAD-IM, Products, Quality and Background Information, http://www.gmes-atmosphere.eu/documents/deliverables/r-ens/D_R-ENS_1.3.4_EURAD_Dossier4.pdf
Metadata standard	NetCDF Climate and Forecast (CF) Metadata Conventions, Version 1.4
Support facilities provided	Not yet available
Conditions on use	SLA
Conditions of access	SLA
Standard(s) of reference	/
Publication(s)	Huijnen et al., 2010 [26].
Additional information	

Product 1 specifications


Product name	European-scale AQ forecast for every hour of the next time period up to 72h ahead by EURAD-IM
Product brief description	AQ forecast of key air pollutants on a domain covering whole Europe with a horizontal resolution of 15 km.
Product developer(s)	Rheinisches Institut für Umweltforschung an der Universität zu Köln, e-mail: he@eurad.uni-koeln.de , telephon #: +49 221 4002220
Targeted applications	Operational European-scale regional AQ service, production of ensemble products, public information
Available version number(s)	1.0
Differences between available versions (summary)	/
Product display	Website https://www.gmes-atmosphere.eu/services/raq/raq_nrt/
Main current user(s)	LANUV, BSC
Digital format	NetCDF, grib2
Parameters	
Parameter / physical quantity	Gas-phase: O ₃ , NO, NO ₂ , CO, SO ₂ , NMVOC Aerosol-phase: PM _{2.5} , PM ₁₀ , SO ₄ ²⁻ , NH ₄ ⁺ , NO ₃ ⁻ , secondary organic aerosol, anthropogenic primary particulate matter, sea salt, mineral dust
Unit	µg/m ³
Generation method	Simulated
Platform / instrument / observational network / technique / model	EURAD-IM (see EURAD-IM, Products, Quality and Background Information, http://www.gmes-atmosphere.eu/documents/deliverables/r-ens/D_R-ENS_1.3.4_EURAD_Dossier4.pdf)
Immediacy	Forecast.
Temporal coverage	72 h
Time resolution	Hourly

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Geographic coverage	Europe
Horizontal resolution	15 km
Vertical extent	Surface to 100 hPa
Vertical resolution	Non-equidistant, 36 m for the near-surface layer, about 16 layers below 3000 m
Other independent variables	/
Typical range of values	Dependent on season, weather conditions, geographical region
Quality indicator(s)	Bias, modified mean bias, root mean square error, fractional gross error, correlation (see Table in Section 3.1.2)
Standard(s) of reference	/
Publication(s)	Huijnen et al., 2010 [26].
Additional information	

Product 2 specifications

Product name	European-scale AQ analysis for every hour of the previous day by EURAD-IM
Product brief description	AQ analysis of key air pollutants on a domain covering whole Europe with a horizontal resolution of 15 km.
Product developer(s)	Rheinisches Institut für Umweltforschung an der Universität zu Köln, e-mail: he@eurad.uni-koeln.de , telephon #: +49 221 4002220
Targeted applications	Operational European-scale regional AQ service, production of ensemble products, public information
Available version number(s)	1.0
Differences between available versions (summary)	/
Product display	Website https://www.gmes-atmosphere.eu/services/raq/raq_nrt/
Main current user(s)	LANUV, BSC
Digital format	NetCDF, grib2
Observations used for assimilation	MACC-RAQ NRT surface in situ observations of O ₃ , NO, NO ₂ , CO, SO ₂ , PM _{2.5} , PM ₁₀ NO ₂ column retrievals from OMI, SCIAMACHY, and GOME-2
Parameters	
Parameter / physical quantity	Gas-phase: O ₃ , NO, NO ₂ , CO, SO ₂ Aerosol-phase: PM _{2.5} , PM ₁₀
Unit	µg/m ³
Generation method	3d-var analysis
Platform / instrument / observational network / technique / model	EURAD-IM (see EURAD-IM, Products, Quality and Background Information, http://www.gmes-atmosphere.eu/documents/deliverables/r-ens/D_R-ENS_1.3.4_EURAD_Dossier4.pdf)
Immediacy	NRT
Temporal coverage	24 h
Time resolution	Hourly
Geographic coverage	Europe
Horizontal resolution	15 km
Vertical extent	Surface to 100 hPa
Vertical resolution	Non-equidistant, 36 m for the near-surface layer, about 16 layers below

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	3000 m
Other independent variables	/
Typical range of values	Dependent on season, weather conditions, geographical region
Quality indicator(s)	Bias, root mean square error, correlation (see Section 3.1.2)
Standard(s) of reference	/
Publication(s)	Simplified version of Strunk et al., 2011 [32] Elbern et al., 2007 [23] Strunk et al., 2010 [31]
Additional information	

3.1.2 Product generation and validation

The European-scale pre-operational air quality forecast has been set up using the continental-to-local scale chemical data assimilation system EURAD-IM (Hass, 1991 [25]; Ackermann et al., 1998 [22]; Memmesheimer et al., 2004 [29]; Friese and Ebel, 2010 [24]). This model system consists of 5 major parts: the meteorological driver MM5, the pre-processors ECP and PREP for preparation of meteorological fields and observation data, the emission model EEM and the chemistry transport model EURAD-IM. The data flow of the EURAD-IM system is depicted in Figure 1. EURAD-IM is a meso-scale chemistry transport model involving transport, diffusion, chemical transformation, wet and dry deposition and sedimentation of tropospheric trace gases and aerosols. It includes 3d-var and 4d-var chemical data assimilation (Elbern et al., 2007 [23]) and is able to run in nesting mode.

Based upon the IFS operational meteorological forecast from 12:00 UTC of the previous day, a 72h forecast of key air pollutants is regularly delivered. Predicted concentrations of O₃, NO, NO₂, SO₂, PM_{2.5}, and PM₁₀ contribute to a multi-model ensemble forecast. Chemical initial values are provided by the EURAD-IM pre-operational 3d-var analysis for the previous day. Chemical boundary values are taken from the pre-operational global MOZART-IFS air quality forecast (MACC sub-project G-RG). Concentration fields are currently available at about 04:00 UTC at ECMWF for further processing. Results are accessible on the MACC web page.

Based upon the IFS operational meteorological forecast from 00:00 UTC, an analysis of the concentrations of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ is daily delivered. Chemical initial values are provided by the EURAD-IM 3d-var analysis of the previous day. Chemical boundary values are taken from the pre-operational global MOZART-IFS air quality forecast. NRT MACC-RAQ surface in-situ measurements of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ as well as NO₂ columns retrievals from OMI, GOME-2, and SCIAMACHY are assimilated every full hour using intermittent 3d-var. Concentration fields are currently available at about 02:00 UTC at ECMWF for further processing. Results are accessible on the MACC web page.

For the forecast as well as analysis, emission input data are derived from the newly available 2005 TNO emission inventory.

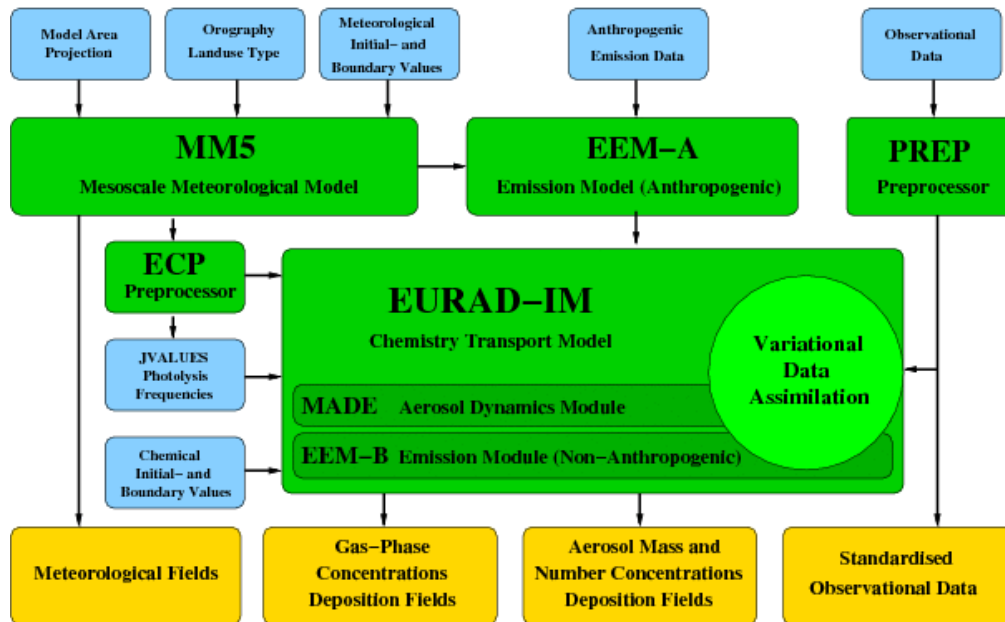


Figure 1: Flowchart of the EURAD-IM model system containing the meteorological driver MM5, the pre-processors ECP and PREP, the emission model EEM and the chemistry transport model EURAD-IM (input parameters are shaded in blue, output parameters are shaded in yellow and procedural parts are shaded in green).

Results of the EURAD-IM AQ forecast are validated on a daily basis on the MACC-RAQ webpage and are compared to results of the ensemble forecast system in quarterly QC/QA dossiers. The MACC-RAQ NRT data is used for verification. This data consists of surface in situ measurements of O₃, NO₂, SO₂, CO, PM_{2.5}, and PM₁₀ from an increasing number of European countries. Quality indicators used for validation are bias, modified mean bias, root mean square error, fractional gross error, and correlation (Jolliffe and Stephenson, 2003 [27]). Averaged quality indicators are displayed on the MACC-RAQ webpage for the next 72h forecast period and as time-series at 03:00 UTC and 15:00 UTC for the last week and for the last three month. Figure 2 exhibits exemplary quality indicators taken from the EURAD-IM QC/QA dossier for September to November 2010.

The EURAD-IM AQ service is validated against the MACC User Requirements Document.

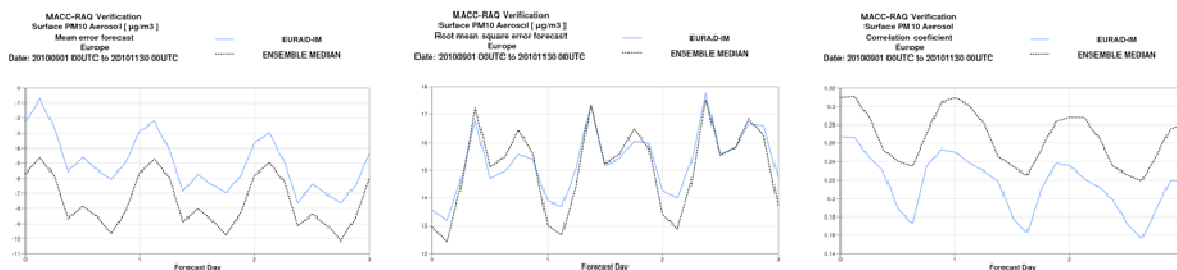



Figure 2: Bias (left), root mean square error (middle), and correlation (right) of near surface PM₁₀ concentrations averaged over the time span from September 1 to November 31, 2010. Blue: EURAD-IM forecast, black: MACC-RAQ ensemble forecast.


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Validation of intermediate and final products

Product name	European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by EURAD-IM
Brief product description	AQ forecast/analysis of key air pollutants on a domain covering whole Europe with a horizontal resolution of 15 km.
Validation method	Calculation of skill scores for surface in situ measurements of O ₃ , NO ₂ , SO ₂ , CO, PM ₁₀ , and PM _{2.5}
Validation data 1	MACC-RAQ NRT data
Quality indicator 1	Mean bias [27]
Quality indicator 2	Modified mean bias [27]
Quality indicator 3	Root mean square error [27]
Quality indicator 4	Fractional gross error [27]
Quality indicator 5	Correlation [27]
Information content analysis	Not operationally
Assessment of product against user requirements	Assessment against the MACC User Requirements Document [2]
Standard(s) of reference	/
Publication(s)	Semestral QC/QA dossiers for EURAD-IM. http://www.gmes-atmosphere.eu/documents/deliverables/r-ens/dossiers/

Validation data

Dataset name	MACC-RAQ NRT data
Dataset provider / source	Environmental agencies of several European countries, collected at Meteo France
Parameter / physical quantity	O ₃ , NO, NO ₂ , CO, SO ₂ , PM _{2.5} , PM ₁₀
Unit	kg/m ³
Generation method	Observed
Platform / instrument / network / model name	Surface in situ measurement sites
Immediacy	NRT
Temporal coverage	24 h
Time resolution	10 min to 1 h depending on originating country
Vertical extent	Surface
Vertical resolution	/
Geographic coverage	Europe
Horizontal resolution	/
Other independent variables	/
Typical range of values over the domain of definition	Dependent on season, weather conditions, geographical region
Accuracy / precision	?
Format	BUFR
Publication(s)	
Additional information	

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3.1.3 Quality control

The supervisor monitor scheduler developed at ECMWF is used to control the production of the daily EURAD-IM AQ forecast and AQ analysis. SMS enables users to run a large number of programs in a controlled environment. It provides reasonable tolerance for hardware and software failures, combined with good restart capabilities.

SVN, a revision control system, is used to document changes of the EURAD-IM source code. Changes of the AQ service are reported in the quarterly EURAD-IM QC/QA dossiers. Furthermore, the dossiers provide performance and availability statistics. The performance statistic consists of graphical representations of mean quality indicators (bias, root mean square error, and correlation) for predicted near surface O₃, NO₂, and PM₁₀ concentrations.

Quality control


Product name	European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by EURAD-IM
Version numbering	SVN
Version documentation	Model development is reported in semestral QC/QA dossiers http://www.gmes-atmosphere.eu/documents/deliverables/r-ens/dossiers/
Frequency of quality checks	Daily
Confidence interval monitoring	MOS system available but not yet operational
Provision of QI(s)	Not used
Graphic representation of QI(s)	https://www.gmes-atmosphere.eu/services/raq/raq_nrt/
Criteria for flagging or discarding new data	/
Data corruption	E-mail alarming and reporting, file transfer errors are reported.
Product degradation	Use of sophisticated algorithms, use of data on the model grid whenever possible
False alerts / failure rate	QC/QA dossiers http://www.gmes-atmosphere.eu/documents/deliverables/r-ens/dossiers/
Monitoring of delivery regularity	QC/QA dossiers http://www.gmes-atmosphere.eu/documents/deliverables/r-ens/dossiers/
User feedback mechanism	
Additional information	

3.2 Origin of forecasted pollution episodes (graphic presentation)

3.2.1 Product and service description

Following the source-receptor (SR) methodology described in Wind et al. (2004) [33], a system for the estimation of country allocated contributions to forecasted air pollution episodes (or air quality emergencies) has been implemented. The system is based on the MACC pre-operational 3-day forecast set-up of the Unified EMEP model.

In practice, when a severe air pollution episode is forecasted by the MACC system, calculations of source-receptor relationships can be performed on request. A user interface has been set up at

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http://www.emep.int/gmes/macc_opol.html. On the same page one also finds examples of source-allocation diagrams.


One example of country-allocated forecasts is shown in the next section, where the newly developed tools have been applied to an Air Pollution episode in the past. They were presented at the 1st policy user workshop under the lead of EIONET in Dessau in October 2010.

Product specifications

Product name	Origin of forecasted pollution episodes (graphic presentation)
Product brief description	Identification of main emission source areas that contribute to a given air pollution episode
Product developer(s)	Norwegian Meteorological Institute (met.no), Alvaro Valdebenito <alvaro.valdebenito@met.no>
Targeted applications	Science based air quality policy measures
Available version number(s)	ver1
Differences between available versions (summary)	n.a.
Product display	http://www.emep.int/gmes/macc_opol.html
Main current user(s)	
Digital format	png
Parameters	
Parameter / physical quantity	percentage contribution of a country or area to a given air pollution episode
Unit	%
Generation method	Derived from model simulations
Platform / instrument / observational network / technique / model	High performance computer / chemical and dispersion modeling / atmospheric chemistry model
Immediacy	Record, delayed or forecast
Temporal coverage	3 to 10 days
Time resolution	1 hour
Geographic coverage	Receptor area (affected by air pollution episode): user defined within Europe, source areas: either countries or seas
Horizontal resolution	0.2 degrees
Vertical extent	
Vertical resolution	20 layers from surface to 100 hPa, lowermost layer 20 m thick If relevant, approximate number of levels in boundary layer, free troposphere, UTLS, middle atmosphere.
Other independent variables	MACC emission data, ECMWF meteorology, EMEP/MSC-W software
Typical range of values	0...100%
Quality indicator(s)	Model skill scores (routine model evaluation within EMEP and MACC)
Standard(s) of reference	
Publication(s)	None yet.

Service specifications

Delivery service name	
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Service description / purpose	
Service provider(s)	Norwegian Meteorological Institute
Service URL	
Contact details	alvaro.valdebenito@met.no, michael.gauss@met.no
Operational stage	Under development / partly operational (explain) / fully operational.
Date of entry into operation	
Upstream external information providers	
Delivery mode	"pull"
Delivery medium / channel	web download
Update regularity / frequency	On demand
Update delay	n.a.
Delivery delay	1 day
Historical record	Yes
Historical record availability	Yes
Historical record time coverage	n.a.
Backup frequency	
Documentation provided	website
Metadata standard	ascii
Support facilities provided	png, website
Conditions on use	
Conditions of access	
Standard(s) of reference	
Publication(s)	None yet
Additional information	

3.2.2 Product generation and validation

The system for the estimation of country allocated contributions to forecasted air pollution episodes was developed within MACC. The current SR ensemble includes more than 200 forecasts performed by the EMEP/MS-CW model for each single day. In each run the emissions are reduced for one specific country and one emitted component at a time. Through a post-processing procedure the percentage contribution from each country to a given air quality episode can be calculated.

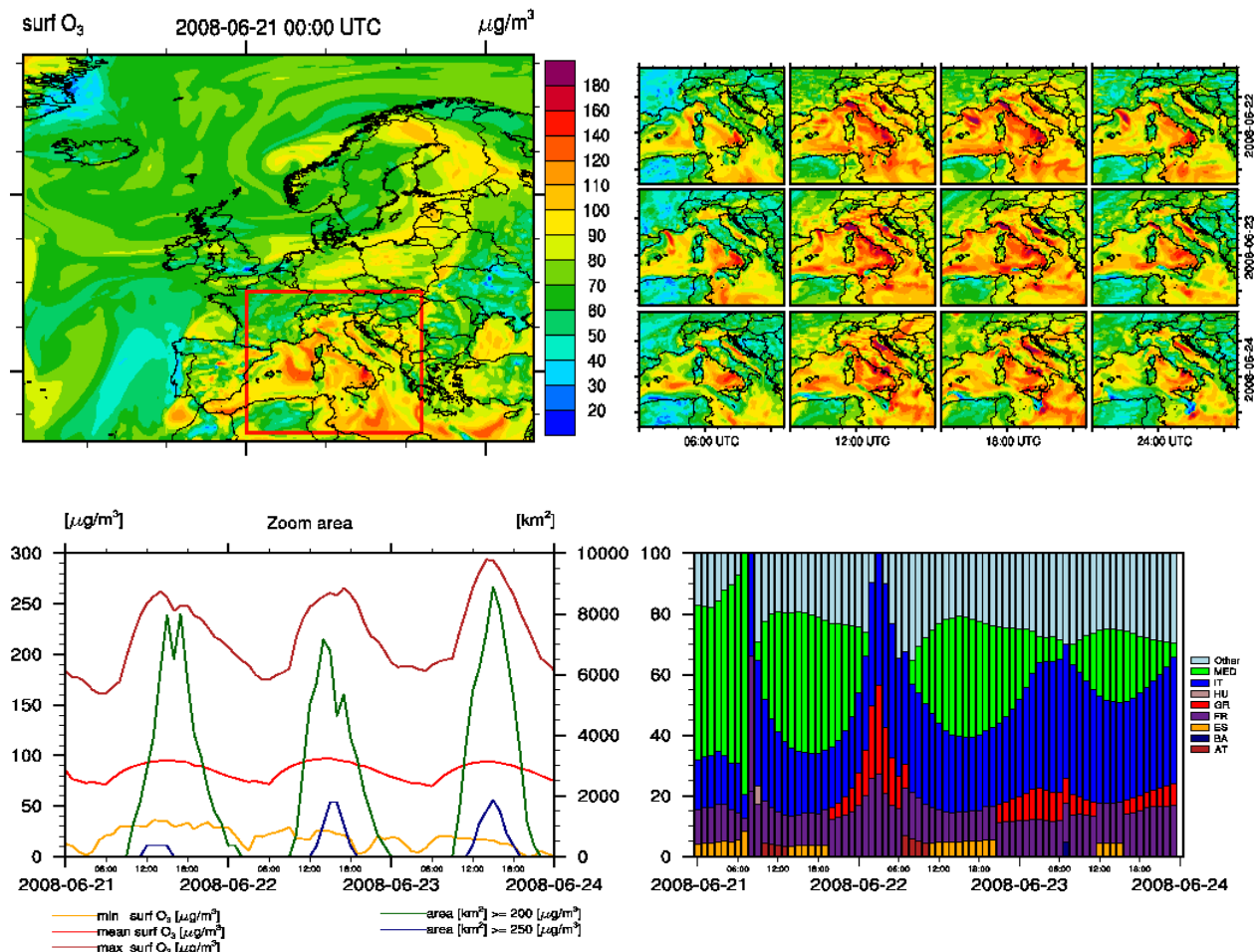
For a given episode, two sets of SR forecast ensembles can be defined:

- Quick response: SR ensemble initialized at the first day of the episode. This ensemble is dedicated to identifying the potential effect of reductions implemented as soon as the episode is forecasted.
- Attribution: SR ensemble initialized 20 days before the first day of the episode. This ensemble is dedicated to allocating the main precursor areas, over the weeks leading to the episode.

As an example, the figure below shows horizontal plots of the forecast of the high ozone episode in 2008, regenerated with the EMEP model in the upper two panels. The right panel shows the zoomed area

(receptor area) for the three days of the forecast and for different times of day. The lower left panel shows time evolutions of main pollutants in the receptor area. The contributors to the receptor area, and the time evolution of their relative contributions are shown in the lower right panel.

3-day Forecast O₃ Episode



Validation data

Dataset name	EMEP measurement data base, Airbase
Dataset provider / source	NILU
Parameter / physical quantity	Various chemical components
Unit	Dependent on component (ppv, ppmv, ug/m3).
Generation method	Observed / derived from observation
Platform / instrument / network / model name	


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Immediacy	Record / annual
Temporal coverage	
Time resolution	
Vertical extent	
Vertical resolution	
Geographic coverage	
Horizontal resolution	
Other independent variables	
Typical range of values over the domain of definition	
Accuracy / precision	
Format	
Publication(s)	
Additional information	

3.2.3 Quality control

The EMEP/MSC-W model is evaluated regularly against a large set of measurements. Evaluation reports can be found at <http://www.emep.int>

The model is also continuously evaluated within the MACC project. Quarterly model dossiers are available through MACC.

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4 DELAYED MODE – GLOBAL PRODUCTS

4.1 Global CO₂ Source and Sink Inversions


4.1.1 Product and service description

The space-time gradients of CO₂ mixing ratios in the atmosphere are determined by CO₂ exchange with the Earth's surface and by atmospheric transport. Thus the joint availability of atmospheric measurements of CO₂ mixing ratios and of numerical models of the atmospheric transport allows the inference of CO₂ surface fluxes over the globe. The present MACC product relies on the flux inversion scheme of Chevallier et al. (2005) [34] that implements Bayesian estimation in the form of the minimization of a cost function. The inversion system computes the Best Linear Unbiased Estimate (BLUE) of the CO₂ surface fluxes given the input information, their Bayesian uncertainty, and the number of degrees of freedom for signal (Chevallier et al. 2007 [35]). The BLUE fluxes are simply called inverted fluxes hereafter.

The inversion system has been operated for the period 2000-2010, with surface air-sample measurements as input observations. Fluxes are estimated on a global longitude-latitude grid of regular mesh 3.75x2.5o at a temporal resolution of 8 days, with day-time and night-time separated. 3-hourly variations within the 8-day segments are prescribed a priori in the inversion. Prior fluxes come from the combination of a flux climatology, of emission inventories and of a model simulation as described in Chevallier et al. (2010) [36]. The operator that links the flux space and the retrieval space in the inversion scheme is the general circulation model of the Laboratoire de Météorologie Dynamique (LMDZ, Hourdin et al. 2006 [37]), nudged to ECMWF winds. Tracer transport is simulated on the same 3.75x2.5o horizontal grid as the fluxes with 19 layers between the surface and the top of the atmosphere. The prior initial conditions (i.e. the 3D field of CO₂ at the start of the inversion window) are taken from the global analysis of surface air-sample measurements for the period 1988-2008 made by Chevallier et al. (2010) [36]. They are adjusted within the inversion. The present inversion configuration follows the one used by Chevallier et al. (2010) [36] with only minor adaptations to process years 2009 and 2010.

Product specifications


Product name	Global CO₂ source & sink inversions
Product brief description	Global distribution of CO ₂ surface fluxes at resolution weekly and 3.75 x 2.5 deg ²
Product developer(s)	LSCE, frederic.chevallier_at_lsce.ipsl.fr
Targeted applications	Studies of the global and regional carbon cycle
Available version number(s)	10.1
Differences between available versions (summary)	The first number of the version id corresponds to the last two digits of the last year of the inversion (currently 2010), the second number identifies the release (currently 1/1)
Product display	None yet, to be done
Main current user(s)	No SLA or MoU signed yet
Digital format	NetCDF
Parameters	

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Parameter / physical quantity	CO ₂ surface flux
Unit	kgC/m ² /hour, with fluxes counted positive towards the atmosphere
Generation method	Data assimilation
Platform / instrument / observational network / technique / model	Air -sample surface networks - Data from four databases: the NOAA Earth System Research Laboratory archive (Conway et al., 2011; Thoning et al., 2010; Andrews et al., 2009), the CarboEurope atmospheric archive, the World Data Centre for Greenhouse Gases (WDCGG) archive and the Réseau Atmosphérique de Mesure des Composés à Effet de Serre (RAMCES) database.
Immediacy	Delayed
Temporal coverage	2000-2010
Time resolution	3 hourly
Geographic coverage	Globe
Horizontal resolution	3.75 degrees in longitude and 2.5 deg in latitude
Vertical extent	/
Vertical resolution	/
Other independent variables	/
Typical range of values	-2.e-3 / 5.e-4
Quality indicator(s)	Bayesian uncertainty, available on request for any space-time target
Standard(s) of reference	Bayesian inversion
Publication(s)	
Additional information	

Service specifications

Delivery service name	Global CO₂ source & sink inversions
Service description / purpose	Global CO ₂ source & sink inversions
Service provider(s)	LSCE
Service URL	http://www-lscedods.cea.fr/invzat/PYVAR10_MACC/V1/
Contact details	frederic.chevallier_at_lsce.ipsl.fr
Operational stage	fully operational
Date of entry into operation	15 August 2011
Upstream external information providers	See the reference publication
Delivery mode	Pull
Delivery medium / channel	web download
Update regularity / frequency	annual
Update delay	12 months
Delivery delay	2 months
Historical record	Yes
Historical record availability	Yes
Historical record time coverage	2000-2010
Backup frequency	At each release

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Documentation provided	Self-documented files
Metadata standard	NetCDF
Support facilities provided	Help desk
Conditions on use	Free
Conditions of access	Free
Standard(s) of reference	Bayesian inversion
Publication(s)	Chevallier et al., 2010 [36].
Additional information	/

4.1.2 Product generation and validation

The evaluation of this product is based on 1) comparison with the fluxes from other inversions, and 2) comparison of CO₂ mixing ratios calculated from the inverted fluxes with independent aircraft measurements. In particular, the latter test confirms that the inversion has improved the quality (i.e. reduced the uncertainty) of the surface fluxes compared to the assumed or prior fluxes. The product quality is documented by the associated Bayesian uncertainty, that can be provided on demand for any space-time target, from the grid-point weekly scale to the annual global scale. The realism of this uncertainty estimate has been demonstrated with independent data.

Validation of intermediate and final products

Product name	Global CO₂ source & sink inversions
Brief product description	Global distribution of CO ₂ surface fluxes at resolution weekly and 3.75 x 2.5 deg ²
Validation method	Independent CO ₂ measurements
Validation data	HIPPO aircraft campaign (PI S. Wofsy); Wofsy et al. (Phil. Trans. R. Soc. A, 2011)
Quality indicator	TCCON retrievals of the CO ₂ total column (https://tcccon-wiki.caltech.edu/); Wunch et al. (Phil. Trans. R. Soc. A, 2011)
Information content analysis	CONTRAIL measurements (PI: Machida, Matsueta, Sawa) ; Machida et al. (J. Atmos. Oceanic. Technol., 2008)
Assessment of product against user requirements	Official QC of HIPPO data
Standard(s) of reference	Bayesian uncertainty of TCCON data
Publication(s)	Chevallier et al., 2010 [36].

4.1.3 Quality control

Quality control

Product name	Global CO₂ source & sink inversions
Version numbering	Yes
Version documentation	Yes
Frequency of quality checks	At each release
Confidence interval monitoring	Yes
Provision of QI(s)	No, because of the large diversity of space-time targets (from



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	local/3hrly to global decadal)
Graphic representation of QI(s)	Yes
Criteria for flagging or discarding new data	see details in Chevallier et al. (JGR, 2010) [36]
Data corruption	Visual QC of all data
Product degradation	Comparison of global totals before and after the interpolation
False alerts / failure rate	/
Monitoring of delivery regularity	Yearly delivery, like the input data
User feedback mechanism	frederic.chevallier_at_lsce.ipsl.fr
Additional information	/

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5 DELAYED MODE – REGIONAL PRODUCTS

5.1 SOLEMI

5.1.1 Product and service description


Meteosat images are received at DLR. This station is external to the service SOLEMI and acts as a provider of images. Images are quality-controlled for all channels. They are then cut into overlapping tiles, which are stored into a database. This database is part of the DIMS system of DLR (Data Information and Management System).

The SOLEMI service exploits data every 30 min for the Meteosat and every 15 minutes for the Meteosat Second Generation satellites. The processing to produce an irradiance product is made only on-request. Standard requests are for time-series for a given site, or for maps. Inputs are latitude, longitude, and elevation of the site of interest.

Meteosat visible images are extracted from DIMS and calibrated. For MSG, the two images in the visible band are combined to create an image of broadband radiance (Cros et al., 2006 [40]). Other inputs to the method Heliosat-2 in SOLEMI (Rigollier et al., 2004 [43]) are aerosol properties, total water column, and total column ozone. These parameters are read from databases containing monthly or daily values and interpolated for the day under concern if needed. The clear-sky irradiance is computed by the Bird model (Bird et al., 1981 [39]). Using a database of ground albedo, the cloud-index, then the clear-sky index, and finally the irradiance are computed. Products are created by aggregating irradiance values over the requested aggregation period, e.g., hour, day, month.

Product specifications


Product name	SOLEMI
Product brief description	Surface solar irradiance
Product developer(s)	DLR, M. Schroedter-Homscheidt, m.schroedter-homscheidt@dlr.de and C. Hoyer-Klick, carsten.hoyer-klick@dlr.de
Targeted applications	Solar energy
Available version number(s)	6.14
Differences between available versions (summary)	
Product display	On request production of timeseries as ASCII files and maps in GIS formats
Main current user(s)	commercial agreements exist with various solar energy project developers, projects on behalf of regional/national authorities are ongoing
Digital format	ASCII or GIS formats
Parameters	
Parameter / physical quantity	Global and direct normal irradiance as derived with the Heliosat-2 method; hourly data in pixel resolution is provided – a 5x5 pixel averaging is typically performed; hourly data is derived from averaging all Meteosat images in the hour
Unit	W/m ²
Generation method	Derived from geostationary satellites using the Heliosat-2 method

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Platform / instrument / observational network / technique / model	Meteosat satellites, Meteosat Second Generation starting with 2004
Immediacy	Historical data sets
Temporal coverage	1984-2005 for Meteosat, since 2004 for Meteosat Second Generation 1995-2005 for Central Asia and the Indian Ocean
Time resolution	Hourly time series, monthly or annual sums in maps
Geographic coverage	Meteosat field of view (Europe, Africa, Middle East, Central Asia, India)
Horizontal resolution	Point for time series, 1 km for maps
Vertical extent	N/A (surface product)
Vertical resolution	N/A
Other independent variables	
Typical range of values	
Quality indicator(s)	Benchmarking report as provided by the MESOR D1.1.3 Handbook on Benchmarking
Standard(s) of reference	Benchmarking follows the MESOR D1.1.3 Handbook on Benchmarking, project report EU MESOR
Publication(s)	User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]
Additional information	

Service specifications

Delivery service name	SOLEMI Service
Service description / purpose	Delivery of time series and maps for solar energy users
Service provider(s)	DLR
Service URL	On request processing
Contact details	Marion Schroedter-Homscheidt (marion.schroedter-homscheidt@dlr.de) Carsten Hoyer-Klick (carsten.hoyer-klick@dlr.de)
Operational stage	fully operational service
Date of entry into operation	
Upstream external information providers	
Delivery mode	on request, consultation
Delivery medium / channel	FTP, email
Update regularity / frequency	Monthly
Update delay	depending on requests
Delivery delay	depending on data amount requested
Historical record	satellite data since 1984 is available for the product generation
Historical record availability	N/A (on request processing)
Historical record time coverage	N/A (on request processing)
Backup frequency	
Documentation provided	Metadata in the common format description header following the MESOR 'D1.1.2 Existing Ground data sets' report is provided in each data file; the User's Guide from the MACC project is describing static information about the product

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Metadata standard	MESOR 'D1.1.2 Existing Ground data sets'
Support facilities provided	Scientist contact
Conditions on use	Commercial until the transfer into the GMES atmosphere service has officially started
Conditions of access	On request (depending on data amount)
Standard(s) of reference	As described in the User's Guide document [44]
Publication(s)	User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]
Additional information	

5.1.2 Product generation and validation

The principles of Heliosat rely on the fact, that in most cases, a cloud exhibits a larger reflectance than the ground. The magnitude of the difference between both targets is related to the depletion of the downwards radiation by the atmosphere. Heliosat comprises a modelling of the SSI that should be observed by the sensor if the sky were cloud-free for any pixel. The method Heliosat is divided into two parts regarding the physical modelling: converting the satellite image into a cloud index and converting the cloud index in irradiance.


Rigollier et al. (2004) [43] designed Heliosat-2 using calibrated Meteosat images instead of gray values. The irradiance is the irradiance for the clear-sky case multiplied by the clear-sky index quantifying cloud extinction. The clear-sky index is derived from a cloud index comparing the pixel's reflectance versus brightest clouds and the ground. The cloud index is close to 0 when the observed reflectance is close to the ground reflectance, i.e., when the sky is clear. The cloud index increases as the clouds are appearing. It can be greater than 1 for clouds that are optically very thick. An empirical relationship was derived from coincident ground measurements linking cloud index and clear-sky index.

The clear-sky model for SOLEMI is the model of Bird (Bird et al., 1981 [39]) requiring auxiliary input on aerosols, water vapour and ozone. SOLEMI currently is an on request processing, so different aerosol data sets are selected based on comparisons with local ground data (if available) or on a regional basis (e.g. GACP and AeroCom tend to match better in European areas whereas MATCH/DLR showed best results on the Arabian Peninsula).

A daily total water vapour column data set of the NCEP/NCAR-Reanalysis of the Climate Diagnostic Center (CDC-NOAA) with a spatial resolution of 2.5° x 2.5° is used. For ozone, a data set from the Total Ozone Mapping Spectrometer (TOMS) sensor is used. The derived ozone columns from the level 2 product are gridded into a 1° latitude by 1.25° longitude level product. As the daily products only have a 90 % coverage and the influence of ozone is relatively small, a monthly data set is used.

Validation of intermediate and final products

Product name	SOLEMI
Brief product description	Surface solar irradiance
Validation method	Comparison to ground measurements
Validation data	
Quality indicator	
Information content analysis	

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Assessment of product against user requirements	
Standard(s) of reference	MESOR D1.1.3 Handbook on Benchmarking
Publication(s)	MESOR D1.1.3 Handbook on Benchmarking; User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]


Validation data

Dataset name	Several ground measurement networks
Dataset provider / source	Baseline Surface Radiation Network (BSRN), Global Atmospheric Watch (GAW), International Daylight Measurement Programme (IDMP), World Radiation Data Center (WRDC), national meteorological services, research organisations as DLR, CIEMAT, CRES
Parameter / physical quantity	Global and direct normal irradiance
Unit	W/m ²
Generation method	Observed
Platform / instrument / network / model name	Pyrheliometers, rotating shadowband pyranometers, pyranometers
Immediacy	record
Temporal coverage	Various
Time resolution	Various, hourly used
Vertical extent	N/A
Vertical resolution	N/A
Geographic coverage	Europe, Africa
Horizontal resolution	Point measurements
Other independent variables	
Typical range of values over the domain of definition	
Accuracy / precision	1 to 5% in RMSE depending on instrument
Format	various
Publication(s)	MESOR D1.1.2 Ground Data report, EU MESOR project provides a summary and original references
Additional information	

5.1.3 Quality control

There are a number of control points in the workflow for monitoring the smooth running of the processing. Each time a failure is observed, reporting is made.

A manual inspection of the product is made based on scientific experience, taking into account the history available in the archive. Such procedures include comparing monthly means, e.g. all months of January in a period spanning several years, or comparing annual patterns and frequency distributions of single years against each other. If larger areas are processed a visual inspection of satellite raw data in movies is done.

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Comparison between irradiance products and measurements at ground by well-calibrated instruments is made as often as possible. This is not systematic as the access to such data is limited. The results of such comparisons are used:

- to document the uncertainty in the retrieval displayed on the Web site,
- to detect possible flaws in the method or processing workflow, and correct them.

The usual way of assessing the quality of retrievals of SSI derived from satellite images is to compare these SSI to coincident measurements performed at ground level. The typical accuracy of SSI measured in the global meteorological network is 3 to 5 % in terms of root mean square error. Therefore, the ground measurements can be seen as an accurate reference against which one may compare the SSI derived from satellite.


However, the actual situation is not that simple. Several limitations exist that make the assessment of the quality of retrieved irradiances a very difficult task. Zelenka et al. (1999) analyzed the real accuracy of satellite estimations of hourly SSI. They suggest that for a relative deviation of 23 % (root mean square error) between ground measurements and satellite estimations, only half of it is due to the estimation method itself. The difference comes from:

- error on the measurements provided by the pyranometer (3 to 5 %);
- error due to the spatial variability of solar radiation within the pixel (5 to 8 %)
- error due to spatial and temporal heterogeneity of the compared data, e.g. assuming ergodicity (3 to 5 %).

Guidelines of the benchmarking procedures of solar radiation products derived from satellite data, have been proposed by the MESoR project, in order to measure the quality of these products with a common scheme (Beyer et al., 2008 [38]). The quality of a product is defined by various statistical quantities that measure the discrepancies between products and ground data considered as a reference.

Quality control

Product name	SOLEMI
Version numbering	Yes
Version documentation	yes
Frequency of quality checks	On request, depending on the availability of ground measurements
Confidence interval monitoring	yes
Provision of QI(s)	N/A
Graphic representation of QI(s)	N/A
Criteria for flagging or discarding new data	N/A
Data corruption	on request data delivery with personal contact
Product degradation	Metadata header
False alerts / failure rate	N/A
Monitoring of delivery regularity	N/A
User feedback mechanism	Existing through direct contact
Additional information	

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5.2 SoDa

5.2.1 Product and service description

Meteosat images are received every 15 min by Armines. Only the two channels in the visible band are kept. The images are stored into a database. The near-real-time processing is triggered at the end of the day by the reception of the last images at 21:00 UT. The first operation is the control of the quality of Meteosat images. It consists in looking for the missing lines if any and in the check of the position of extreme lines and columns in each image. If a failure is observed, the processing stops.

Meteosat images are calibrated using the calibration coefficients supplied in the flow emitted by Meteosat, resulting into two images of radiance every 15 min. MSG visible images are then combined to create an image of broadband radiance (Cros et al. 2006 [40]).

Inputs to the method Heliosat-2 are the latitude, longitude, and elevation of the current pixel. Another input is the Linke turbidity factor characterising the optical state of the clear atmosphere. It is read from a database containing monthly values and interpolated for the day under concern. The clear-sky irradiation for the 15 min period is computed by the ESRA model, (Rigollier et al., 2000 [43]; Geiger et al., 2002 [41]). Then, using a database of ground albedo, the cloud-index, then the clear-sky index, and finally the irradiation G15 for the 15 min period are computed. The irradiation is stored in the HelioClim-3 database.


Request for products are made through the Web site of the SoDa Service (www.soda-is.com). There are two types of requests: manual and automated. Manual requests are made by the means of a browser. Automated requests are emitted by computers. They typically request for hourly values of irradiance every day for large numbers of geographical sites.

A request can be for a time-series (the standard product) or for a map. For the time-being, the processing is the same; a map is considered as made of independent pixels that are processed separately.

Automated requests are processed in the same way than the manual requests, except that their processing is part of the near-real-time processing and takes part immediately after the updating of the HelioClim-3 database.

Product specifications


Product name	SoDa
Product brief description	Surface solar irradiance
Product developer(s)	Armines, Lucien.wald@mines-paristech.fr
Targeted applications	Solar energy
Available version number(s)	
Differences between available versions (summary)	
Product display	Regular production of timeseries as ASCII files and maps in GIS formats
Main current user(s)	commercial agreements exist with various solar energy project developers, projects on behalf of regional/national authorities are ongoing
Digital format	ASCII or GIS formats
Parameters	
Parameter / physical quantity	Global and direct normal irradiance as derived with the Heliosat-2 method; hourly data or 15 min data in pixel resolution is provided

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Unit	W/m ²
Generation method	Derived from geostationary satellites using the Heliosat-2 method
Platform / instrument / observational network / technique / model	Meteosat satellites, Meteosat Second Generation starting with 2004
Immediacy	Historical data sets, delayed production mode
Temporal coverage	1984-2005 for Meteosat, since 2004 for Meteosat Second Generation
Time resolution	Hourly time series, monthly or annual sums in maps
Geographic coverage	Meteosat field of view (Europe, Africa, Middle East)
Horizontal resolution	Point for time series, km for maps
Vertical extent	N/A (surface product)
Vertical resolution	N/A
Other independent variables	
Typical range of values	
Quality indicator(s)	Benchmarking report as provided by the MESOR D1.1.3 Handbook on Benchmarking
Standard(s) of reference	Benchmarking follows the MESOR D1.1.3 Handbook on Benchmarking, project report EU MESOR
Publication(s)	User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]
Additional information	

Service specifications

Delivery service name	SoDa Service
Service description / purpose	Delivery of time series and maps for solar energy users
Service provider(s)	ARMINES
Service URL	Delayed mode processing, web service access http://www.soda-is.com
Contact details	Lucien Wald (lucien.wald@mines-paristech.fr)
Operational stage	fully operational service
Date of entry into operation	
Upstream external information providers	
Delivery mode	pull, consultation
Delivery medium / channel	web service
Update regularity / frequency	Monthly
Update delay	several days
Delivery delay	depending on data amount requested
Historical record	satellite data since 1984 is available for the product generation
Historical record availability	
Historical record time coverage	
Backup frequency	
Documentation provided	

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Metadata standard	
Support facilities provided	help desk
Conditions on use	Commercial until the transfer into the GMES atmosphere service has been declared operational
Conditions of access	
Standard(s) of reference	As described in the User's Guide document.
Publication(s)	User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]
Additional information	

5.2.2 Product generation and validation


The principles of Heliosat rely on the fact, that in most cases, a cloud exhibits a larger reflectance than the ground. The magnitude of the difference between both targets is related to the depletion of the downwards radiation by the atmosphere. Heliosat comprises a modelling of the SSI that should be observed by the sensor if the sky were cloud-free for any pixel. The method Heliosat is divided into two parts regarding the physical modelling: converting the satellite image into a cloud index and converting the cloud index in irradiance.

Rigollier et al. (2004) [43] designed Heliosat-2 using calibrated Meteosat images instead of gray values. The irradiance is the irradiance for the clear-sky case multiplied by the clear-sky index quantifying cloud extinction. The clear-sky index is derived from a cloud index comparing the pixel's reflectance versus brightest clouds and the ground. The cloud index is close to 0 when the observed reflectance is close to the ground reflectance, i.e., when the sky is clear. The cloud index increases as the clouds are appearing. It can be greater than 1 for clouds that are optically very thick. An empirical relationship was derived from coincident ground measurements linking cloud index and clear-sky index.

The database HelioClim-3 is constructed by the means of the clear-sky model ESRA (European Solar Radiation Atlas). It is based on Kasten's (1996) [42] Rayleigh optical depth parameterization and the Linke turbidity factor at air mass 2. Details can be found in Rigollier et al. (2000) [43] with revision proposed by Page and Remund and reported in Geiger et al. (2002) [41].

Validation of intermediate and final products

Product name	SoDa
Brief product description	Surface solar irradiance
Validation method	Comparison to ground measurements
Validation data	
Quality indicator	
Information content analysis	
Assessment of product against user requirements	
Standard(s) of reference	MESOR D1.1.3 Handbook on Benchmarking
Publication(s)	MESOR D1.1.3 Handbook on Benchmarking; User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]

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Validation data

Dataset name	Several ground measurement networks
Dataset provider / source	Baseline Surface Radiation Network (BSRN), Global Atmospheric Watch (GAW), International Daylight Measurement Programme (IDMP), World Radiation Data Center (WRDC), national meteorological services, research organisations as DLR, CIEMAT, CRES
Parameter / physical quantity	Global and direct normal irradiance
Unit	W/m ²
Generation method	Observed
Platform / instrument / network / model name	Pyrheliometers, rotating shadowband pyranometers, pyranometers
Immediacy	record
Temporal coverage	Various
Time resolution	Various, hourly used
Vertical extent	N/A
Vertical resolution	N/A
Geographic coverage	Europe, Africa
Horizontal resolution	Point measurements
Other independent variables	
Typical range of values over the domain of definition	
Accuracy / precision	1 to 5% depending on instrument
Format	various
Publication(s)	MESOR D1.1.2 Ground Data report, EU MESOR project provides a summary and original references
Additional information	

5.2.3 Quality control

There are a number of control points in the workflow for monitoring the smooth running of the near-real-time processing. Each time a failure is observed, detailed reporting is made to the management, written in a log file and sent by e-mail as well. A visual monitoring is in place to perform visually a gross check of the computed irradiance. It comprises a graph of the irradiances for the last two days for three selected sites: Sophia Antipolis where the chain is operated, and two extreme locations in the East and the West on the Equator. A Web page is updated that provides access to the archive of log files and graphs.

Multiple benchmarking activities demonstrated a few biases in the raw irradiation data contained in the database. A posteriori corrections are brought to the raw values. In order to cope with gaps and to compute direct and diffuse components, the clear-sky index is interpolated every minute. ESRA algorithms are used to compute direct and diffuse components from the global irradiance every minute. Finally, the 1-min values are summed up to yield the requested aggregation period, e.g. hour, day, month.

Comparison between irradiance products and measurements at ground by well-calibrated instruments is made as often as possible. This is not systematic as the access to such data is limited. The results of such comparisons are used:

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- to document the uncertainty in the retrieval displayed on the Web site,
- to set up a posteriori correction procedures if possible, to improve the quality,
- to detect possible flaws in the method or processing workflow, and correct them,

to establish the model of uncertainty allowing to allocate uncertainty values to each irradiance value.

The usual way of assessing the quality of retrievals of SSI derived from satellite images is to compare these SSI to coincident measurements performed at ground level. The typical accuracy of SSI measured in the global meteorological network is 3 to 5 % in terms of root mean square error. Therefore, the ground measurements can be seen as an accurate reference against which one may compare the SSI derived from satellite.


However, the actual situation is not that simple. Several limitations exist that make the assessment of the quality of retrieved irradiances a very difficult task. Zelenka et al. (1999) analyzed the real accuracy of satellite estimations of hourly SSI. They suggest that for a relative deviation of 23 % (root mean square error) between ground measurements and satellite estimations, only half of it is due to the estimation method itself. The difference comes from:

- error on the measurements provided by the pyranometer (3 to 5 %);
- error due to the spatial variability of solar radiation within the pixel (5 to 8 %)
- error due to spatial and temporal heterogeneity of the compared data, e.g. assuming ergodicity (3 to 5 %).

Guidelines of the benchmarking procedures of solar radiation products derived from satellite data, have been proposed by the MESoR project, in order to measure the quality of these products with a common scheme (Beyer et al., 2008 [38]). The quality of a product is defined by various statistical quantities that measure the discrepancies between products and ground data considered as a reference.

Quality control

Product name	SoDa
Version numbering	
Version documentation	
Frequency of quality checks	On request, depending on the availability of ground measurements
Confidence interval monitoring	Data is checked against typical value ranges.
Provision of QI(s)	Several QI as quoted in Product Specification Table in Section 5.2.1 are provided with the data.
Graphic representation of QI(s)	TBD
Criteria for flagging or discarding new data	Yes, part of QIs.
Data corruption	
Product degradation	
False alerts / failure rate	N/A
Monitoring of delivery regularity	Existing schemes within the SoDa precursor will be used.
User feedback mechanism	Existing feedback mechanisms within the SoDa precursor will be used.
Additional information	

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5.3 RAD-SOLAR

5.3.1 Product and service description

Setting up an operational information system with new capabilities and new processing methods is a lengthy process spanning over a few years. In order to exploit as soon as possible and efficiently the outcomes of the MACC project and other initiatives as they are flowing, a number of intermediate steps are being taken to implement these outcomes. Actually, it is too early to describe in detail many aspects of the transition chains and the operation chain in the RAD-SOLAR Service. An overview can be provided only.

Several data on atmospheric conditions (clouds, aerosol, water vapour, and ozone) and ground albedo will be received from various sources, pre-processed and stored in several databases. These intermediate databases (or tables) will constitute the HelioClim-4 database.

The delivery deadline from each source is still unknown. It could amount to several days. Therefore, the term ‘near-real-time’ has to be interpreted as within 24 hours (preferably) or longer. Operations are triggered by successfully received input data sets.

Currently, the concept to produce products is that the processing is made on-request (on-the-fly). When a request is made for a time-series for a given site and a given period, the irradiance processor will invoke the McClear model with inputs extracted from the database “atm”. Extinction coefficients are then obtained by the cloud processor using inputs from the database “cloud”. Finally, the contribution to the diffuse irradiance due to the ground albedo is computed.

Tests have been made that demonstrate that such an on-the-fly processing is sustainable in the perspective of the RAD-SOLAR Service. Nevertheless, it is likely that databases of irradiance will be pre-computed, at least to best answer to request for maps of daily or monthly values of irradiance.

Presently, there are two series of products in the RAD-SOLAR Service:

- ARCH products: the first series is an archive: 1984-2005, based on Meteosat First Generation (MFG) data. It is denoted by the letters ARCH (for Archive),
- MSG products: the second series is based on Meteosat Second Generation (MSG) series of satellites, starting from 2004 and on-going. It is denoted by the letters MSG.

For both series currently available, core products in the RAD-SOLAR Service are time-series of solar radiation available at ground surface, also called surface solar downward irradiance (SSI).

This includes the total global irradiance (GHI), i.e., the SSI integrated over the whole spectrum available at ground level, on a horizontal surface; the total diffuse irradiance (DifHI), i.e., the diffuse part of the SSI integrated over the whole spectrum available at ground level, on a horizontal surface; and total direct (beam) irradiance (DirHI), i.e., the direct part of the SSI integrated over the whole spectrum available at ground level, on a horizontal surface.

From a practical point of view, and beyond the various issues related to being a recognised customer of the information system, the inputs by users needed to trigger a request for a selected MACC product will be:

- the geographical coordinates of the site of interest, or the name of this site,

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- the elevation of this site above sea-level. By default, the application uses well-known digital elevation models, such as NASA-SRTM,
- the period of time: begin data, end date.


Delivery deadline is the time lag between the moment the request is made and the instant of delivery. The delivery deadline depends on the series of products: ARCH or MSG.

The ARCH products are computed on request and are not available as such on the shelf. Once the request for a product is made, DLR, the author of the products ARCH, selects the best suitable auxiliary data set for the site among global atmospheric data sets (aerosol, water vapour, ozone) from different earth observation sources and climate models. The atmospheric data is gridded to a resolution of $1^{\circ} \times 1^{\circ}$ and the cloud data from Meteosat has a nominal resolution of 2.5 km x 2.5 km at the sub satellite point. The geographical coordinates (latitude, longitude and height above sea level) in decimal degrees and meters have to be delivered to DLR. The product is delivered per e-mail within two weeks.

The MSG products are computed on-the-fly from the database HelioClim. The request is made through the Web site of the SoDa Service (www.soda-is.com) and the answer is provided within a few minutes.

Product specifications

Product name	RAD-SOLAR
Product brief description	Surface solar irradiance
Product developer(s)	Armines, Lucien.wald@mines-paristech.fr ; DLR, Marion.Schroedter-Homscheidt@dlr.de
Targeted applications	Solar energy
Available version number(s)	yes
Differences between available versions (summary)	
Product display	regular production of timeseries as ASCII files
Main current user(s)	solar energy project developers, regional/national authorities
Digital format	ASCII
Parameters	
Parameter / physical quantity	Global, diffuse and direct irradiance as derived with the Heliosat-4 method; hourly data (archive) or 15 min (near real time) data in pixel resolution is provided
Unit	W/m ²
Generation method	Derived from geostationary satellites using the Heliosat-4 method and making use of MACC re-analyses for aerosols, ozone and water vapour and MODIS for ground albedo.
Platform / instrument / observational network / technique / model	Meteosat Second Generation starting with 2004
Immediacy	Historical data sets, few days delayed production mode
Temporal coverage	since 2004
Time resolution	Hourly time series for archived data, 15 min for near-real-time processing
Geographic coverage	Meteosat Second Generation field of view (Europe, Africa, Middle East)
Horizontal resolution	Point for time series

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Vertical extent	N/A (surface product)
Vertical resolution	N/A
Other independent variables	
Typical range of values	
Quality indicator(s)	Benchmarking report as provided by the MESOR D1.1.3 Handbook on Benchmarking
Standard(s) of reference	Benchmarking follows the MESOR D1.1.3 Handbook on Benchmarking, project report EU MESOR
Publication(s)	User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]
Additional information	

Service specifications

Delivery service name	RAD-SOLAR Service
Service description / purpose	Delivery of time series for solar energy users
Service provider(s)	ARMINES in collaboration with DLR
Service URL	Delayed mode, on request and near real time processing, web service access http://www.soda-is.com
Contact details	Lucien Wald (lucien.wald@mines-paristech.fr), Marion Schroedter-Homscheidt (marion.schroedter-homscheidt@dlr.de)
Operational stage	fully operational service in 2014 foreseen
Date of entry into operation	
Upstream external information providers	
Delivery mode	pull, consultation
Delivery medium / channel	web service
Update regularity / frequency	Monthly or daily
Update delay	several days in delayed mode
Delivery delay	depending on data amount requested
Historical record	satellite data since 2004 is available for a product generation starting in 2014
Historical record availability	tbd
Historical record time coverage	tbd
Backup frequency	tbd
Documentation provided	User's Guide RAD-SOLAR
Metadata standard	Metadata are available to describe the RAD-SOLAR products in GEOSS-compliant portals. These are discovery metadata that permit the cataloguing of these products and therefore to users to discover the products. These metadata obey to INSPIRE implementation rules (Ménard et al. 2009).
Support facilities provided	help desk
Conditions on use	free if GAS is operational, reproduction costs may apply
Conditions of access	
Standard(s) of reference	As described in the User's Guide document.
Publication(s)	User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]

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5.3.2 Product generation and validation

The new Heliosat-4 method is based on the principle that the SSI for a cloudy atmosphere can be considered as equal to the product of the irradiance obtained under a clear sky and a function modelling the extinction of the radiation by clouds and the contribution due to the ground albedo. The possibility of considering several spatial and temporal resolutions is of practical importance in MACC. MACC outcomes should be daily values or every 3 h but by no means every hour. The expected spatial resolution should be in the range 50 km - 200 km. The cloud properties can be derived from the processing of Meteosat images as done by DLR with the adapted APOLLO chain. Such products will be available every 15 min for each Meteosat pixel.

Recent initiatives from NCAR (USA, MATCH scheme) and the EU-funded project GEMS yielded to more accurate and detailed assessments of optical properties of the aerosols with capability of producing daily maps. MACC will produce aerosol properties using a method similar or enhanced if compared to GEMS. Therefore, the expertise gained with these GEMS products will be efficiently used in the RAD-SOLAR Service.

In the meantime, other parameters such as the column content in water vapour or ozone are available daily over the world. MACC is producing such parameters as well as other sources. In the same manner than for the aerosol properties, these recent results will be ingested.


The availability of these atmospheric parameters as well as the increase in computing power advocate for an increase in the complexity of the models used to compute the clear-sky models, which should result in an increase in accuracy. Such a model is being developed, called McClear. Inputs to this model will be outputs from MACC, except for site coordinates, solar angles, elevation, atmospheric profile, and ground albedo. The current ESRA model will be replaced by this new model McClear. This will be a major step towards the operational RAD-SOLAR Service. It will lead to major changes in the workflow though it is too early to provide details.

Validation of intermediate and final products

Product name	RAD-SOLAR
Brief product description	Surface solar irradiance
Validation method	Comparison to ground measurements
Validation data	
Quality indicator	
Information content analysis	
Assessment of product against user requirements	
Standard(s) of reference	MESOR D1.1.3 Handbook on Benchmarking
Publication(s)	MESOR D1.1.3 Handbook on Benchmarking; User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service [44]

Validation data

Dataset name	Several ground measurement networks
Dataset provider / source	Baseline Surface Radiation Network (BSRN), Global Atmospheric Watch (GAW), International Daylight Measurement Programme

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	(IDMP), World Radiation Data Center (WRDC), national meteorological services, research organisations as DLR, CIEMAT, CRES
Parameter / physical quantity	Global and direct normal irradiance
Unit	W/m ²
Generation method	Observed
Platform / instrument / network / model name	Pyrheliometers, rotating shadowband pyranometers, pyranometers
Immediacy	record
Temporal coverage	Various
Time resolution	Various, hourly used
Vertical extent	N/A
Vertical resolution	N/A
Geographic coverage	Europe, Africa
Horizontal resolution	Point measurements
Other independent variables	
Typical range of values over the domain of definition	
Accuracy / precision	1 to 5% in RMSE depending on instrument
Format	various
Publication(s)	MESOR D1.1.2 Ground Data report, EU MESOR project provides a summary and original references
Additional information	


5.3.3 Quality control

A quality control must be performed everyday by comparing the core products to measurements performed by ground stations and to re-analyses. The first aim of this quality control is to monitor possible trends in products and decide for appropriate corrections. In that sense, what is important is the change of differences between products and measurements or re-analyses with time outside the expected range of variation. To do so, a model should be available that explains these discrepancies as a function of known explanatory variables such as the solar zenithal angle or the temporal variability of the SSI. Therefore, the distance between products and re-analyses can be predicted. It will be used to monitor the quality of products: large values should indicate suspect products.

The second aim of this quality control is to perform a benchmarking of the products against a reference. This can be done only with quality-proven measurements. By comparison, one will obtain the uncertainty parameters synthesizing the difference between products and reference following the methodology recommended by the projects IEA SHC 36 and MESoR. These uncertainty parameters will be displayed on the Web pages of the RAD-SOLAR Service to support the documentation on the quality of products.

Based on the results of such comparisons, a model of uncertainty can be established or improved that provides for any instant the plausible uncertainty level of the SSI, given known explanatory variables.


To perform the quality control, operations should be established to collect in an automatic way re-analyses values from ECMWF and ground measurements from selected sites or from the World Radiation

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Data Center. Quality control procedures must be also implemented that apply onto these measurements and re-analyses.

Quality control

Product name	RAD-SOLAR
Version numbering	Tbd
Version documentation	tbd
Frequency of quality checks	Tbd, depending on the availability of ground measurements
Confidence interval monitoring	New data is checked against typical value ranges.
Provision of QI(s)	Several QI as quoted in Product Specification Table in Section 5.3.1 are provided with the data.
Graphic representation of QI(s)	TBD
Criteria for flagging or discarding new data	Yes, part of QIs.
Data corruption	
Product degradation	
False alerts / failure rate	N/A
Monitoring of delivery regularity	Existing schemes within the SoDa precursor will be used.
User feedback mechanism	Existing feedback mechanisms within the SoDa precursor will be used.
Additional information	

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6 REANALYSIS MODE – GLOBAL PRODUCTS

6.1 BASCOE Reanalysis of Ozone and Ozone-Related Species

6.1.1 Product and service description

Product specifications

Product name	BASCOE reanalysis of ozone and ozone-related species
Product brief description	Reanalyses of stratospheric ozone and related chemical species (O ₃ , H ₂ O, HNO ₃ , HCl, HOCl, N ₂ O) by the BASCOE data assimilation system using UARS/MLS, Envisat/MIPAS or Aura/MLS level 2 satellite observations – the list of assimilated species depends on the instrument. The reanalyses of UARS/MLS and MIPAS include only ozone.
Product developer(s)	BIRA-IASB, Ringlaan 3, B-1180 Brussel, Contact by e-mail: macc@aeronomie.be
Targeted applications	<ul style="list-style-type: none"> • Detection and evaluation of trends in processes related to polar stratospheric ozone depletion, e.g. PSC formation, chlorine activation, denitrification, dehydration, etc. • Validation of the stratospheric composition delivered for MACC by the IFS-MOZART reanalysis fbov (where only ozone is assimilated in the stratosphere) • Evaluation of the stratospheric composition delivered by multi-year simulations of Chemistry-Climate Models (project CCMVal of SPARC)
Available version number(s)	BASCOE/UARS-MLS: v4q09 BASCOE/MIPAS: v4q30a BASCOE/AURA-MLS: q02.13
Differences between available versions (summary)	<ul style="list-style-type: none"> • v4q09 is driven by winds and Temperature from ERA-40 reanalysis. Assimilated species: O₃, ClO, H₂O. The delivered product includes only O₃. • v4q30a is driven by winds and Temperature from ECMWF operational analyses. Assimilated species: O₃, HNO₃, NO₂, CH₄, H₂O, N₂O. The delivered product includes only O₃. • q02.13 (algorithm identical to v06q21) is driven by winds and Temperature from ERA-Interim reanalysis, uses an improved solver for the adjoint chemistry module, and the chemical reaction rates were updated to JPL2006. Assimilated species: O₃, H₂O, HNO₃, HCl, N₂O, HOCl. The delivered product includes all the assimilated species.
Product display	<ul style="list-style-type: none"> • Monthly averaged maps of O₃ and NO_x interpolated at 1, 50, 100 hPa pressure levels; O₃ total columns • Time-series of the same quantities (without monthly averaging) • Movies comparing the seasonal evolution of the ozone hole during years 2004 to 2010
Main current user(s)	SPARC CCMVal, MACC
Digital format	HDF-4, PNG
Parameters	
Parameter / physical quantity	volume mixing ratio
Unit	dimensionless (mole/mole)

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Generation method	Observations assimilated into a model
Platform / instrument / observational network / technique / model	BASCOE Data Assimilation System
Immediacy	Record
Temporal coverage	BASCOE/UARS-MLS v4q09: 1992/01/01 – 1999/12/31 BASCOE/MIPAS v4q30a: 2002/07/15 – 2004/03/31 BASCOE/AURA-MLS q02.13: 2004/08/08 – 2010/12/31
Time resolution	24h (analyses valid at 12h UT)
Geographic coverage	global
Horizontal resolution	5°x 3.75° (lon x lat)
Vertical extent	0.1 hPa to the surface (data should not be used in the troposphere)
Vertical resolution	37 levels, most of them lying in the stratosphere.
Other independent variables	Surface pressure (Pa) global,
Typical range of values	depends on species O3: 0 – 12e-6 H2O: 0 – 0.05 HNO3: 0 – 15e-9 HCl: 0 - 6e-9 N2O: 0 – 0.5e-6 HOCl: 0 – 20e-9 (Note: this species is not validated – see Section 6.1.2)
Quality indicator(s)	N/A
Standard(s) of reference	N/A
Publication(s)	Lefever et al., 2011b [10].
Additional information	/


Service specifications

See Section 2.1.1.

6.1.2 Product generation and validation

Validation of intermediate and final products

Product name	BASCOE reanalysis of ozone and ozone-related species
Brief product description	Reanalyses of stratospheric ozone and related chemical species (O3, H2O, HNO3, HCl, HOCl, N2O) by the BASCOE data assimilation system using UARS/MLS, Envisat/MIPAS or Aura/MLS level 2 satellite observations – the list of assimilated species depends on the instrument. The reanalyses of UARS/MLS and MIPAS include only ozone.
Validation method	Vertically resolved mean bias and standard deviations of differences w.r.t. independent observations for 5 latitude bands (90°S-60°S, 60°S-30°S, 30°S-30°N, 30°N-60°N, 60°N-90°N)
Validation data 1	HALOE (see table below).
Quality indicator 1	N/A
Validation data 2	POAM (see table below).
Quality indicator 1	N/A

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Information content analysis	N/A
Assessment of product against user requirements	No
Standard(s) of reference	N/A
Publication(s)	Errera et al., 2008 [4]. Errera, Q., S. Viscardy and F. Baier, 2009 [5]. Geer et al., 2006 [6]. Lahoz et al., 2007 [7]. Lahoz, W.A, Q. Errera, S. Viscardy, and G.L. Manney, 2011 [8]. Thornton et al., 2009 [11]. Vigouroux et al., 2007 [12]. Viscardy et al., in press [13]. Lefever et al., 2011a [9].

Validation data

Dataset name	HALOE
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Validation data

Dataset name	POAM
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6.1.3 Quality control

Quality control

Product name	BASCOE reanalyses of stratospheric ozone and related species (i.e. this table applies to the 2 NRT products defined in T1)
Version numbering	Versions are numbered following vXqYYz where X denotes major version changes, YY minor version changes and z is a configuration label.
Version documentation	Internal documentation on the wiki of the intranet.
Frequency of quality checks	N/A
Confidence interval monitoring	
Provision of QI(s)	N/A
Graphic representation of QI(s)	N/A
Criteria for flagging or discarding new data	N/A
Data corruption	N/A
Product degradation	N/A
False alerts / failure rate	N/A
Monitoring of delivery regularity	N/A
User feedback mechanism	email to macc@aeronomie.be
Additional information	

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6.2 Global Fire Emission Database (GFED)


6.2.1 Product and service description

Product specifications

Product name	Global Fire Emission Database (GFED)
Product brief description	Biomass burning emissions of carbon & various trace species based on observed Burnt Area (BA) for 2010 (GFED3.1)
Product developer(s)	VUA
Targeted applications	input for global aerosol, reactive gas and greenhouse gas models and regional air quality models of MACC
Available version number(s)	3.0, 3.1
Differences between available versions (summary)	The parameters that changed were mostly depth of burning in tropical peatlands and organic soils in boreal regions. In addition, the algorithm that combines burned area and active fire detections to estimate deforestation rates was revised.
Product display	
Main current user(s)	MACC
Digital format	grib, ASCII
Parameters	
Parameter / physical quantity	dry matter combustion rate, species emission, burnt area monthly averages
Unit	kg/s/m ² , kg/s/m ² , m ²
Generation method	derived from observational data
Platform / instrument / observational network / technique / model	mostly MODIS aboard Terra and Aqua (LEO)
Immediacy	retrospective
Temporal coverage	1997-2010
Time resolution	1 month
Geographic coverage	global
Horizontal resolution	0.5deg
Vertical extent	N/A
Vertical resolution	N/A
Other independent variables	N/A
Typical range of values	> 0
Quality indicator(s)	N / A
Standard(s) of reference	N / A
Publication(s)	
Additional information	

Service specifications

Delivery service name	
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Service description / purpose	
Service provider(s)	VUA, ECMWF
Service URL	http://www.falw.vu/~gwerf/GFED/index.html , gmes-atmosphere.eu/fire
Contact details	guido.van.der.werf@falw.vu.nl
Operational stage	N / A
Date of entry into operation	N / A
Upstream external information providers	NASA
Delivery mode	"pull"
Delivery medium / channel	web download, MARS retrieval
Update regularity / frequency	annually
Update delay	N / A
Delivery delay	N / A
Historical record	yes
Historical record availability	yes
Historical record time coverage	since 1997
Backup frequency	N / A
Documentation provided	with product, online, scientific literature
Metadata standard	N / A
Support facilities provided	online data visualisation
Conditions on use	
Conditions of access	
Standard(s) of reference	N / A
Publication(s)	van der Werf et al., 2010 [Error! Reference source not found.].
Additional information	

6.2.2 Product generation and validation

Validation of intermediate and final products


Product name	
Brief product description	
Validation method	see van der Werf et al., 2010 [Error! Reference source not found.].
Validation data 1	
Quality indicator 1	
Information content analysis	
Assessment of product against user requirements	
Standard(s) of reference	
Publication(s)	

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6.2.3 Quality control

Quality control

Product name	Global Fire Emission Dataset (GFED)
Version numbering	yes
Version documentation	yes
Frequency of quality checks	N / A
Confidence interval monitoring	yes
Provision of QI(s)	N / A
Graphic representation of QI(s)	N / A
Criteria for flagging or discarding new data	N / A
Data corruption	N / A
Product degradation	The processing is performed consistently in high resolution.
False alerts / failure rate	N / A
Monitoring of delivery regularity	N / A
User feedback mechanism	email
Additional information	

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8 ABBREVIATIONS, ACRONYMS, NAMES & LINKS

AERONET	<i>Aerosol Robotic Network</i> of NASA ☞ http://www.esrl.noaa.gov/gmd/obop/mlo/programs/coop/nasa/aeronet/aeronet.html
AOD	Aerosol Optical Depth
AQ	Air Quality
BASCOE	<i>Belgian Assimilation System for Chemical Observations</i> ☞ http://bascoe.oma.be/
BSC	Commission on the Protection of the Black Sea against Pollution (the <i>Black Sea Commission</i>) ☞ http://www.blacksea-commission.org/
BUFR	Binary Universal Form for the Representation of Meteorological Data
DLR	Deutsche Forschungs- und Versuchsanstalt für Luft- und Raumfahrt ☞ http://www.dlr.de/
EC	<i>European Commission</i> ☞ http://ec.europa.eu/
ECMWF	<i>European Centre for Medium-range Weather Forecasts</i> ☞ http://www.ecmwf.int/
EU	Europe, European, European Union
EURAD-IM	<i>European Air Pollution Dispersion Model – Inverse Modelling Version</i>
FMI	<i>Finnish Meteorological Institute</i> ☞ http://ilmatieteenlaitos.fi/
FP6, FP7	<i>Sixth and Seventh Framework Programmes</i> of the EC ☞ http://ec.europa.eu/research/fp7/
FRP	Fire Radiative Power
GAS	<i>GMES Atmospheric Service</i> ☞ http://www.gmes.info/pages-principales/services/atmosphere-monitoring/
GEMS	<i>Global and Regional Earth-System (Atmosphere) Monitoring Using Satellite and In-Situ Data</i> , FP6 project (2005-2009) ☞ http://gems.ecmwf.int/
GFAS	<i>Global Fire Assimilation System</i>
GFED	<i>Global Fire Emission Database</i>
GMES	<i>Global Monitoring for Environment and Security</i> , joint initiative of the EC and ESA for the establishment of a European capacity for EO ☞ http://www.gmes.info/
GRIB2	<i>Gridded Binary</i> (second edition)

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IASB-BIRA	<i>Belgian Institute for Space Aeronomy</i> ☞ http://www.aeronomie.be/
IFS	<i>Integrated Forecast System of the ECMWF</i> ☞ http://www.ecmwf.int/research/ifsdocs/
LANUV	<i>Landesamt für Natur, Umwelt und Verbraucherschutz Nordrhein-Westfalen</i> ☞ http://www.lanuv.nrw.de/
MACC	<i>Monitoring Atmospheric Composition and Climate, FP7 project (June 2009 – October 2011)</i> ☞ http://www.gmes-atmosphere.eu/
MARS	<i>Meteorological Archival and Retrieval System of the ECMWF</i> ☞ http://www.ecmwf.int/services/archive/
MOS	Model Output Statistic
MoU	Memorandum of Understanding
NASA	<i>National Aeronautics and Space Administration</i> ☞ http://www.nasa.gov/
NetCDF	<i>Network Common Data Form</i>
NRT	Near-Real Time
QA4EO	<i>Quality Assurance Framework for Earth Observation</i> ☞ http://qa4eo.org/
QC/QA	Quality control/quality assessment
QI	Quality Indicator
RAQ	Regional Air Quality
REA	<i>Research Executive Agency of the EC</i> ☞ http://ec.europa.eu/research/rea/index.cfm
RIUUK	<i>Rheinisches Institut für Umweltforschung an der Universität zu Köln</i> ☞ http://www.eurad.uni-koeln.de
SLA	Service Level Agreement
SVN	<i>Subversion</i> (version control system)
URD	User Requirement Document
UV	Ultra Violet
WRF	<i>Weather Research and Forecasting model</i> ☞ http://www.wrf-model.org



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Annex 1 - MACC portfolio

Data production temporal mode	Geo-graphic scale	Physical parameter category	Product	Delivery date	Update frequency	Lead provider
NRT and forecast	Global	RG	NRT analyses and forecasts of global RG	Jun 2009		ECMWF
			SACADA assimilated NRT global stratospheric ozone	Sep 2009		DLR
			BASCOE NRT analysis of stratospheric ozone	Sep 2009	Daily	IASB
			BASCOE NRT analysis of ozone-related species	Sep 2010	Daily	IASB
			TM3DAM global total ozone monitoring and forecast	Sep 2009		KNMI
			NRT ozone & NO ₂ data from OMI, SCIAMACHY, GOME & GOME-2	Sep 2009		DLR
			MOZART total ozone forecast			
		Aerosol	NRT analyses and forecasts of global aerosol	Jun 2009		ECMWF
			SYNAER NRT aerosol data	Jun 2009		DLR
			ATSR-DV global aerosol	Nov 2009		FMI
	Emissions	SEVIRI aerosol data	Nov 2009		ICARE	
		Global Fire Assimilation System (GFAS)	Jun 2009	Daily	ECMWF	
	Solar radiation	RAD-UV - Monitoring and forecasting UV radiation		Daily	ECMWF	
	Regional	Aerosol	Dust NRT regional monitoring and forecast based on satellites & the Aeronet network	May 2010		AEMet
			ATSR-DV NRT aerosol over Europe	Jun 2009		FMI
		AQ	European-scale ensemble hourly AQ analyses of the previous day and forecast up to 72h ahead	Sep 2010	Daily	CNRM
			European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by CHIMERE	Sep 2010	Daily	
European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by EMEP			Sep 2011	Daily		
European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by EURAD			Sep 2012	Daily		
European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by LOTOS-EUROS			Sep 2013	Daily		



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			European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by MATCH	Sep 2014	Daily	
			European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by MOCAGE	Sep 2015	Daily	
			Web-oriented warning & information system about health impacts of poor AQ (preoperational)	Oct 2011		CHMI
			Origin of forecasted pollution episodes (graphic presentation)	Nov 2010		MET.NO
			Regional AQ forecasts with source-allocation capabilities (internet-based)	Oct 2011		MET.NO
Delayed	Global	GHG	Reprocessed analyses of global GHG, RG & aerosol	Dec 2010		ECMWF
			Global CH ₄ source & sink inversions	May 2010	Every 6 months	JRC
			Global CO ₂ source & sink inversions	May 2010	Quarterly	CEA
				May 2011	Monthly	
			Stand-alone CO ₂ & CH ₄ retrievals from AIRS & IASI over 2003-2009	Nov 2010		LMD
		Stand-alone CO ₂ & CH ₄ retrievals from AIRS & IASI over 2009-2010	Sep 2011		LMD	
		Aerosol	Reprocessed analyses of global aerosol	Dec 2010		ECMWF
			Global aerosol source & sink inversions	Oct 2011		CEA
			Global aerosol climate forcing	Oct 2011		UKMET
			SYANER aerosol data record	Oct 2011		DLR
	Emissions	Updated inventory of global emissions based on RETRO	May 2011		CEA	
		Biomass burning emissions of carbon & various trace species based on observed Burnt Area (BA) for 2010 (GFED3.1)	Aug 2011	Once	VUA	
	Regional	AQ	Library of test cases for AQ emergency scenarios	Oct 2011		INERIS
		Emissions	Updated inventory of European emissions based on RETRO	May 2011		CEA
		Solar radiation	SOLEMI archive of surface solar irradiance			
SoDa surface solar irradiance						
		RAD-SOLAR				
Reanalysis	Global	GHG	Extension of GEMS global GHG reanalysis to 2009	May 2010		ECMWF
			Global GHG new reanalysis over 2003-2010	Oct 2011		ECMWF
	RG	Extension of GEMS global RG reanalysis to 2009	May 2010		ECMWF	
		Global RG new reanalysis over 2003-2010	Oct 2011		ECMWF	
		SACADA assimilated historical global stratospheric ozone	Sep 2009		DLR	
		BASCOE reanalysis of ozone and ozone-related species	Sep 2009	Once	IASB	



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			TM3DAM global total ozone record	Sep 2009		KNMI
			Total ozone multi sensor reanalysis			
	Aerosol		Extension of GEMS global aerosol reanalysis to 2009	May 2010		ECMWF
			Global aerosol new reanalysis over 2003-2010	Oct 2011		ECMWF
			AEROCOM modelled & observational global aerosol comparisons	May 2011	Monthly	CEA
			Long-term retrospective analysis of dust (DREAM model) & aerosol index (TOMS-OMI) with meningitis epidemics data	Jan 2011		AEMet
	Emissions		Global fire emission database (GFED)	Apr 2010	Once	VUA
	Regional	AQ	Ensemble regional AQ reanalysis for Years 2007, 2008 & 2009 (web-based)	Feb 2010		INERIS
Combined	Global	All	Web-based graphical display and supply of data from global MACC production, monitoring and validation	Sep 2009		ECMWF
	Regional	AQ	Toolbox for AQ emergency scenarios (distributed through internet)	May 2011		INERIS

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Annex 2 - Abstracts

As requested by the MACC Management Board, two-page abstracts of all products or services documented in this report are presented below. They were written by the product providers or derived from the information they supplied, and were formatted using a uniform template. Separate leaflets have also been issued, to be integrated into the MACC website as downloadable documents.

The abstracts that follow relate to

- BASCOE NRT analysis of stratospheric ozone, NRT analysis of ozone-related species, reanalysis of ozone and ozone-related species
- SYNAER aerosol data in NRT and delayed modes;
- Global Fire Assimilation System (GFAS)
- RAD-UV – Monitoring and forecasting UV radiation
- European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by EURAD-IM
- Origin of forecasted pollution episodes (graphic presentation)
- Global CO₂ source and sink inversions
- SOLEMI
- SoDa
- RAD-SOLAR
- Global Fire Emission Database (GFED)



BASCOE

NRT analysis of stratospheric ozone

NRT analysis of ozone-related species

Reanalysis of ozone and ozone-related species

Product and service description

1. Analyses of stratospheric ozone by the BASCOE data assimilation system using Aura/MLS-SCI level 2 (v2.2) satellite observations
2. Analyses of chemical species related to stratospheric ozone (H₂O, HNO₃, HCl, N₂O, HOCl, NO_x) by the BASCOE data assimilation system using Aura/MLS-SCI level 2 (v2.2) satellite observations.
3. Reanalyses of stratospheric ozone and related chemical species (O₃, H₂O, HNO₃, HCl, HOCl, N₂O) by the BASCOE data assimilation system using UARS/MLS, Envisat/MIPAS or Aura/MLS level 2 satellite observations – the list of assimilated species depends on the instrument. The reanalyses of UARS/MLS and MIPAS include only ozone.
4. The MACC stratospheric ozone service is delivered through the website <http://www.gmes-stratosphere.eu>. It is described in Lefever et al (2011b) (available on the web site under More info > User Guide)

Product generation and validation

See the product description: the datasets consist in satellite observations assimilated into the BASCOE Chemical Data Assimilation System.

Quality control

- Source codes are versioned and maintained under the Subversion versioning software
- Version changes are documented within the versioning software, in file Manifest.txt and on the internal wiki of BIRA-IASB
- The maxima of the typical value range (see T1) are not implemented yet. Negative values are clipped automatically and result in warnings in the log files.
- QI are provided in filenames and content of the daily generated log files.
- Emails with processing status are sent daily to macc@aeronomie.be
- Logfiles are listed on the web (with automatic and daily updates). Their names depend on basic processing events (no satellite data available; assimilation failed and forward modelling was used instead). Hence a quicklook on current and past processing outcome is available anytime and everywhere: see http://macc.aeronomie.be/logs/bascoe_AMLS_NRT_loglist.txt
- User feedback mechanism: email to macc@aeronomie.be

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Product and service description

Total aerosol optical depth (AOD) and aerosol type retrieved from satellite-borne sensors, delivered in near-real time (less than 24h delay). Global coverage at 60 x 30 km² resolution. Format: HDF4.

Online pre-calculated GIF daily and monthly maps available.

Data archive spanning 2003-2011.

Parameters include

- the AOD at 550 nm;
- the aerosol type number;
- derived parameters such as
 - multi-spectral AOD;
 - Angström coefficient;
 - fine/coarse mode AOD;
 - components AOD (sulfate, dust, soot, sea salt);
 - single scattering albedo.

Service provider: Deutsche Forschungs- und Versuchsanstalt für Luft- und Raumfahrt (DLR).

- http://www.gmes-atmosphere.eu/services/gac/aerosol_record/
- http://wdc.dlr.de/php/indexer_r.php?dir_index=16&url=/data_products/AEROSOLS/synaer_orbit_hdf_archive.php

Contact: Thomas Holzer-Popp - thomas.holzer-popp@dlr.de

Product generation and validation

Product generation

Combined retrievals from

- AATSR radiometer AATSR + SCIAMACHY spectrometer (on board Envisat);
- AVHRR radiometer + GOME-2 spectrometer (on board MetOP).

Product validation

Comparison with the NASA AERONET ground-based observations by CIMEL photometers (± 60 min ± 50 km) of multi-spectral AOD and other parameters.

Quality indicators provided: bias, RMSE, envelope.

Error on reflectances and critical retrieval parameters are taken into account in the information content analysis.

Plan: additional validation data to be used in the future include MACC, AEROCOM, MODIS/MISR data.

Quality control

About-daily quality checks are performed. Version numbers are documented on the website.

References

Holzer-Popp, T., M. Schroedter, and G., Gesell, Retrieving aerosol optical depth and type in the boundary layer over land and ocean from simultaneous GOME spectrometer and ATSR-2 radiometer measurements, 1, Method description, Journal of Geophysical Research, 107, D21, pp. AAC16-1 – AAC16-17, 2002a.

Holzer-Popp, T., M. Schroedter, and G., Gesell, Retrieving aerosol optical depth and type in the boundary layer over land and ocean from simultaneous GOME spectrometer and ATSR-2 radiometer measurements, 2, Case study application and validation, Journal of Geophysical Research, 107, D24, pp. AAC10-1 – AAC10-8, 2002b.

Holzer-Popp T., Schroedter-Homscheidt, M., Breikreuz, H., Klüser, L., Martynenko, D., Improvements of synergetic aerosol retrieval for ENVISAT, Atmospheric Chemistry and Physics, 8, 7651-7672, 2008.

Holzer-Popp T., M. Schroedter-Homscheidt, H. Breikreuz, D. Martynenko, and L. Klüser, Benefits and limitations of the synergistic aerosol retrieval SYNAER, in Kokhanovsky A. and de Leeuw G., Aerosol Remote Sensing over Land, Springer, Berlin, 2009.

Holzer-Popp, T., SYNAER Validation Report, MACC D_D-SAT_3.1.2, DLR, 2010.

December 2011



Product and service description

Global emission fluxes for 40+ species from open biomass burning based on satellite-based FRP observations in gif, kml, grin and netcdf formats, developed by ECMWF, FZJ, KCL and VUA. The product includes daily averages of fire radiative power (FRP) areal density, combustion rate areal density, species emission areal density over a global coverage, obtained by NRT assimilation of MODIS and SEVIRI data. The product is updated daily within a 10-min delay.

Horizontal resolution: T159 (V0), 0.5 deg (V1.0), 0.1 deg (V1.1).

Available archive: since 2003.

Data are retrievable by web download from the MARS system. Online documentation, data visualisation, extraction example scripts, email support are provided.

Service providers:

ECMWF

<http://www.gmes-atmosphere.eu/fire/>

FZJ

http://macc.icg.kfa-juelich.de:50080/access?catalog=http://macc.icg.kfa-juelich.de:58080/MACC_wildfire

Product generation and validation

See Kaiser et al., 2011.

Quality control

Quality indicators are provided. Quality checks are performed daily, including monitoring of values based on a confidence interval and monitoring of the delivery regularity.

Reference

Kaiser, J. W., Heil, A., Andreae, M. O., Benedetti, A., Chubarova, N., Jones, L., Morcrette, J.-J., Razinger, M., Schultz, M. G., Suttie, M., and van der Werf, G. R. (2011). Biomass burning emissions estimated with a global fire assimilation system based on observed fire radiative power. BGD, 8(4):7339–7398.

Product and service description

As part of the GEMS/MACC analysis and forecast project, UV-radiation has been computed in the IFS model with a dedicated UV-processor (Morcrette and Arola, 2007). Surface irradiance in 5 nm wide spectral intervals is computed on-line within the forecast model, and the UV-index is computed from the distribution of the spectral irradiance using a standard skin response function.

The UV-Index is available from the ECMWF MARS archive.

Product generation and validation

Each step of the development and improvement of the system has been accompanied by comparison against both ground-based and satellite-based UV data, as extensively as possible. During GEMS AER sub-project, prognostic aerosol model was developed for IFS, which has since been coupled with the UV processor. A re-analysis run, including the UV processor with prognostic aerosols, was launched earlier in the MACC project. FMI has carried out a validation work in RAD sub-project, comparing UV processor against ground-based UV data. The special focus has been on the aerosol effect on UV through the prognostic aerosols. Therefore satellite-UV, that does not account properly for absorbing aerosols, has not been included in these comparisons. In addition to UV comparisons, aerosol loading (AOD) and other optical properties (e.g. single scattering albedo) from the processor have been compared against measurements from the Aerosol Robotic Network (AERONET).

Quality control

The version numbering follows the numbering of ECMWF operational cycles.

Reference

Morcrette, J.-J., and A. Arola (2007), A processor to get UV-A and UV-B radiation products in/from the ECMWF IFS. ECMWF Technical Memorandum No.528, 25 pp.

<http://www.ecmwf.int/publications/library/do/references/list/14>



European-scale AQ analysis for every hour of the previous day and forecast for every hour of the next time period up to 72h ahead by EURAD-IM

Product and service description

The comprehensive chemical data assimilation scheme EURAD-IM, developed at the Rhenish Institute of Environmental Research at the University of Cologne provides daily 72h AQ forecasts and AQ analyses for the previous day on a domain covering whole Europe with 15 km horizontal resolution using a Lambert conformal projection. Predicted hourly concentrations of O₃, NO, NO₂, CO, SO₂, total NMVOC, PM_{2.5}, PM₁₀, and concentrations of the particulate matter constituents SO₄²⁻, NO₃⁻, NH₄⁺, secondary organics, sea salt, mineral dust and primary anthropogenic material as well as analysed hourly concentrations of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ are regularly delivered in NetCDF format. Physical dimension of gas phase and aerosol phase species is ppb and µg/m³, respectively. The air pollutant concentrations are available on 23 non-equidistant terrain following layers between the surface and 100 hPa. Thickness of the near surface layer is about 35 m, 16 layers are below 3000 m.

Hourly concentrations of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ are also available in grib2 format on a latitude/longitude grid covering the region from 15° W to 35° E and 35° N to 70° N with a resolution of 0.15° x 0.125° in the near surface layer and at 500 m, 1000 m, 3000 m, and 5000 m. Physical dimension of air pollutants in grib2 format is kg/m³.

The EURAD-IM AQ forecast and analysis is used for the generation of ensemble products and for public information purposes.

Product generation and validation

The European-scale pre-operational air quality forecast has been set up using the continental-to-local scale chemical data assimilation system EURAD-IM (Hass, 1991, Ackermann et al., 1998, Memmesheimer et al., 2004, Friese and Ebel, 2010). This model system consists of 5 major parts: the meteorological driver MM5, the pre-processors ECP and PREP for preparation of meteorological fields and observation data, the emission model EEM and the chemistry transport model EURAD-IM. The data flow of the EURAD-IM system is depicted in Figure 1. EURAD-IM is a meso-scale chemistry transport model involving transport, diffusion, chemical transformation, wet and dry deposition and sedimentation of tropospheric trace gases and aerosols. It includes 3d-var and 4d-var chemical data assimilation (Elbern et al., 2007) and is able to run in nesting mode.

Based upon the IFS operational meteorological forecast from 12:00 UTC of the previous day, a 72h forecast of key air pollutants is regularly delivered. Predicted concentrations of O₃, NO, NO₂, SO₂, PM_{2.5}, and PM₁₀ contribute to a multi-model ensemble forecast. Chemical initial values are provided by the EURAD-IM pre-operational 3d-var analysis for the previous day. Chemical boundary values are taken from the pre-operational global MOZART-IFS air quality forecast (MACC sub-project G-RG). Concentration fields are currently available at about 04:00 UTC at ECMWF for further processing. Results are accessible on the MACC web page.

Based upon the IFS operational meteorological forecast from 00:00 UTC, an analysis of the concentrations of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ is daily delivered. Chemical initial values are provided by the EURAD-IM 3d-var analysis of the previous day. Chemical boundary values are taken from the pre-operational global MOZART-IFS air quality forecast. NRT MACC-RAQ surface in-situ measurements of O₃, NO, NO₂, CO, SO₂, PM_{2.5}, and PM₁₀ as well as NO₂ columns retrievals from OMI, GOME-2, and SCIAMACHY are assimilated every full hour using intermittent 3d-var. Concentration fields are currently available at about 02:00 UTC at ECMWF for further processing. Results are accessible on the MACC web page.

For the forecast as well as analysis, emission input data are derived from the newly available 2005 TNO emission inventory.

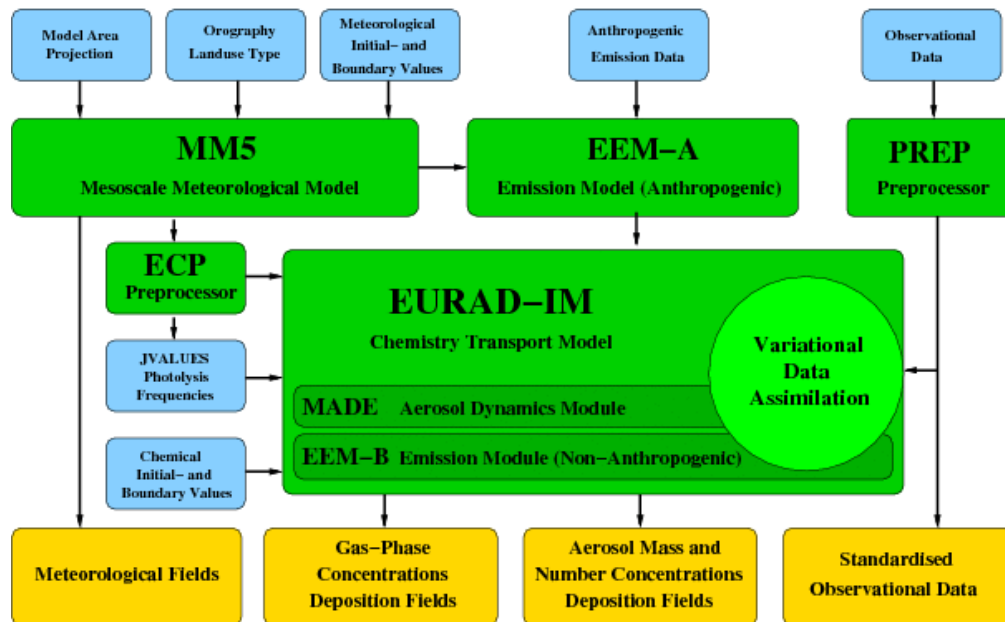


Figure 1: Flowchart of the EURAD-IM model system containing the meteorological driver MM5, the pre-processors ECP and PREP, the emission model EEM and the chemistry transport model EURAD-IM (input parameters are shaded in blue, output parameters are shaded in yellow and procedural parts are shaded in green).

Results of the EURAD-IM AQ forecast are validated on a daily basis on the MACC-RAQ webpage and are compared to results of the ensemble forecast system in quarterly QC/QA dossiers. The MACC-RAQ NRT data is used for verification. This data consists of surface in situ measurements of O₃, NO₂, SO₂, CO, PM_{2.5}, and PM₁₀ from an increasing number of European countries. Quality indicators used for validation are bias, modified mean bias, root mean square error, fractional gross error, and correlation (Jolliffe and Stephenson, 2003). Averaged quality indicators are displayed on the MACC-RAQ webpage for the next 72h forecast period and as time-series at 03:00 UTC and 15:00 UTC for the last week and for the last three months. Figure 2 exhibits exemplary quality indicators taken from the EURAD-IM QC/QA dossier for September to November 2010.

The EURAD-IM AQ service is validated against the MACC User Requirements Document.

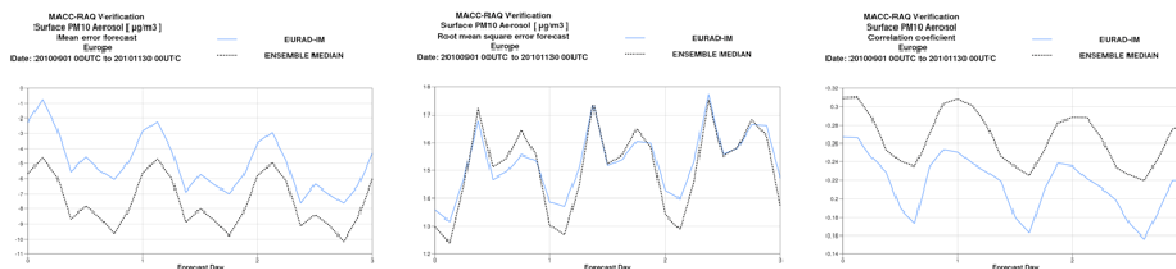


Figure 2: Bias (left), root mean square error (middle), and correlation (right) of near surface PM₁₀ concentrations averaged over the time span from September 1 to November 31, 2010. Blue: EURAD-IM forecast, black: MACC-RAQ ensemble forecast.

Quality control

The supervisor monitor scheduler developed at ECMWF is used to control the production of the daily EURAD-IM AQ forecast and AQ analysis. SMS enables users to run a large number of programs in a controlled environment. It provides reasonable tolerance for hardware and software failures, combined with good restart capabilities.

SVN, a revision control system, is used to document changes of the EURAD-IM source code. Changes of the AQ service are reported in the quarterly EURAD-IM QC/QA dossiers. Furthermore, the dossiers provide performance and availability statistics. The performance statistic consists of graphical representations of mean quality indicators (bias, root mean square error, and correlation) for predicted near surface O₃, NO₂, and PM₁₀ concentrations.

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Elbern, H., A. Strunk, H. Schmidt, and O. Talagrand, Emission rate and chemical state estimation by 4-dimensional variational inversion, *Atmos. Chem. Phys.*, **7**, 1-59, 2007.

Friese, E. and A. Ebel, Temperature dependent thermodynamic model of the system H⁺-NH₄⁺-Na⁺-SO₄²⁻-NO₃⁻-Cl⁻-H₂O, *J. Phys. Chem. A*, **114**, 11595-11631, 2010.

Hass, H., Description of the EURAD Chemistry-Transport-Model version 2 (CTM2), vol 83, Mitteilungen aus dem Institut für Geophysik und Meteorologie der Universität zu Köln, 1991.

Huijnen, V. et al., Comparison of OMI NO₂ tropospheric columns with an ensemble of global and European regional air quality models, *Atmos. Chem. Phys.*, **10**, 3273-3296, 2010.

Jolliffe, I. and D. Stephenson, Environmental Forecast Verification: A Practitioner's Guide in Atmospheric Science, Wiley, 2003.

Martynenko, D. et al., Understanding the aerosol information content in multi-spectral reflectance measurements using a synergetic retrieval algorithm, *Atmos. Meas. Tech.*, **3**, 1589-1598, 2010.

Memmesheimer, M., E. Friese, A. Ebel, H. J. Jakobs, H. Feldmann, C. Kessler and G. Piekorz, Long-term simulations of particulate matter in Europe on different scales using sequential nesting of a regional model, *Int. J. Environm. and Pollution*, **22**, (1-2), 108-132, 2004.

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Strunk, A. et al., Using Satellite Observations for Air Quality Assessment with an Inverse Model System. In: Numerical Methods and Applications, Lecture Notes in Computer Science, Eds. I. Dimov, S. Dimov., and N. Kolkovska, Volume 6046, 174-181, 2011.



Origin of forecasted pollution episodes (graphic presentation)

Product and service description

Following the source-receptor (SR) methodology described in Wind et al. (2004), a system for the estimation of country allocated contributions to forecasted air pollution episodes (or air quality emergencies) has been implemented. The system is based on the MACC pre-operational 3-day forecast set-up of the Unified EMEP model.

In practice, when a severe air pollution episode is forecasted by the MACC system, calculations of source-receptor relationships can be performed on request. A user interface has been set up at http://www.emep.int/gmes/macc_opol.html. On the same page one also finds examples of source-allocation diagrams.

One example of country-allocated forecasts is shown in the next section, where the newly developed tools have been applied to an Air Pollution episode in the past. They were presented at the 1st policy user workshop under the lead of EIONET in Dessau in October 2010.

Product generation and validation

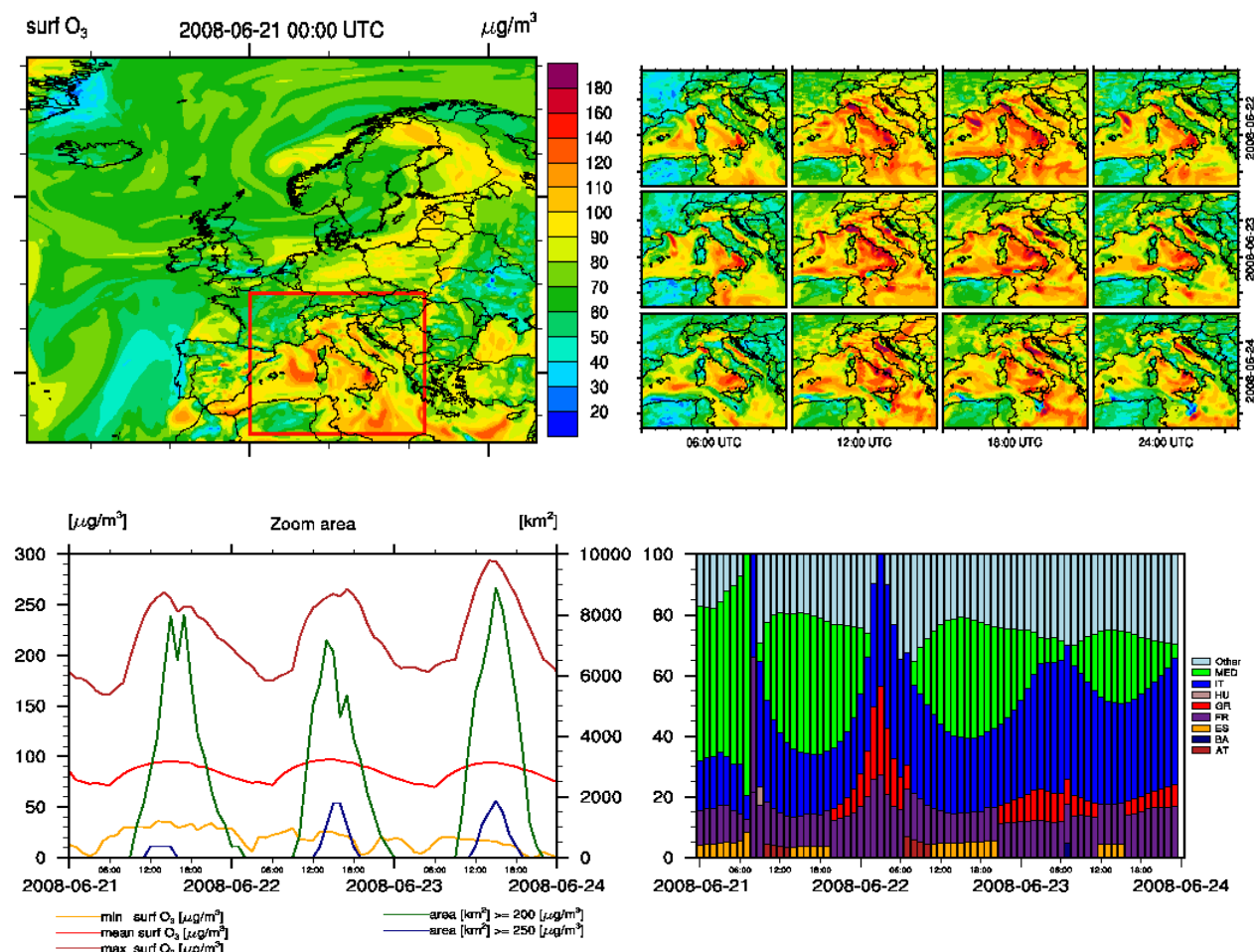
The system for the estimation of country allocated contributions to forecasted air pollution episodes was developed within MACC. The current SR ensemble includes more than 200 forecasts performed by the EMEP/MS-CW model for each single day. In each run the emissions are reduced for one specific country and one emitted component at a time. Through a post-processing procedure the percentage contribution from each country to a given air quality episode can be calculated.

For a given episode, two sets of SR forecast ensembles can be defined:

- Quick response: SR ensemble initialized at the first day of the episode. This ensemble is dedicated to identifying the potential effect of reductions implemented as soon as the episode is forecasted.
- Attribution: SR ensemble initialized 20 days before the first day of the episode. This ensemble is dedicated to allocating the main precursor areas, over the weeks leading to the episode.

As an example, the figure below shows horizontal plots of the forecast of the high ozone episode in 2008, regenerated with the EMEP model in the upper two panels. The right panel shows the zoomed area (receptor area) for the three days of the forecast and for different times of day. The lower left panel shows time evolutions of main pollutants in the receptor area. The contributors to the receptor area, and the time evolution of their relative contributions are shown in the lower right panel.

3-day Forecast O₃ Episode



Quality control

The EMEP/MSC-W model is evaluated regularly against a large set of measurements. Evaluation reports can be found at <http://www.emep.int>

The model is also continuously evaluated within the MACC project. Quarterly model dossiers are available through MACC.

Reference

Wind, P., D. Simpson & L. Tarrasón, Source-receptor calculations. In Transboundary acidification, eutrophication and ground level ozone in Europe. EMEP Status Report 1/2004, The Norwegian Meteorological Institute, Oslo, Norway, 2004, 49-75.



Global CO₂ source and sink inversions

Product description

The space-time gradients of CO₂ mixing ratios in the atmosphere are determined by CO₂ exchange with the Earth's surface and by atmospheric transport. Thus the joint availability of atmospheric measurements of CO₂ mixing ratios and of numerical models of the atmospheric transport allows the inference of CO₂ surface fluxes over the globe. The present MACC product relies on the flux inversion scheme of Chevallier et al. (2005) that implements Bayesian estimation in the form of the minimization of a cost function. The inversion system computes the Best Linear Unbiased Estimate (BLUE) of the CO₂ surface fluxes given the input information, their Bayesian uncertainty, and the number of degrees of freedom for signal (Chevallier et al. 2007). The BLUE fluxes are simply called inverted fluxes hereafter.

The inversion system has been operated for the period 2000-2010, with surface air-sample measurements as input observations. Fluxes are estimated on a global longitude-latitude grid of regular mesh 3.75°x2.5° at a temporal resolution of 8 days, with day-time and night-time separated. 3-hourly variations within the 8-day segments are prescribed a priori in the inversion. Prior fluxes come from the combination of a flux climatology, of emission inventories and of a model simulation as described in Chevallier et al. (2010). The operator that links the flux space and the retrieval space in the inversion scheme is the general circulation model of the Laboratoire de Météorologie Dynamique (LMDZ, Hourdin et al. 2006), nudged to ECMWF winds. Tracer transport is simulated on the same 3.75°x2.5° horizontal grid as the fluxes with 19 layers between the surface and the top of the atmosphere. The prior initial conditions (i.e. the 3D field of CO₂ at the start of the inversion window) are taken from the global analysis of surface air-sample measurements for the period 1988-2008 made by Chevallier et al. (2010). They are adjusted within the inversion. The present inversion configuration follows the one used by Chevallier et al. (2010) with only minor adaptations to process years 2009 and 2010.

Product validation

The evaluation of this product is based on 1) comparison with the fluxes from other inversions, and 2) comparison of CO₂ mixing ratios calculated from the inverted fluxes with independent aircraft measurements. In particular, the latter test confirms that the inversion has improved the quality (i.e. reduced the uncertainty) of the surface fluxes compared to the assumed or prior fluxes. The product quality is documented by the associated Bayesian uncertainty, that can be provided on demand for any space-time target, from the grid-point weekly scale to the annual global scale. The realism of this uncertainty estimate has been demonstrated with independent data.

References

Chevallier, F., et al. (2005), Inferring CO₂ sources and sinks from satellite observations: method and application to TOVS data. *J. Geophys. Res.*, 110, D24309, doi:10.1029/2005JD006390.

Chevallier, F., F.-M. Bréon, P. J. Rayner (2007), The contribution of the Orbiting Carbon Observatory to the estimation of CO₂ sources and sinks: Theoretical study in a variational data assimilation framework. *J. Geophys. Res.*, 112, D09307, doi:10.1029/2006JD007375.

Chevallier, F., et al. (2010), CO₂ surface fluxes at grid point scale estimated from a global 21-year reanalysis of atmospheric measurements. *J. Geophys. Res.*, 115, D21307, doi:10.1029/2010JD013887.

Hourdin, F., et al. (2006), The LMDZ4 general circulation model: climate performance and sensitivity to parametrized physics with emphasis on tropical convection, *Climate Dynamics*, 27, 787-813, doi:10.1007/s00382-006-0158-0.

December 2011



Product and service description

Meteosat images are received at DLR. This station is external to the service SOLEMI and acts as a provider of images. Images are quality-controlled for all channels. They are then cut into overlapping tiles, which are stored into a database. This database is part of the DIMS system of DLR (Data Information and Management System).

The SOLEMI service exploits data every 30 min for the Meteosat and every 15 minutes for the Meteosat Second Generation satellites. The processing to produce an irradiance product is made only on-request. Standard requests are for time-series for a given site, or for maps. Inputs are latitude, longitude, and elevation of the site of interest.

Meteosat visible images are extracted from DIMS and calibrated. For MSG, the two images in the visible band are combined to create an image of broadband radiance (Cros et al., 2006). Other inputs to the method Heliosat-2 in SOLEMI (Rigollier et al., 2004) are aerosol properties, total water column, and total column ozone. These parameters are read from databases containing monthly or daily values and interpolated for the day under concern if needed. The clear-sky irradiance is computed by the Bird model (Bird et al., 1981). Using a database of ground albedo, the cloud-index, then the clear-sky index, and finally the irradiance are computed. Products are created by aggregating irradiance values over the requested aggregation period, e.g., hour, day, month.

Product generation and validation

The principles of Heliosat rely on the fact, that in most cases, a cloud exhibits a larger reflectance than the ground. The magnitude of the difference between both targets is related to the depletion of the downwards radiation by the atmosphere. Heliosat comprises a modelling of the SSI that should be observed by the sensor if the sky were cloud-free for any pixel. The method Heliosat is divided into two parts regarding the physical modelling: converting the satellite image into a cloud index and converting the cloud index in irradiance.

Rigollier et al. (2004) designed Heliosat-2 using calibrated Meteosat images instead of gray values. The irradiance is the irradiance for the clear-sky case multiplied by the clear-sky index quantifying cloud extinction. The clear-sky index is derived from a cloud index comparing the pixel's reflectance versus brightest clouds and the ground. The cloud index is close to 0 when the observed reflectance is close to the ground reflectance, i.e., when the sky is clear. The cloud index increases as the clouds are appearing. It can be greater than 1 for clouds that are optically very thick. An empirical relationship was derived from coincident ground measurements linking cloud index and clear-sky index.

The clear-sky model for SOLEMI is the model of Bird (Bird et al., 1981) requiring auxiliary input on aerosols, water vapour and ozone. SOLEMI currently is an on request processing, so different aerosol data sets are selected based on comparisons with local ground data (if available) or on a regional basis (e.g. GACP and Aerocom tend to match better in European areas whereas MATCH/DLR showed best results on the Arabian Peninsula).

A daily total water vapour column data set of the NCEP/NCAR-Reanalysis of the Climate Diagnostic Center (CDC-NOAA) with a spatial resolution of $2.5^{\circ} \times 2.5^{\circ}$ is used. For ozone, a data set from the Total Ozone Mapping Spectrometer (TOMS) sensor is used. The derived ozone columns from the level 2 product are gridded into a 1° latitude by 1.25° longitude level product. As the daily products only have a 90 % coverage and the influence of ozone is relatively small, a monthly data set is used.

Quality control

There are a number of control points in the workflow for monitoring the smooth running of the processing. Each time a failure is observed, reporting is made.

A manual inspection of the product is made based on scientific experience, taking into account the history available in the archive. Such procedures include comparing monthly means, e.g. all months of January in a period spanning several years, or comparing annual patterns and frequency distributions of single years against each other. If larger areas are processed a visual inspection of satellite raw data in movies is done.

Comparison between irradiance products and measurements at ground by well-calibrated instruments is made as often as possible. This is not systematic as the access to such data is limited. The results of such comparisons are used:

- to document the uncertainty in the retrieval displayed on the Web site,
- to detect possible flaws in the method or processing workflow, and correct them.

The usual way of assessing the quality of retrievals of SSI derived from satellite images is to compare these SSI to coincident measurements performed at ground level. The typical accuracy of SSI measured in the global meteorological network is 3 to 5 % in terms of root mean square error. Therefore, the ground measurements can be seen as an accurate reference against which one may compare the SSI derived from satellite.

However, the actual situation is not that simple. Several limitations exist that make the assessment of the quality of retrieved irradiances a very difficult task. Zelenka et al. (1999) analyzed the real accuracy of satellite estimations of hourly SSI. They suggest that for a relative deviation of 23 % (root mean square error) between ground measurements and satellite estimations, only half of it is due to the estimation method itself. The difference comes from:

- error on the measurements provided by the pyranometer (3 to 5 %);
- error due to the spatial variability of solar radiation within the pixel (5 to 8 %)
- error due to spatial and temporal heterogeneity of the compared data, e.g. assuming ergodicity (3 to 5 %).

Guidelines of the benchmarking procedures of solar radiation products derived from satellite data, have been proposed by the MESoR project, in order to measure the quality of these products with a common scheme (Beyer et al., 2008). The quality of a product is defined by various statistical quantities that measure the discrepancies between products and ground data considered as a reference.

References

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Cros S., Albuisson M., Wald L., 2006. Simulating Meteosat-7 broadband radiances at high temporal resolution using two visible channels of Meteosat-8. *Solar Energy*, 80, 3, 361-367, doi: 10.1016/j.solener.2005.01.012.

Rigollier C., Bauer O., Wald L., 2000. On the clear sky model of the 4th European Solar Radiation Atlas with respect to the Heliosat method. *Solar Energy*, 68(1), 33-48.

Product and service description

Meteosat images are received every 15 min by Armines. Only the two channels in the visible band are kept. The images are stored into a database. The near-real-time processing is triggered at the end of the day by the reception of the last images at 21:00 UT. The first operation is the control of the quality of Meteosat images. It consists in looking for the missing lines if any and in the check of the position of extreme lines and columns in each image. If a failure is observed, the processing stops.

Meteosat images are calibrated using the calibration coefficients supplied in the flow emitted by Meteosat, resulting into two images of radiance every 15 min. MSG visible images are then combined to create an image of broadband radiance (Cros et al. 2006).

Inputs to the method Heliosat-2 are the latitude, longitude, and elevation of the current pixel. Another input is the Linke turbidity factor characterising the optical state of the clear atmosphere. It is read from a database containing monthly values and interpolated for the day under concern. The clear-sky irradiation for the 15 min period is computed by the ESRA model, (Rigollier et al., 2000; Geiger et al., 2002). Then, using a database of ground albedo, the cloud-index, then the clear-sky index, and finally the irradiation G15 for the 15 min period are computed. The irradiation is stored in the HelioClim-3 database.

Request for products are made through the Web site of the SoDa Service (www.soda-is.com). There are two types of requests: manual and automated. Manual requests are made by the means of a browser. Automated requests are emitted by computers. They typically request for hourly values of irradiance every day for large numbers of geographical sites.

A request can be for a time-series (the standard product) or for a map. For the time-being, the processing is the same; a map is considered as made of independent pixels that are processed separately.

Automated requests are processed in the same way than the manual requests, except that their processing is part of the near-real-time processing and takes part immediately after the updating of the HelioClim-3 database.

Product generation and validation

The principles of Heliosat rely on the fact, that in most cases, a cloud exhibits a larger reflectance than the ground. The magnitude of the difference between both targets is related to the depletion of the downwards radiation by the atmosphere. Heliosat comprises a modelling of the SSI that should be observed by the sensor if the sky were cloud-free for any pixel. The method Heliosat is divided into two parts regarding the physical modelling: converting the satellite image into a cloud index and converting the cloud index in irradiance.

Rigollier et al. (2004) designed Heliosat-2 using calibrated Meteosat images instead of gray values. The irradiance is the irradiance for the clear-sky case multiplied by the clear-sky index quantifying cloud extinction. The clear-sky index is derived from a cloud index comparing the pixel's reflectance versus brightest clouds and the ground. The cloud index is close to 0 when the observed reflectance is close to the ground reflectance, i.e., when the sky is clear. The cloud index increases as the clouds are appearing. It can be greater than 1 for clouds that are optically very thick. An empirical relationship was derived from coincident ground measurements linking cloud index and clear-sky index.

The database HelioClim-3 is constructed by the means of the clear-sky model ESRA (European Solar Radiation Atlas). It is based on Kasten's (1996) Rayleigh optical depth parameterization and the Linke

turbidity factor at air mass 2. Details can be found in Rigollier et al. (2000) with revision proposed by Page and Remund and reported in Geiger et al. (2002).

Quality control

There are a number of control points in the workflow for monitoring the smooth running of the near-real-time processing. Each time a failure is observed, detailed reporting is made to the management, written in a log file and sent by e-mail as well. A visual monitoring is in place to perform visually a gross check of the computed irradiance. It comprises a graph of the irradiances for the last two days for three selected sites: Sophia Antipolis where the chain is operated, and two extreme locations in the East and the West on the Equator. A Web page is updated that provides access to the archive of log files and graphs.

Multiple benchmarking activities demonstrated a few biases in the raw irradiation data contained in the database. A posteriori corrections are brought to the raw values. In order to cope with gaps and to compute direct and diffuse components, the clear-sky index is interpolated every minute. ESRA algorithms are used to compute direct and diffuse components from the global irradiance every minute. Finally, the 1-min values are summed up to yield the requested aggregation period, e.g. hour, day, month.

Comparison between irradiance products and measurements at ground by well-calibrated instruments is made as often as possible. This is not systematic as the access to such data is limited. The results of such comparisons are used:

- to document the uncertainty in the retrieval displayed on the Web site,
- to set up a posteriori correction procedures if possible, to improve the quality,
- to detect possible flaws in the method or processing workflow, and correct them,

to establish the model of uncertainty allowing to allocate uncertainty values to each irradiance value.

The usual way of assessing the quality of retrievals of SSI derived from satellite images is to compare these SSI to coincident measurements performed at ground level. The typical accuracy of SSI measured in the global meteorological network is 3 to 5 % in terms of root mean square error. Therefore, the ground measurements can be seen as an accurate reference against which one may compare the SSI derived from satellite.

However, the actual situation is not that simple. Several limitations exist that make the assessment of the quality of retrieved irradiances a very difficult task. Zelenka et al. (1999) analyzed the real accuracy of satellite estimations of hourly SSI. They suggest that for a relative deviation of 23 % (root mean square error) between ground measurements and satellite estimations, only half of it is due to the estimation method itself. The difference comes from:

- error on the measurements provided by the pyranometer (3 to 5 %);
- error due to the spatial variability of solar radiation within the pixel (5 to 8 %)
- error due to spatial and temporal heterogeneity of the compared data, e.g. assuming ergodicity (3 to 5 %).

Guidelines of the benchmarking procedures of solar radiation products derived from satellite data, have been proposed by the MESoR project, in order to measure the quality of these products with a common scheme (Beyer et al., 2008). The quality of a product is defined by various statistical quantities that measure the discrepancies between products and ground data considered as a reference.

References

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Kasten F., 1996. The Linke turbidity factor based on improved values of the integral Rayleigh optical thickness. *Solar Energy*, 56 (3), 239-244.

Rigollier C., Bauer O., Wald L., 2000. On the clear sky model of the 4th European Solar Radiation Atlas with respect to the Heliosat method. *Solar Energy*, 68(1), 33-48.

December 2011



Product and service description

Setting up an operational information system with new capabilities and new processing methods is a lengthy process spanning over a few years. In order to exploit as soon as possible and efficiently the outcomes of the MACC project and other initiatives as they are flowing, a number of intermediate steps are being taken to implement these outcomes. Actually, it is too early to describe in detail many aspects of the transition chains and the operation chain in the RAD-SOLAR Service. An overview can be provided only.

Several data on atmospheric conditions (clouds, aerosol, water vapour, and ozone) and ground albedo will be received from various sources, pre-processed and stored in several databases. These intermediate databases (or tables) will constitute the HelioClim-4 database.

The delivery deadline from each source is still unknown. It could amount to several days. Therefore, the term 'near-real-time' has to be interpreted as within 24 hours (preferably) or longer. Operations are triggered by successfully received input data sets.

Currently, the concept to produce products is that the processing is made on-request (on-the-fly). When a request is made for a time-series for a given site and a given period, the irradiance processor will invoke the McClear model with inputs extracted from the database "atm". Extinction coefficients are then obtained by the cloud processor using inputs from the database "cloud". Finally, the contribution to the diffuse irradiance due to the ground albedo is computed.

Tests have been made that demonstrate that such an on-the-fly processing is sustainable in the perspective of the RAD-SOLAR Service. Nevertheless, it is likely that databases of irradiance will be pre-computed, at least to best answer to request for maps of daily or monthly values of irradiance.

Presently, there are two series of products in the RAD-SOLAR Service:

- ARCH products: the first series is an archive: 1984-2005, based on Meteosat First Generation (MFG) data. It is denoted by the letters ARCH (for Archive),
- MSG products: the second series is based on Meteosat Second Generation (MSG) series of satellites, starting from 2004 and on-going. It is denoted by the letters MSG.

For both series currently available, core products in the RAD-SOLAR Service are time-series of solar radiation available at ground surface, also called surface solar downward irradiance (SSI).

This includes the total global irradiance (GHI), i.e., the SSI integrated over the whole spectrum available at ground level, on a horizontal surface; the total diffuse irradiance (DifHI), i.e., the diffuse part of the SSI integrated over the whole spectrum available at ground level, on a horizontal surface; and total direct (beam) irradiance (DirHI), i.e., the direct part of the SSI integrated over the whole spectrum available at ground level, on a horizontal surface.

From a practical point of view, and beyond the various issues related to being a recognised customer of the information system, the inputs by users needed to trigger a request for a selected MACC product will be:

- the geographical coordinates of the site of interest, or the name of this site,
- the elevation of this site above sea-level. By default, the application uses well-known digital elevation models, such as NASA-SRTM,
- the period of time: begin data, end date.

Delivery deadline is the time lag between the moment the request is made and the instant of delivery. The delivery deadline depends on the series of products: ARCH or MSG.

The ARCH products are computed on request and are not available as such on the shelf. Once the request for a product is made, DLR, the author of the products ARCH, selects the best suitable auxiliary data set for the site among global atmospheric data sets (aerosol, water vapour, ozone) from different earth observation sources and climate models. The atmospheric data is gridded to a resolution of $1^\circ \times 1^\circ$ and the cloud data from Meteosat has a nominal resolution of 2.5 km x 2.5 km at the sub satellite point. The geographical coordinates (latitude, longitude and height above sea level) in decimal degrees and meters have to be delivered to DLR. The product is delivered per e-mail within two weeks.

The MSG products are computed on-the-fly from the database HelioClim. The request is made through the Web site of the SoDa Service (www.soda-is.com) and the answer is provided within a few minutes.

Product generation and validation

The new Heliosat-4 method is based on the principle that the SSI for a cloudy atmosphere can be considered as equal to the product of the irradiance obtained under a clear sky and a function modelling the extinction of the radiation by clouds and the contribution due to the ground albedo. The possibility of considering several spatial and temporal resolutions is of practical importance in MACC. MACC outcomes should be daily values or every 3 h but by no means every hour. The expected spatial resolution should be in the range 50 km - 200 km. The cloud properties can be derived from the processing of Meteosat images as done by DLR with the adapted APOLLO chain. Such products will be available every 15 min for each Meteosat pixel.

Recent initiatives from NCAR (USA, MATCH scheme) and the EU-funded project GEMS yielded to more accurate and detailed assessments of optical properties of the aerosols with capability of producing daily maps. MACC will produce aerosol properties using a method similar or enhanced if compared to GEMS. Therefore, the expertise gained with these GEMS products will be efficiently used in the RAD-SOLAR Service.

In the meantime, other parameters such as the column content in water vapour or ozone are available daily over the world. MACC is producing such parameters as well as other sources. In the same manner than for the aerosol properties, these recent results will be ingested.

The availability of these atmospheric parameters as well as the increase in computing power advocate for an increase in the complexity of the models used to compute the clear-sky models, which should result in an increase in accuracy. Such a model is being developed, called McClear. Inputs to this model will be outputs from MACC, except for site coordinates, solar angles, elevation, atmospheric profile, and ground albedo. The current ESRA model will be replaced by this new model McClear. This will be a major step towards the operational RAD-SOLAR Service. It will lead to major changes in the workflow though it is too early to provide details.

Quality control

A quality control must be performed everyday by comparing the core products to measurements performed by ground stations and to re-analyses. The first aim of this quality control is to monitor possible trends in products and decide for appropriate corrections. In that sense, what is important is the change of differences between products and measurements or re-analyses with time outside the expected range of variation. To do so, a model should be available that explains these discrepancies as a function of known explanatory variables such as the solar zenithal angle or the temporal variability of the SSI. Therefore, the distance between products and re-analyses can be predicted. It will be used to monitor the quality of products: large values should indicate suspect products.

The second aim of this quality control is to perform a benchmarking of the products against a reference. This can be done only with quality-proven measurements. By comparison, one will obtain the uncertainty parameters synthesizing the difference between products and reference following the methodology

recommended by the projects IEA SHC 36 and MESoR. These uncertainty parameters will be displayed on the Web pages of the RAD-SOLAR Service to support the documentation on the quality of products.

Based on the results of such comparisons, a model of uncertainty can be established or improved that provides for any instant the plausible uncertainty level of the SSI, given known explanatory variables.

To perform the quality control, operations should be established to collect in an automatic way re-analyses values from ECMWF and ground measurements from selected sites or from the World Radiation Data Center. Quality control procedures must be also implemented that apply onto these measurements and re-analyses.

Reference

User's Guide to the SODA and SOLEMI services – Towards the solar energy radiation resources RAD-SOLAR service, deliverable D_R-RAD_2.2_1, v1.0, MACC project.

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Product and service description

Biomass burning emissions of carbon & various trace species based on observed Burnt Area (BA) for 2010 (GFED3.1). Dry matter combustion rate, species emission, burnt area monthly averages derived from various observational data, mostly MODIS aboard Terra and Aqua (LEO).

Temporal coverage: 1997-2010.

Global coverage.

0.5 deg x 0.5 deg resolution.

Data retrievable via web download from MARS.

Service providers:

VUA

<http://www.falw.vu/~gwerf/GFED/index.html>

ECMWF

http://gmes-atmosphere.eu/about/project_structure/input_data/d_fire/

Contact: guido.van.der.werf@falw.vu.nl

Product generation and validation

See van der Werf et al., 2010.

Quality control

See van der Werf et al., 2010.

Reference

van der Werf et al., Global fire emissions and the contribution of deforestation, savanna, forest, agricultural, and peat fires (1997–2009), ACPD Vol. 10, 2010.

PROJECT:	MACC	Monitoring Atmospheric Composition and Climate
SUB-PROJECT / CLUSTER:	MAN	Management and System Engineering
WORK PACKAGE / TASK:	MAN_3	System engineering for the GMES Atmospheric Service
DELIVERABLES:	D_MAN_3.5 (b), D_MAN_3.6, D_MAN_3.7	