



GSE – PROMOTE
C6 Validation Report

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TITLE:

GMES SERVICE ELEMENT
PROMOTE
C6 Validation Report
AIR QUALITY RECORDS SERVICE
Version 1



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C6 Validation Report

AQ Records

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DOCUMENT CHANGE RECORD

Issue	Date	Modified Items / Reason for Change
Version 1		
0.1	22.02.2007	Draft document created
0.2	22.03.2007	Implementation of SLA requirements in draft document
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Version 2		
1.05	20.03.2008	Reception validation plan
1.1	09.05.2008	template updated and distributed
1.2	21.05.2008	document updated (KNMI, RIU, IUP, BIRA)
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LIST OF ACRONYMS

3DVAR	three-dimensional variational data assimilation
ADEME	Agence De l'Environnement et de la Maîtrise de l'Energie
AEROCOM	Aerosol model intercomparison
AERONET	Aerosol sun photometer network
AOD	aerosol optical depth
APOLLO	AVHRR processing scheme for clouds over land and ocean
ARPA	Regional Agency for the Prevention and the Environment
AQ	air quality
BIRA-IASB	Belgian Institute for Space Aeronomy
CREATE	Construction, use and delivery of an European aerosol database
CTM	Chemistry Transport Model
DLR	German Aerospace Centre
DOAS	Differential Optical Absorption Spectrometry
ECMWF	European Centre for Medium-Range Weather Forecasts
EMEP	cooperative programme for monitoring and evaluation of long-range transmission of air pollutants in Europe
EPA	Environmental Protection Agency
EURAD	EUropean Air pollution Dispersion model
FRESCO	Fast Retrieval Scheme for Cloud Observables
GOME	Global Ozone Monitoring Instrument
HDF	hierarchical data format
KNMI	Royal Netherlands Meteorological Institute
LANUV	Environmental Protection Agency of Northrhine-Westfalia
LISA	Laboratoire Interuniversitaire des Systèmes Atmosphériques
LMN	Limb Nadir Matching
LUA	Environmental Protection Agency of Northrhine-Westfalia (now LANUV)
MSG	Meteosat Second Generation
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
NNORSY	Neural Network Ozone Retrieval System
NRT	Near Real Time
OI	optimal interpolation
PM	Particulate Matter
RIU	Rhenish Institute for Environmental Research at the Univ. of Cologne
RIVM	National Institute of Public Health and the Environment
ROSE/DLR	DLR CTM
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CartographY
SYNAER	SYNergetic Aerosol Retrieval
WHO	World Health Organization
WMO	World Meteorological Organization
N/A	Not Available
n.a.	not applicable
n.s.	not specified



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1 AQ RECORDS SERVICE

1.1 Service Summary

Description: Optimal assessments of both background and regional/local air quality conditions and their long term evolution by combining novel satellite data in situ data and model results using data assimilation algorithms.

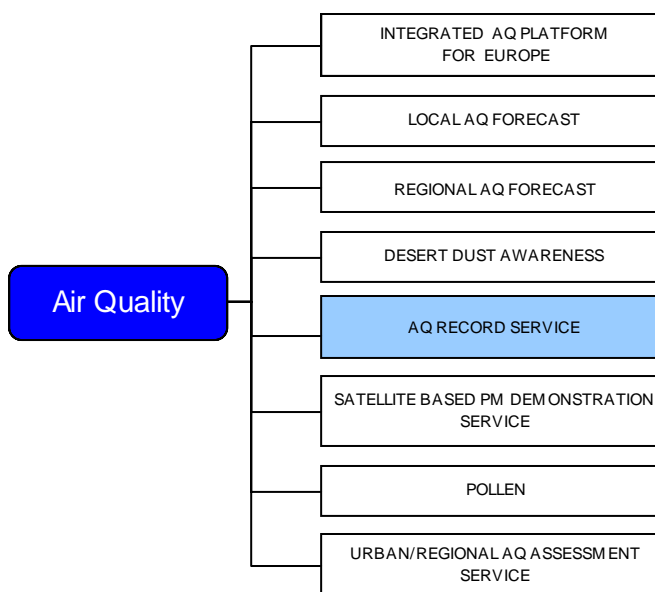


Figure 1.1-1 Structure and position of the AQ Records Service within PROMOTE 2 Air Quality.

Service is/will be operational since/after: Operational since 01/05/2007.

Research partners: University Bremen

Provider: BIRA, DLR, KNMI, RIU

Validation contact: Hendrik Elbern, RIU (e-mail: he at eurad dot uni-koeln dot de)

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1.1.1 Products characterization

The following list of products includes both global and regional concentration fields. Near surface concentration fields are produced by the Regional assimilated near surface pollutants sub-service, while the tropospheric column information for NO₂ and HCHO are produced by the two retrieval sub-services.

NO₂	
Parameter	Near Surface Concentration Field
Typical range	10-500
Determination of the typical range (Method, criteria)	Regulatory monitoring with in-situ measurement stations
Maximum range	0 - n.a.
Units	µg/m ³
<i>Standards</i>	<i>European Directive on atmospheric limit values for SO₂, NO_x, NO₂, PM₁₀ and Pb- 22/04/1999 – 1999/30/CE</i>
NO₂	
Parameter	Tropospheric NO ₂ columns from satellite
Typical range	0 - 20 10 ¹⁵ molecules/cm ²
Determination of the typical range (Method, criteria)	Analysis of historic data
Maximum range	-5 10 ¹⁵ - 200 10 ¹⁵
Units	molecule/cm ²
<i>Standards</i>	<i>none</i>
O₃	
Parameter	Near Surface Concentration Field
Typical range	20-360
Determination of the typical range (Method, criteria)	Regulatory monitoring with in-situ measurement stations
Maximum range	0 - n.a.



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Units	$\mu\text{g}/\text{m}^3$
<i>Standards</i>	<i>European Directive on ambient ozone- 12/02/2002- 2002/03/CE</i>
SO₂	
Parameter	Near Surface Concentration Field
Typical range	10-600
Determination of the typical range (Method, criteria)	Regulatory monitoring with in-situ measurement stations
Maximum range	0 - n.a.
Units	$\mu\text{g}/\text{m}^3$
<i>Standards</i>	<i>European Directive on atmospheric limit values for SO₂, NO_x, NO₂, PM₁₀ and Pb- 22/04/1999 – 1999/30/CE</i>
HCHO	
Parameter(s)	Near Surface Concentration Field
Typical range	0-100
Determination of the typical range (Method, criteria)	Regulatory monitoring with in-situ measurement stations
Maximum range	0 - n.a.
Units	$\mu\text{g}/\text{m}^3$
<i>Standards</i>	<i>n.s.</i>
HCHO observations from Satellite	
Parameter(s)	HCHO Vertical Columns from Satellite (GOME-SCIAMACHY)
Typical range	0-5 10^{16} molec/cm ²
Determination of the typical range (Method, criteria)	Statistical analysis of satellite data and comparison with tropospheric models.
Maximum range	0-1 10^{17} molec/cm ²
Units	molec/cm ²
<i>Standards</i>	<i>none</i>

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CO	
Parameter(s)	Near Surface Concentration Field
Typical range	0-100
Determination of the typical range (Method, criteria)	Regulatory monitoring with in-situ measurement stations
Maximum range	0 - n.a.
Units	mg/m ³
<i>Standards</i>	<i>European Directive on atmospheric limit values for benzene and carbon monoxide in ambient air 16/11/2000 - 2000/69/EC</i>
PM2.5	
Parameter(s)	Near Surface Concentration Field
Typical range	10-300
Determination of the typical range (Method, criteria)	Regulatory monitoring with in-situ measurement stations
Maximum range	0 - n.a.
Units	µg/m ³
<i>Standards</i>	<i>n.s.</i>
PM10	
Parameter(s)	Near Surface Concentration Field
Typical range	10-300
Determination of the typical range (Method, criteria)	Regulatory monitoring with in-situ measurement stations
Maximum range	0 - n.a.
Units	µg/m ³
<i>Standards</i>	<i>European Directive on atmospheric limit values for SO₂, NO_x, NO₂, PM₁₀ and Pb- 22/04/1999 – 1999/30/CE</i>

Table 1.1-1 Characterization of the products provided by the AQ Records service

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1.1.2 Validation plan and validation data

1.1.2.1 Global tropospheric NO₂ Column

Phase 1: N/A

Phase 2: Comparison between tropospheric NO₂ data from SCIAMACHY, OMI and GOME-2. For a few individual sites an comparison with ground data will be performed. The last activity will be extended into phase 3.

1.1.2.2 Tropospheric Formaldehyde Column

Although few ground-based measurements of HCHO are currently available, different data sources can be envisaged to validate HCHO

(1) First within the Network for the Detection of Atmospheric Composition Change (NDACC) several research groups are currently improving their algorithms with the aim to retrieve HCHO total columns and deliver these measurements, in particular for satellite validation purposes. In this context, the integrated EU project GEOMON has for objective to unify and harmonize the main Europeans networks of surface and aircraft-based measurements. One of its tasks is to set up and deliver consolidated FTIR and MAX-DOAS data sets in support of GMES (<http://geomon.ipsl.jussieu.fr/index.html>). In Australia for example, the University of Wollongong (Nicholas Jones) is using a Bomem DA8 since 1994 and has recently produced interesting time-series of HCHO columns. Similarly at Jungfraujoch (Switzerland), the University of Liège is using a Bruker 120HR since 1990 and has recently demonstrated its ability to retrieve HCHO columns. In Bremen-Germany, the IUP (Justus Notholt) perform retrievals with a Bruker 125HR since 2004 and the FTIR observations are complemented by microwave and DOAS measurements. In the tropical region, the same group uses a Bruker 120M for campaign in Paramaribo-Surinam (September/November 2004, February/March, 2005, and October 2005). MAX-DOAS measurements allow retrieving HCHO columns and profiles. Such measurements are currently performed by several groups, among them the Bremen University which operates instruments at a number of stations from the BREMDOM network [see e.g. Wittrock, 2007]. Other MAX-DOAS instruments are expected to complete the observational network for HCHO in the framework of the GEOMON project. For example, measurement campaigns are performed by BIRA-IASB at St Denis, Ile de La Réunion, using ground-based MAXDOAS and FTIR measurements (see figure 1, courtesy of C.Vigouroux, M.De Mazière, F.Hendrick, M.Van Roozendael). The day to day variations are well captured. On October 12, CH₂O enhancement is related to biomass burning in Madagascar. It is well correlated with enhancements observed in other FTIR gases like CO, C₂H₆, and has been confirmed by FLEXPART runs.

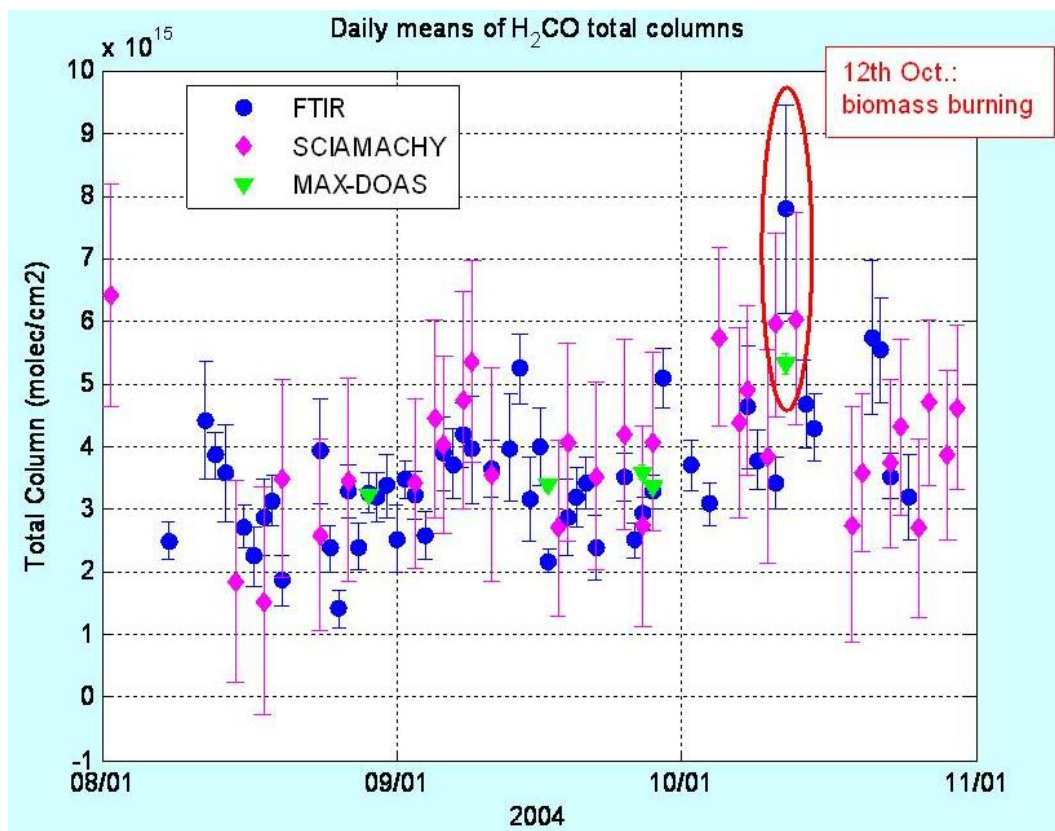


Figure 1.1-2: FTIR retrievals of CH₂O at 2400-3310 cm⁻¹; MAXDOAS retrievals of CH₂O at 336-358 nm between August and November 2004 at St Denis.

(2) In complement to ground-based data, aircraft measurements of HCHO tropospheric profiles can also be used for the validation of satellite column measurements. In particular, several aircraft campaigns have been used to validate the model HCHO profiles used for the AMF calculation. This has been done using composite data sets from a number of airborne observations including PEM-Tropics (1999), Topse (2000), TraceA (1992) and TraceP (2001) [Emmons, 2000]. More recently, the INTEX-A campaign over North America (2004) also provided HCHO profiles suitable for the validation of HCHO AMFs and total columns [Millet, 2004].

(3) Other useful sources of comparison are HCHO profiles obtained from 3D chemical transport models like the IMAGES model [Müller, 1995] or TM model [Heskes, 2003]. As can be seen in Figure 1, consistency checks performed comparing the PROMOTE HCHO data sets with simulations from the IMAGES model show satisfying results for both GOME and SCIAMACHY (Figure 1.1-4).



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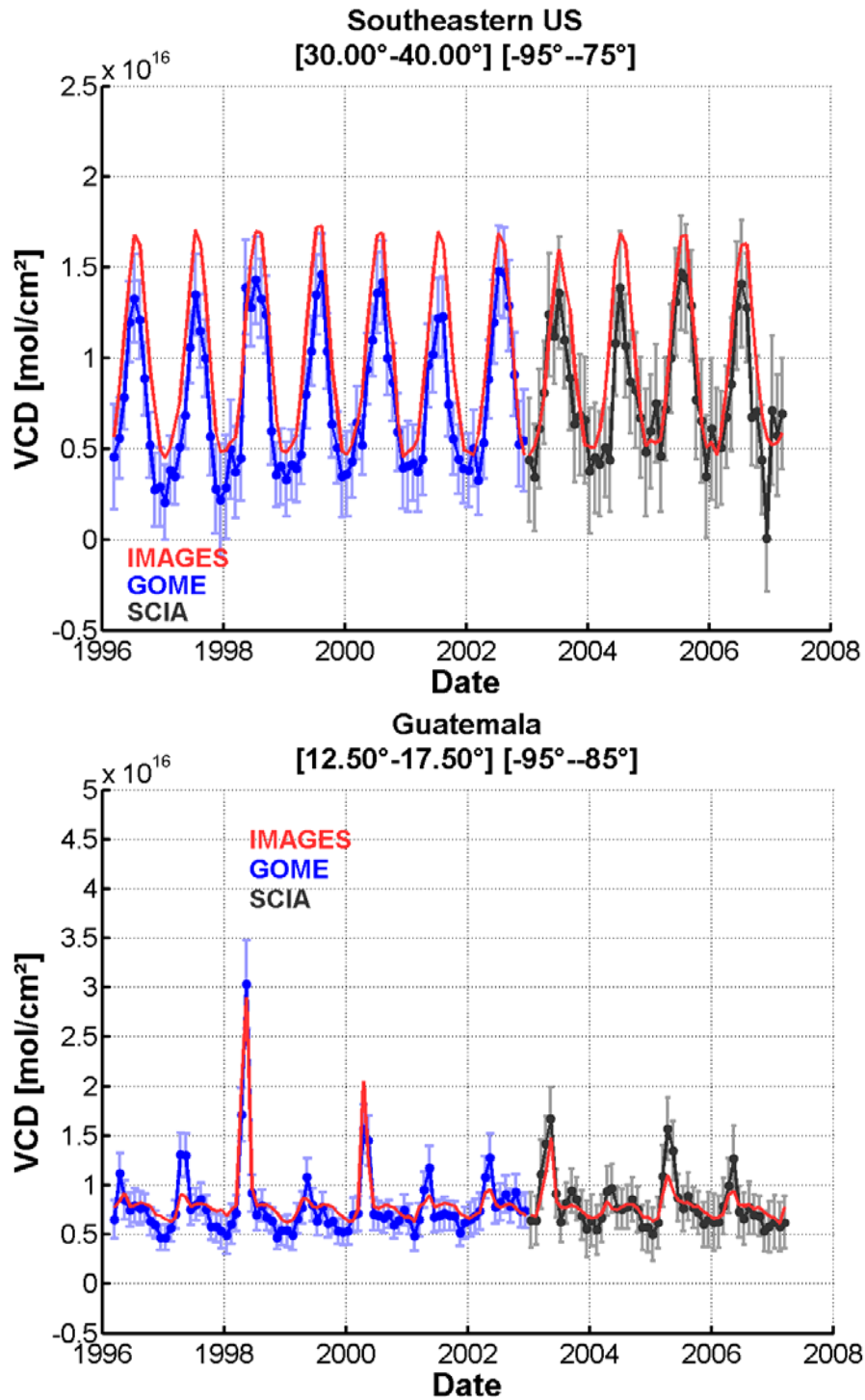


Figure 1.1-3 Comparison between monthly mean HCHO measurements from GOME (in blue)/SCIAMACHY (in black) and IMAGES 3D-CTM (in red)

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(4) Intercomparison exercises with other satellite products are also ongoing: for example with the SCIAMACHY Bremen product in Europe (Wittrock, Dufour) or the GOME Harvard product in Australia (Palmer, Jones). Other satellite measurements as those recently derived from the OMI instrument onboard the AURA platform [Kurosu, 2004] are suitable sources of independent measurements of potential interest for validation purposes.

1.1.2.3 Regional assimilated near surface pollutants

The analysis of daily synoptic maps of key constituents on regular grids over Europe includes ozone, sulphur dioxide, nitrogen dioxide, carbon monoxide, formaldehyde, and particulate matter PM10 and PM2.5. While doing 3d-var data assimilation, the forecast skill and the analysis quality will be evaluated using observed and modelled time series. The strategy selected here is the standard data assimilation validation, performed by the compilation of forecast – observation and analysis – observation statistics. This includes χ^2 -testing.

Evaluation procedure is underway with currently producing data flows for Phase 2. The validation includes studies on background error covariance matrix definition and the characterisation of measurement sites.

The 3d-var system is a reduced algorithm in comparison with the as yet too resource consuming 4d-var chemical data assimilation scheme, the validation of which can be obtained in e.g. Elbern *et al.*, 2007. The 3d-var is of sufficient benefit, when not non-observed species are to be analysed, which are chemically coupled with observed constituents.

VALIDATION DATA	
Ground based observations	
AIRBASE Phase: 1+2	<i>Data availability and access:</i> free; validated database managed by the European Environment Agency which gather measurements from regulatory networks (http://air-climate.eionet.europa.eu/databases/airbase/) <i>Spatial coverage and resolution:</i> EU 25; resolution depends on the pollutants and the country <i>Temporal coverage and resolution:</i> hourly or daily values depending on the pollutant updated on an annual basis <i>Location(s) (coordinates):</i> N/A <i>Accuracy:</i> in line with the accuracy asked by the Directives
In-situ observations	
Airplane measurements Phase: 1+2	<i>Data availability and access:</i> via campaigns (within the OMI validation programme, MOZAIC) <i>Spatial coverage and resolution:</i> global <i>Temporal coverage and resolution:</i> n.s. <i>Location(s) (coordinates)/orbits:</i> South-East USA, global Accuracy: N/A
EO Data	

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Name SCIAMACHY Phase: 1+2	<i>Data availability and access:</i> since October 2002 via KNMI <i>Spatial coverage and resolution:</i> Global coverage each 6 days <i>Temporal coverage and resolution:</i> Daily at 10.00 local time <i>Location(s) (coordinates)/orbits:</i> all orbits <i>Accuracy:</i> 40-100 %
Name OMI Phase: 1+2	<i>Data availability and access:</i> since October 2004 via KNMI <i>Spatial coverage and resolution:</i> Global coverage each day <i>Temporal coverage and resolution:</i> Daily at 13.30 local time <i>Location(s) (coordinates)/orbits:</i> all orbits <i>Accuracy:</i> 40-100 %
Name GOME Phase: 1+2	<i>Data availability and access:</i> NO2-columns: 01/2002 - 06/2003 at KNMI; O3-profiles: 01/2002 – 06-2003 at ZSW-BW (NNORSY retrievals) <i>Spatial coverage and resolution:</i> Global coverage each day <i>Temporal coverage and resolution:</i> n.a. <i>Location(s) (coordinates)/orbits:</i> all orbits <i>Accuracy:</i> 5-30%
Name MOPITT CO columns Phase: 1+2	<i>Data availability and access:</i> 01/2002 - 12/2005 at NASA <i>Spatial coverage and resolution:</i> Global coverage each day <i>Temporal coverage and resolution:</i> n.a. <i>Location(s) (coordinates)/orbits:</i> all orbits <i>Accuracy:</i> 10-100%
Name SYNAER PM10/AOT columns Phase: 2	<i>Data availability and access:</i> selected months out of 01/2002 - 12/2005 at DLR <i>Spatial coverage and resolution:</i> Global coverage each day <i>Temporal coverage and resolution:</i> n.a. <i>Location(s) (coordinates)/orbits:</i> all orbits <i>Accuracy:</i> n.s.
Name GOME-2 Phase: 2+3	<i>Data availability and access:</i> since April 2007 at KNMI <i>Spatial coverage and resolution:</i> Global coverage each day <i>Temporal coverage and resolution:</i> Daily at 9.30 local time <i>Location(s) (coordinates)/orbits:</i> all orbits <i>Accuracy:</i> 40-100 %

Table 1.1-2 Data used for the validation of the AQ Records service

1.1.3 Validation of individual components

1.1.3.1 Global Tropospheric Formaldehyde Column

HCHO columns are retrieved with the DOAS method. Slant column densities are retrieved using the WINDOAS software, which has been developed at BIRA-IASB and has been validated through participation at various intercomparison exercises [Hofmann, 1995], [Roscoe, 1999], [Aliwell, 2002]. Statistical analyses of the slant columns and detailed sensitivity tests [Boersma, 2004] have been performed to evaluate the errors on the slant columns and to separate the systematic part from the random part. The total error

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on the slant columns are estimated to be between 15% and 40%. Tropospheric air mass factors are needed to obtain the HCHO vertical columns. They are calculated independently from the slant columns, using the radiative transfer model DISORT [Kylling, 1995] and HCHO monthly a-priori profile shapes from the 3D-CTM IMAGES [Müller, 1995]. Albedo values are taken from the monthly database of Koelemeijer [2003]. A correction for cloudy pixels is applied using the independent pixels approximation and the FRESCO algorithm [Koelemeijer, 2001 and 2002], which provides the necessary cloud parameters (cloud fraction, cloud top height and cloud albedo). The estimation of the error made on the air mass factor is based on the study of Millet [2006]. It leads to an error of 5 to 20% depending on the cloud fraction and selecting only pixels with cloud fraction lower than 0.4. A full sensitivity study of the air mass factors including the impact of aerosols has still to be performed for our product. Combining the errors on the slant columns and the errors on the AMFs, the total error on the tropospheric HCHO vertical columns is estimated to be comprised between 16 and 50% depending on the conditions of observations (cloud fraction, ozone absorption, solar zenith angle). Averaging kernels and error estimates are provided for each satellite pixel.

VALIDATION OF INDIVIDUAL COMPONENTS	
Quality assessment methods and parameters	
Quality checks:	Inspection of fitting residuals and automated verification of the RMS fit residual value, which should always lie within a pre-defined confidence interval. Identification and rejection of outliers using filter approach defined below.
Identification of outliers	HCHO: Criterion for bad days filter: Mean HCHO above Pacific Ocean at Equator should be between -0.5×10^{16} and 1×10^{16} mol/cm ² .
Identification of bad retrievals	HCHO: RMS (fit residual) threshold: 1×10^{-3} ; Cloud fraction range: 0-0.4
Uncertainty evaluation	HCHO: Between 16 and 50%.
Accuracy	HCHO: N/A.
Retrievals error analysis (slant column density, stratospheric slant column density, tropospheric air-mass factor, averaging kernels)	See De Smedt <i>et al.</i> 2008 (submitted to ACP)
Best estimator: BIAS	$\text{BIAS} = \sum_i C_{obs,i} - C_{mod,i}$

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Error bar: Root mean square Error	$RMSE = \sqrt{\frac{\sum_{i=1}^N (C_{obs,i} - C_{mod,i})^2}{N}}$
MODELS /ALGORITHMS/ASSIMILATION	
FRESCO (SC-v4)	Validation and sensitivity in Koelemeijer <i>et al.</i> , 2001 and in Koelemeijer <i>et al.</i> , 2002
WinDOAS HCHO slant column density retrieval	WinDOAS algorithm (Van Roozendaal, 1999) Windoas software manual (Fayt, 2001) WinDOAS validation (Hofmann, 1995; Roscoe, 1999; Aliwell, 2002)
HCHO vertical column density retrieval	IMAGES profile shapes (Müller, 1995 and 2005) Fresco Cloud parameters (Koelemeijer, 2001 and 2002) Albedo LER monthly climatology (Koelemeijer, 2003) See S5 Document for details See De Smedt <i>et al.</i> , 2006 and De Smedt <i>et al.</i> , 2007.

Table 1.1-3 Validation of individual components for global tropospheric formaldehyde.

1.1.3.2 Global Tropospheric NO2 Column

The retrieval of tropospheric NO₂ is based on a combined retrieval/data assimilation approach. The data assimilation of the measured NO₂ is used for estimating the stratospheric NO₂ and for estimating the shape of the vertical distribution of the tropospheric NO₂.

VALIDATION OF INDIVIDUAL COMPONENTS	
Quality assessment methods and parameters	
Quality checks	The measured slant column of NO ₂ and auxiliary parameters are checked for their range. The chi-square and the error estimate of the results are given in the output files.
Identification of outliers	None. All retrieved results are made available.
Identification of bad retrievals	The chi-square and the RMS error is calculated.
Uncertainty evaluation	NO ₂ : See Boersma <i>et al.</i> 2004

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Retrievals error analysis (slant column density, stratospheric slant column density, tropospheric air-mass factor, averaging kernels)	See Boersma <i>et al.</i> 2004
Best estimator	$\text{BIAS} = \sum_i C_{obs,i} - C_{mod,i}$
Error bar: Root mean square Error	$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^N (C_{obs,i} - C_{mod,i})^2}{N}}$
MODELS /ALGORITHMS/ASSIMILATION	
FRESCO (SC-v4)	Validation and sensitivity in Koelemeijer <i>et al.</i> , 2001 and in Koelemeijer <i>et al.</i> , 2002
WinDOAS NO2 slant column density retrieval	WinDOAS algorithm (Van Roozendael, 1999) Windoas software manual (Fayt, 2001) WinDOAS validation (Hofmann, 1995; Roscoe, 1999; Aliwell, 2002) (See S5 Document for details on fitting)
Tropospheric NO2 column density retrieval SCIA:1.1.1 OMI: 1.0.2	See Boersma <i>et al.</i> 2004, Blond <i>et al.</i> 2007, Boersma <i>et al.</i> 2007a, Boersma <i>et al.</i> 2007b, Schaub <i>et al.</i> , 2007, Eskes <i>et al.</i> 2003 A product specification document with version changes is made available on the web-site.
Validation	
Vs. satellite data [SCIAMACHY, OMI, GOME-2]	Bias and rms will be calculated
Vs. Ground observations [in-situ and DOAS observations]	Bias and rms will be calculated . Correlations will be analysed.

Table 1.1-4 Validation of individual components for global tropospheric NO2 column.



1.1.3.3 European tropospheric assimilation based analysis

The validity of the assimilation results can be shown satisfactorily by independent observations. Retaining observations from assimilation and preserving them for quality check is the usual way to demonstrate assimilation improvements. Given the task to ameliorate forecasts, an improved prediction skill also provides a means of validation, when chemical state forecasts with and without data assimilation are compared. Both modes will be presented.

VALIDATION OF INDIVIDUAL COMPONENTS	
Quality assessment methods and parameters	
Best estimator (1): 3d-var cost function	Cost function (3d-var): $J = \frac{1}{2}(x - x_b)^T B^{-1}(x - x_b) + \frac{1}{2}(y - Hx)^T R^{-1}(y - Hx)$ with <ol style="list-style-type: none"> 1) x = model state 2) x_b = background model state 3) y = observations 4) H = observation operator 5) R = observation error covariance matrix 6) B = background error covariance matrix
Bias	BIAS= $\sum (y - Hx)$
Best estimator (2.1): OmA	Observation minus analysis departures (OmA): $\mathbf{OmA} = (y - Hx_a)$
Best estimator (2.2): OmB	Observation minus Background departures (OmB): $\mathbf{OmB} = (y - Hx_b)$
Best estimator (2.3): BmA	Background minus analysis departures (BmA): $\mathbf{BmA} = (Hx_b - Hx_a)$



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Error bar: NRMSE with
OmA terms

$$\text{NRMSE} = \sqrt{\frac{\sum \left(\frac{(y - Hx_a)}{\Delta y} \right)^2}{N}}$$

MODELS /ALGORITHMS/ASSIMILATION

3D-var Assimilation

Please see the following document for a (technical) description of the 3d-var data assimilation system:

- o http://db.eurad.uni-koeln.de/promote/dasys_descr.pdf

First evaluation based on statistics gathered on the European grid (45 km resolution):

Against ground-based in-situ data (in [ppb] for gas phase species and in [$\mu\text{g}/\text{m}^3$] for PM10):

SO₂: 2 to -0.5 (BIAS), < 5 (RMSE)

NO₂: 5 to -3 (BIAS), < 10 (RMSE)

NO: 15 to -5 (BIAS), < 20 (RMSE)

O₃: 2 to -2 (BIAS), < 5 (RMSE)

CO: 80 to -40 (BIAS), < 150 (RMSE)

PM10: 10 to -2 (BIAS), < 20 (RMSE)

EURAD against SCIAMACHY/GOME NO₂ column retrievals (by KNMI in [10^{15} molec/cm²]):

GOME: -0.5 to 0.2 (BIAS), < 2 (RMSE);

SCIAMACHY: -1.0 to 0.4 (BIAS), < 3 (RMSE)

The 4d-var data assimilation system within EURAD (Elbern *et al.* (1997), Elbern and Schmidt (2001)) has been applied to several campaign studies. The evaluation of which has been conducted by costs statistics, withheld observations and forecast improvement studies. An example:

- European scale, 54 km resolution, 03.08.-20.08.1997. 4d-var applications using pure initial value optimization, pure emission rate optimization and joint emission rate/initial value optimization. Observational data: European Environmental Agency (EEA), environmental protection agencies from the German state Northrhine Westfalia (LANUV) and the federal state (UBA), Switzerland, Austria, The Netherlands, Denmark, United Kingdom, Species: O₃, SO₂, CO, NO, NO₂; Reference: Elbern *et al.* (2007).

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	<p>See Figure 1.1-4 (next page)</p> <p>Phase 2: 1.1-5 shows the Chi-square testing results for 2003. The costs per observation are given on a daily basis for ground based NO₂ and O₃ observations from EEA, NO₂ satellite columns (GOME and SCIAMACHY) and NNORSY ozone profiles.</p> <p>For further information about validation documents, please see the given references.</p>
--	--

EURAD	<p><u>Evaluated reference dataset:</u></p> <p>SO₂, NO₂, NO, Nox, O₃, CO, PM₁₀ at regional scale down to urban scale (by nesting 54-18-6-2 km), 21.07.-30.07.1994 (Memmesheimer <i>et al.</i>, 1999). Observational data: German federal state environmental protection agency (UBA), O₃, NO, CO; German state Northrhine-Westfalia environmental protection agency LUA, O₃, NO, NO₂, NO_x, SO₂, CO, PM₁₀.</p> <p><u>Model intercomparison:</u></p> <p>European scale, 25 km resolution, April - September 1995, SO₂, NO₂, NH₃, HNO₃, VOC, SO₄⁻, NO₃⁻, NH₄⁺, TNH₄, TNH₃ (Hass <i>et al.</i>, 2003). Observational data: EMEP measurement network.</p> <p>Additionally, please see the following documents for a detailed description of the model system and references thereof:</p> <ul style="list-style-type: none"> ● Jakobs <i>et al.</i> (1995) ● http://db.eurad.uni-koeln.de/promote/euraddescr_cost.pdf
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Table 1.1-5 Validation of the individual components of the AQ Records sub-service

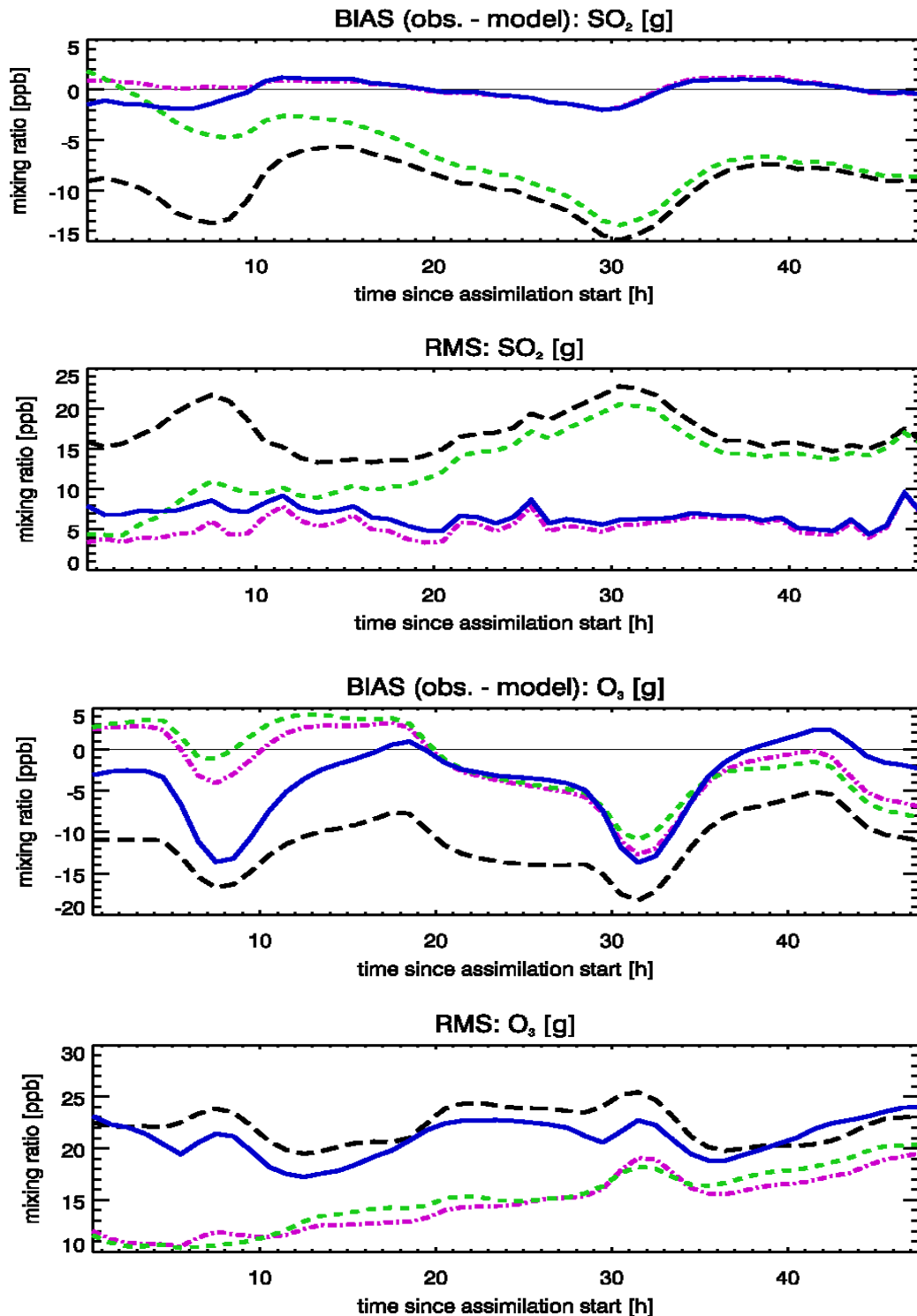


Figure 1.1-4 Mean observation-minus-model differences and RMS differences of all 8 two-day simulations for SO₂ and O₃. Observations assimilated for the first 24 h, with hours 25-48 displayed for quality control only. Green stippled line: only initial value optimisation, blue full line: only emission rate optimisation, pink dash-dotted line: combined initial value/emission rate optimisation. Dashed line: control run without any data assimilation in the case study, for reference only.



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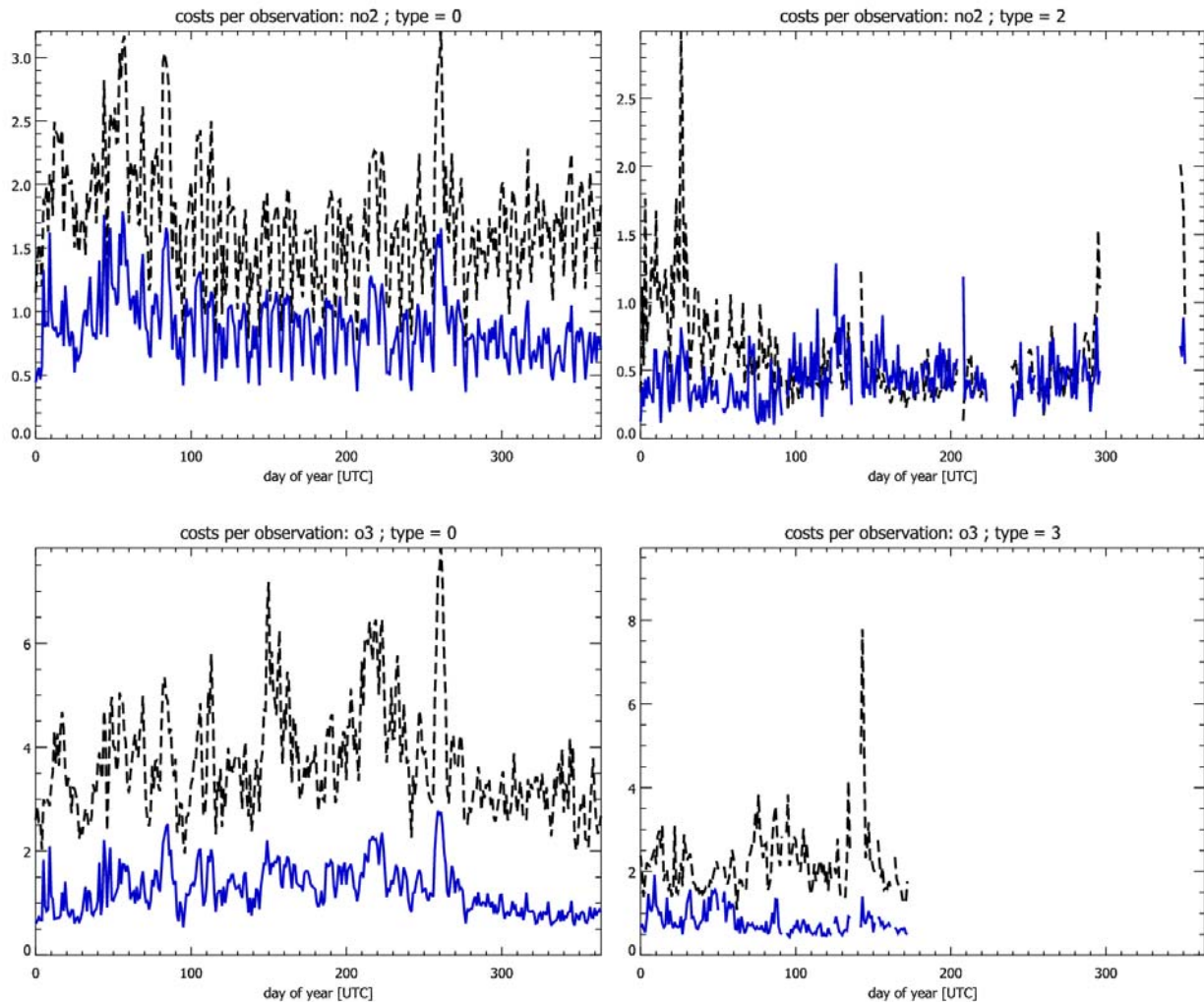


Figure 1.1-5 Costs per observation (Chi-Square testing) for 2003. Background costs are given by the black dashed line, analysis costs by a blue solid line. Upper left: ground based NO₂ observations (EEA); upper right: NO₂ columns (GOME, SCIAMACHY); lower left: ground based O₃ observations (EEA); lower right: O₃ satellite profiles (NNORSY).

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1.1.4 Validation against specifications and against user requirements

The status of compliance with specific Phase 2 SLA defined user requirements for this service can be summarized as follows:

Revise error co-variances in the assimilation: revised correlation lengths for three heights (ground, PBL, model top) and all nest-levels;	done
revised background variance estimates; revised representativeness error specifications on all nest-levels	done
Complement validation methods and skill scores	done
Adapt web presentation to user needs	done
Update of emission inventories	to be done in collaboration with users

1.1.4.1 Global Tropospheric Formaldehyde Column

VALIDATION AGAINST SERVICE SPECIFICATIONS			
No limitations/delays for compliance between theoretical and actual service specifications reported			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	S5	REQUIRED*	ACTUAL
Product	Daily tropospheric HCHO column: tropospheric column of HCHO, error on the tropospheric column of HCHO		
Accuracy	See Boersma <i>et al.</i> 2004 Specified as parameter	n.s.	20-50%
Accuracy minimum	n.s.	n.s.	n.s.
Accuracy target	n.s.	n.s.	n.s.
Spatial coverage	Global Swath 960 km (both GOME and SCIAMACHY), 14 orbits per day, i.e. global coverage in approx. 1-2 weeks	Global	Global Swath 960 km (both GOME and SCIAMACHY), 14 orbits per day, i.e. global coverage in approx. 1-2 weeks
Horizontal resolution	320 x 40 (GOME) and 120 x 30 km ² (SCIAMACHY) except for high latitudes	n.s. ~250x250 km ²	320 x 40 (GOME) and 120 x 30 km ² (SCIAMACHY)



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		$50 \times 50 \text{ km}^2$ $1 \times 1 \text{ km}^2$	except for high latitudes
Vertical resolution	n.s.	n.s.	n.a.
Grid/Projection	Orbit geometry	n.s.	Orbit geometry
Temporal coverage	6 years	1995**-2007	10 years
Temporal resolution	1-2 weeks	n.s.	1-2 weeks
User Interfaces			
PROMOTE Web	n.s.	Complete, operational and up to date	Incomplete, operational and up-to-date
ftp	n.s.	n.s.	yes
On demand/other	n.s.	n.s.	yes
Data formats and data delivery			
Data availability	Online	Phase 1: Global 07/95**-07/03 an: 07/03-07/07 SCI. 01/03-07/07 Phase 2: GOME (ERS-2) : 1996-2003 SCIAMACHY (Envisat) : 2003-today	Online
Data access	Online	Online	Online
Delivery Mode	No NRT	No NRT, offline	GOME (Maps and Daily HDF files) downloadable from PROMOTE Web
Delivery frequency	n.s.	at the end of processing/Phase	3 months
Data Format	HDF, GIF	HDF5	HDF, GIF

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Historical archive	GOME (ERS-2) : 1996-2003 SCIAMACHY (Envisat) : 2003-today	Phase 1: Global 07/95**-07/03 an: 07/03-07/07 SCI. 01/03-07/07 Phase 2: processing of global satellite tropospheric products HCHO column	GOME (ERS-2): 1996-2003 SCIAMACHY (Envisat): 2003-today
Visualization	Images	n.s.	Images
REMARKS			
No remarks			

* Requirements written in *Italics* are only recommended and not compulsory for Phase 2

**GOME data only available from April the 1st 1996 on

Table 1.1-6 Validation against specifications and against user requirements for the AQ Records sub-service Tropospheric Formaldehyde

1.1.4.2 Global Tropospheric NO₂ Column

* Requirements written in *Italics* are only recommended and not compulsory for Phase 2

VALIDATION AGAINST SERVICE SPECIFICATIONS			
No limitations/delays for compliance between theoretical and actual service specifications reported			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	S5	REQUIRED*	ACTUAL
Product	Daily tropospheric NO ₂ columns (level 2) including total column of NO ₂ , tropospheric column of NO ₂ , error on the tropospheric column of NO ₂		
Accuracy	See Boersma <i>et al.</i> 2004	n.s.	See Boersma <i>et al.</i> 2004
Accuracy minimum	n.s.	50%	n.s.
Accuracy target	n.s.	5%	n.s.
Spatial coverage	Swath 960 km (SCIAMACHY), 3000(OMI), 14 orbits per day,	Global	Swath 960 km (SCIAMACHY), 3000(OMI), 14 orbits per day,



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	i.e. global coverage in approx. 1 week (SCIAMACHY) and 1 day (OMI)		i.e. global coverage in approx. 1 week (SCIAMACHY) and 1 day (OMI)
Horizontal resolution	60 x 30 km ² (SCIAMACHY) except for high latitudes 12 x 24 km ² (OMI)	50 x 50 km ² 1 x 1 km ²	60 x 30 km ² (SCIAMACHY) except for high latitudes 12 x 24 km ² (OMI)
Vertical resolution	n.s.	2-4 Layers(troposphere)	Distinction troposphere and stratosphere
Grid/Projection	Orbit geometry	Orbit	Orbit geometry
Temporal coverage	See historical archive	See historical archive <i>Year, all seasons. Records as long as possible</i>	See historical archive
Temporal resolution	24 h	24-1 h	24 h
User Interfaces			
PROMOTE Web	n.s.	Complete, operational and up to date	Available
ftp	n.s.	n.s.	N/A
On demand/other	n.s.	n.s.	TEMIS http://www.temis.nl/
Data formats and data delivery			
Data availability	Operational	n.s.	
Data access	Offline/NRT	Online	online
Delivery Mode	Offline and NRT	n.s.	Downloadable from PROMOTE Web (except OMI)
Delivery frequency	24 h - NRT	NRT	NRT
Data Format	HDF	HDF5	HDF Monthly mean in ASCII

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Historical archive (reprocessed)	GOME (ERS-2) : 1996-2003 SCIAMACHY (Envisat) : 2003-today OMI : 2006-today	GOME 07/95**-07/03 SCI. 01/03-today OMI 10/04-07/07	GOME (ERS-2): 1996-2003 SCIAMACHY (Envisat): 2003-today OMI : 2006-today
Visualization	Images	n.s.	Images
REMARKS			
No remarks			

* Requirements written in *Italics* are only recommended and not compulsory for Phase 2

**GOME data only available from April the 1st 1996 on

Table 1.1-7 Validation against specifications and against user requirements for the AQ Records sub-service for Tropospheric NO₂

1.1.4.3 Regional assimilated near surface pollutants

VALIDATION AGAINST SERVICE SPECIFICATIONS			
No limitations/delays for compliance reported			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	S5	REQUIRED*	ACTUAL
Product	Analyses of daily synoptic maps of ozone, sulphur dioxide, nitrogen dioxide, carbon monoxide, formaldehyde, particulate matter PM ₁₀ , PM _{2.5} on regular grids over Europe		
Accuracy	30-50%	n.s.	n.a.
Accuracy minimum	n.s.	<i>Precision/trueness</i> ~30%	n.a.
Accuracy target	n.s.	<i>Optimal precision/trueness</i> ~7%	n.a.
Spatial coverage	Europe	Europe, EU27	Europe
Horizontal resolution	45 x 45 km ²	50x50 Km ²	45 x 45 km ²
Vertical resolution	Topography following vertical resolution with 40 m in the near surface layer	n.s.	Topography following vertical resolution with 40 m



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			in the near surface layer
Grid/Projection	Gridded fields on Lambert conformal	<i>Georeferenced, regular</i>	Gridded fields on regular Lambert conformal grid
Temporal coverage	(1) 12 months between 2002-2005 (2) 36 months 2002-2005 (3) 36 months 2006-2008	(1) 12 months between 2002-2005 (2) 36 months 2002-2005 (3) 36 months 2006-2008	(1) 16 months between 2002-2005 (2) 48 months between 2002-2005
Temporal resolution	24 h and daily means, monthly means, annual means	24 h	max1h-avg, max08h-avg, max24h-avg, daily max and daily means, monthly means, annual means
User Interfaces			
PROMOTE Web	n.s.	<i>Complete, operational and up to date</i>	<i>Complete, operational and up to date</i>
ftp	n.s.	n.s.	via PROMOTE web page or on demand
On demand/other	n.s.	n.s.	n.s.
Data formats and data delivery			
Data availability	reanalyses 2002-2005: in 2008; reanalyses 2006-2008: in 2009	(Phase 1) 12 months between 2002-2005 (Phase 2) 36 month record 2002-2005	(Phase 1) 16 months between 2002-2005 (Phase 2) 48 months between 2002-2005
Data access	Online	<i>Online</i>	Online
Delivery Mode	No NRT	n.s.	reanalysis mode
Delivery frequency	24 h/ reanalysis 12 months - After production	24 h/ reanalysis 12 months - After production	24 h/ reanalysis after production
Data Format	optional and HDF5	HDF5	optional, HDF5
Historical archive	2002 until project end	Reanalysis 2 summer	(Phase 1)



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	2008	months+two winter months of 1995**, 2002-2005 In situ Observations GOME Jan-Feb/Jul-Aug 2002-2003 (NO2 Col, O3 Prof) SCIAMACHY Jan-Feb/Jul-Aug 2002-2005 (NO2 Col) OMI Jan-Feb/Jul-Aug 2004-2005 MOPITT Jan-Feb/Jul-Aug 2002-2005 (CO Profiles)	Jan/Feb/Jul/Aug 2002-2005 for In situ observations, GOME, SCIAMACHY and MOPITT (Phase 2) Jan-Dec 2002-2005 (Phase 3) 2002 until project end 2008 (in Phase 3)
Visualization	Surface maps	maps	maps

REMARKS

Additional products as input to *Regional assimilated near surface pollutants*:

Global CO total columns from SCIAMACHY nadir observations (demonstration product by University Bremen)

Validation contact: M. Buchwitz (email: Michael dot Buchwitz belongs to iup dot physik dot uni minus bremen dot de)

Parameter: CO total column

Typical range: 0 – 10 x 10¹⁸

Determination of typical range: a-priori knowledge

Unit: molecules/cm²

Standards: n.a. (ground based FTS)

Retrieval Version: WFM-DOAS version 0.6

Spatial Resolution (single pixel): 30 x 120 km

Estimated accuracy: ~10 %

Estimated precision: ~20 %

Algorithm specification and product description document: http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/scia_wfmd_adps_V2.pdf

Validation: Dils *et al.* (2006)



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References: Buchwitz *et al.* (2007)

Data access: Via PROMOTE web page or from

- http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/
- http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/PROMOTE/CO_cols_SCIAMACHY

Data format: ASCII, level 2, 1 file per orbit

Images:

- http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_COv06_figs_2003.html
- http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_COv06_figs_2004.html
- http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_COv06_figs_2005.html

Aerosol optical depth and aerosol speciation for Europe (SYNAER/ENVISAT) (PROMOTE Service Product by DLR-DFD)

Validation contact: T. Holzer-Popp (email: thomas dot holzer-popp belongs to dlr dot de)

Validation document: see at *Greenhouse Gas and Aerosol Service :: Aerosol and Speciation Record*

* Requirements written in *Italics* are only recommended and not compulsory for Phase 2

**GOME data only available from April the 1st 1996 on

Table 1.1-8 Validation against specifications and against user requirements for the AQ Records sub-service for Regional Assimilated Pollutants

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1.1.4.4 SO₂ Slant and Vertical Column data from GOME and SCIAMACHY

Note from the Validation Office: Specifications and validation for GOME, SCHIAMACHY (and GOME 2) SO₂ slant and vertical column densities are available in the framework of the SACS Service.

Compliance of this product with specific SLA defined user requirements for this service can be summarized as follows:

	REQUIRED	ACTUAL
GOME		
Improved Background correction	Yes	N/A
Validation/verification	??	N/A
Systematic processing of data	Yes	To be done
Data Archive	July 1995 - June 2003	Preliminary dataset: Jan. 2000 – June 2003
SCIAMACHY		
Improved Background correction	Yes	2nd version
Validation/verification	??	In progress
Systematic processing of data	Yes	In progress
Data Archive	Jan 2003 - present	Sep. 2004 – Apr. 2008
NRT processing	Yes	Aug.2007 - present
GOME-2		
Improved Background correction	Yes	Preliminary version
Validation/verification	??	In progress
Systematic processing of	Yes	In progress

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data		
Data Archive	Jan 2003 - present	Not yet available
NRT processing	Yes	Feb.2008 - present

Specifications and validation for GOME, SCHIAMACHY (and GOME 2) SO₂ slant and vertical column densities are available in the framework of the SACS Service.

1.1.5 Quality assessment and control procedures

Service delivery start date: n.s.				
Service Quality				
	S5	REQUIRED*	ACTUAL	N checks/Delivery period
Quality checks <i>(NO₂ columns)</i>	Error and averaging kernel calculations for each observation	yes	Error and averaging kernel calculations for each observation	n.s.
Product data confidence interval <i>(NO₂ columns)</i>	n.s.	95%	n.s.	n.s.
Error bar definition and representation <i>(Regional assimilated near surface pollutants)</i>	RMSE with OmA differences	1 σ , 2 σ , total error	1 σ	n.a.
Representation of missing data <i>(Regional assimilated near surface pollutants)</i>	Due to failure safeness there is no missing data expected	-99.99 or similar <0 or interpolation	Missing data is not available	n.a.

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Documentation of process failure <i>(Regional assimilated near surface pollutants)</i>	If reanalysis step fails for a certain day system setup is analysed and reconfigured if necessary until success can be stated	n.s.	e-mail to operator	n.a.
Version control mechanisms and representation <i>(Regional assimilated near surface pollutants)</i>	Enabled. Will be started in Phase 3	<i>References to Quality Control procedures and product version number and last date of modification to be available in background</i>	History in product specification document and CVS, References to Quality Control procedures and product version number and last date of modification to be available in background	n.s.

*Requirements written in *Italics* are only recommended and not compulsory for Phase 2

Table 1.1-9 Quality assessment and control procedures for the AQ Records

1.1.6 References

1.1.6.1 Electronic references and online data access paths

<http://www.temis.nl/>

<http://www.temis.nl/airpollution/no2.html>

http://db.eurad.uni-koeln.de/promote/dasys_descr.pdf

http://db.eurad.uni-koeln.de/promote/euraddescr_cost.pdf

<http://kups.ub.uni-koeln.de/volltexte/2007/1942>

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Boersma, K. F., H. J. Eskes, and E. J. Brinksma, Error Analysis for Tropospheric NO₂ Retrieval from Space, *J. Geophys. Res.*, 109, D04311, 2004.

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Boersma, K.F., H.J. Eskes, J.P. Veefkind, E.J. Brinksma, R.J. van der A, M. Sneep, G.H.J. van den Oord, P.F. Levelt, P. Stammes, J.F. Gleason and E.J. Bucsela (2007b), Near-real time retrieval of tropospheric NO₂ from OMI, *Atm. Chem. Phys.*, 2013-2128, sref:1680-7324/acp/2007-7-2103

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De Smedt, I., M. Van Roozendael, R. Van der A, H. Eskes, J.F. Müller, Retrieval of formaldehyde columns from GOME as part of the GSE PROMOTE and comparison with 3D-CTM calculations, *Proceedings of the Atmospheric Science Conference, ESA*, 2006.

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