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GMES SERVICE ELEMENT
PROMOTE 2

C6 Validation Report

Chapter 2
3D OZONE RECORD SERVICE

Version 3

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CONTRIBUTING AUTHORS	Service leader Service providers	F. Baier F. Baier Q. Errera		
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3	20.10.2009	Chapter number update

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS AND ACRONYMS

4DVAR	Four-dimensional variational assimilation method
ACE-FTS	Atmospheric Chemistry Experiment - Fourier Transform Spectrometer
ASSET	Assimilation of ENVISAT data working group
AURA	NASA scientific research satellite - third component of EOS
BASCOE	Belgian Assimilation System of Chemical Observations from ENVISAT
BIRA-IASB	Belgian Institute for Space Aeronomy
BMBF	Federal Ministry of Education and Research
CCMval	Chemistry Climate Model Validation working group
ClOx	Reactive chlorine oxide family (Cl + ClO)
COMMA	Cologne Model of the Middle Atmosphere
CTM	Chemistry-Transport Model
DFD	German Remote Sensing Data Center
DG Environment	European Commission's Environment Directorate-General
DLR	German Aerospace Center
ECMWF	European Center for Medium range Weather Forecasts
ENVISAT	European Environmental Satellite
EOS	Earth Observation System
GME	Global Model of the German Weather Service
GOME	Global Ozone Mapping Experiment
GOMOS	Global Ozone Monitoring by Occultation of Stars
HALOE	Halogen Occultation Experiment
IASI	Infrared Atmospheric Sounding Interferometer
ICE	Water ice phase PSC constituent
NAT	Nitric acid trihydrate PSC constituent
INVERT	Inversion of vertically resolved trace gas profiles from ERS-2-GOME
KF	Kalman-Filter based assimilation method
METOP	Meteorological Polar-Orbiting Operational Satellite
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MPI	Message Passing Interface – Parallelization Library
MLS	Microwave Limb Sounder
NNORSY	Neural Network Ozone Retrieval System
NAT	Nitric Acid Trihydrate – PSC constituent
NOx	Reactive nitric oxide family (NO + NO2)
OI	Optimum Interpolation based assimilation method
OMF	Observation minus First-guess/Forecast
OmF	Observation minus First-guess/Forecast
PSCs	Polar Stratospheric Clouds
PC cluster	Intel-based multiprocessor computing platform
RIU	Rhenish Institute for Environmental Research
ROSE	Research for Ozone in the Stratosphere and its Evolution
SACADA	Synoptic Analysis of Chemical constituents by Advanced Data Assimilation
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
SCISAT	Canadian Atmospheric Research Satellite
SLA	Service Level Agreement
SPARC	Stratospheric Processes and their Role in Climate
SdA	Service d'Aéronomie

TOMS	Total Ozone Mapping System
UARS	Upper Atmospheric Research Satellite
WDC-RSAT	World Data Center for Remote Sensing of the Atmosphere
WMO	World Meteorological Organization

N/A	Not Available
n.a.	not applicable
n.s.	not specified

TABLE OF CONTENTS

2 3-D OZONE SERVICE VALIDATION

2.1 Service overview

PROMOTE-2 products dealing with ozone records, monitoring and forecast, are provided by two services: the Total Ozone Service, providing ozone columns (i.e. vertically integrated ozone concentrations), and the demonstration 3-D Ozone Service, providing ozone concentration profiles. Figure 2.1-1 shows the structure of the PROMOTE-2 Ozone services.

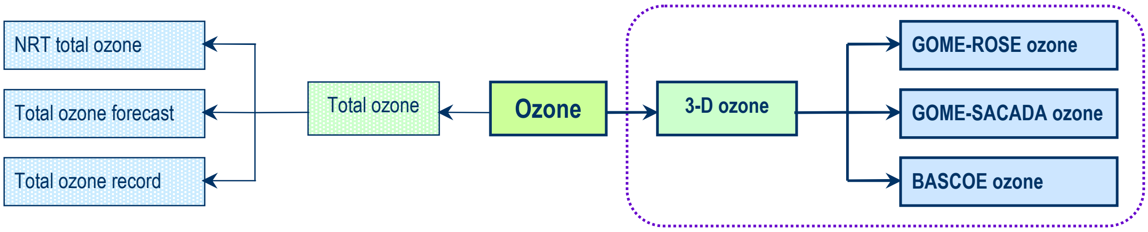


Figure 2.1-1. The 3-D Ozone Service within the PROMOTE-2 Ozone Theme

The 3D Records demonstration service derives long-term three-dimensional ozone record and additional information on ozone related species from the combination of three physic-chemical models, namely, ROSE, SACADA and BASCOE, and satellite observations via data assimilation.

2.2 ROSE Products

ROSE products consist of vertically resolved global synoptic analysis of stratospheric ozone mixing ratios (3D ozone), PSC area densities and accumulated daily ozone loss rates. Analyses are derived by sequential assimilation of GOME/NNORSY and MIPAS trace gas observations. The Assimilation scheme is Optimum Interpolation based with analysis errors propagated via transport and chemistry (Baier *et al.*, 2005). To balance a-priori and observational errors a χ^2 correction is performed dynamically calculated from a three-day running mean. To check the consistency of results and analyse model/instrument bias Observation minus First-guess (OMF) residuals are stored along the ozone analysis and its errors. Additionally comparisons of ozone and related trace gases to independent observations (ground based and satellites) are performed when data is available.

Service is/will be operational since/after: MetOp GOME-2 since July 2008

Research partners: BIRA-IASB

Provider(s): DLR

Validation contact: Frank Baier

2.2.1 ROSE Product Characterization

PRODUCT CHARACTERISATION	
3D gridded fields of synoptic ozone mixing ratios	
Parameter	Ozone concentration
Typical range	0 – 10 ppmv
Determination of the typical range (Method, criteria)	Maximum simulated mean value for single altitude
Units	ppmv
Standards	-
gridded fields of daily accumulated chemical ozone loss rates as mixing ratios per day	
Parameter	Ozone concentration
Typical range	+/- 20 ppbv per day
Determination of the typical range (Method, criteria)	maximum simulated mean value for single altitude
Units	ppmv
Standards	-
3D gridded fields of synoptic PSC area densities	
Parameter	PSC Density
Typical range	0 – 10 μ^2/cm^3
Determination of the typical range (Method, criteria)	Maximum simulated mean value for single altitude
Units	μ^2/cm^3
Standards	-

Table 2.2-1. ROSE Products characterization

2.2.2 Validation plan and validation data

VALIDATION PLAN

There has been an extensive evaluation of ROSE/DLR ozone within the BMBF project INVERT (Bittner and Baier, 2006) and ESA's PROMOTE 1. Comparisons to HALOE, SAGEII and GAW ozone sonde observations showed mean rms (root mean squared) errors well below 15% for the time period 1996-2002 using ERS2-GOME total ozone data and O3/PV correlations and/or a SAGE based bias correction. Similar results where attained by assimilating ENVISAT-MIPAS observations covering the winter period 2003/2004 (see below). In PROMOTE 2 the system is used to deliver first 3D ozone products for the period 1996-2005 and beyond. Results for the half-year of 2003/2004 have been already compared to respective SACADA data and to HALOE observations. The 3D ozone record for the years 1996-2003 GOME/NNORSY has been successfully generated and compared to HALOE. Additional comparisons to ozone sonde data are currently under investigation. Here, we report preliminary results. Evaluation of PSC area densities and ozone loss rates is much more complex (only very limited data or only model data available) and will be part of the follow-on project MACC

VALIDATION DATA	
Ground based observations	
Stations	N/A
***In-situ* observations**	
WOUDC ozone sonde archive	Availability: WOUDC, 1996-2008 Spatial coverage: n.a. Temporal coverage: approx. one sounding per week Location (coordinates): see WOUDC station list Accuracy: N/A
Model outputs	
SACADA-MIPAS	Availability: PROMOTE Spatial coverage: gobal Temporal coverage: 2002-2004 Location (coordinates): -90° South to +90° North Accuracy: <15%
Other EO Data	
UARS/HALOE V19 O3 observations	Availability: NASA DAAC Spatial coverage: two latitude bands (max 10° of width) by day Temporal coverage: 1992 – 2005, approx. 30 profiles per day Location (coordinates): -75° South to +75° North Accuracy: approx. 10%, deteriorates below 20 km altitude (Brühl et al., 1996)

SAGE-II O3 observations	Availability: NASA DAAC Spatial coverage: two latitude bands (max 10° of width) by day Temporal coverage: 1984 - 2005, approx. 30 profiles per day Location (coordinates): -75° South to +75° North Accuracy: approx. 10%, deteriorates below 20 km altitude (Wang et al., 2002)

Table 2.2-2. Data used for validation of the ROSE products

2.2.3 Validation of individual components

VALIDATIONS METHODS APPLIED

To balance *a priori* and observational errors a χ^2 (Chi-Square) correction is performed dynamically calculated from a three-day running mean. To check the consistency of results and analyse model/instrument bias Observation minus First-guess (OMF) residuals are stored along the ozone analysis and its errors. Additionally, comparisons of ozone and related trace gases to independent observations (ground based and satellites) are performed when data is available.

The most actual results concerning the October-March episode 2003/2004 are obtained from comparisons to HALOE occultation measurements. Ground based ozone soundings were performed to derive mean bias and rms errors. Two experiments have been conducted to assess the overall model performance (also in comparison to SACADA, see Section 0) and the impact of meteorological data (UKMO and ECMWF/GME). The quality of ozone analysis using offline chemistry-transport models depends strongly on the external wind and temperature fields. In fact, it was shown that ROSE ozone rms errors decrease by 30% when ECMWF/GME meteo data is applied. The GME forecast model was used to generate 24h forecasts starting with 00:00 GMT ECMWF analyses. This set-up is also used for the SACADA system. Validation results obtained by comparison to HALOE data on O3, H2O, NOx, CH4 and HCl within the altitude region 100 – 2 hPa are given in Table 2.2-3 HALOE HCl and NOx were only considered above 56hPa due to poor data quality in lower altitude regions.

For comparisons to GAW ozone soundings the currently available base product (valid for 12:00 GMT) has been used. Note that the base product covers only the altitude region between 147 hPa (~14 km) and 0.3 hPa (~58 km). For model cross comparisons the full vertical range will be used.

VALIDATION OF INDIVIDUAL COMPONENTS	
Accuracy	
For Uncertainty/Error bars	See Table 2-2.2-5 below (Quality Assessment and control procedures for ROSE)
Quality assessment	
Monitoring of OMF residuals	Daily zonal mean observation minus first-guess (OMF) differences: zonal mean = $\sum$ OMF_i , for all model longitudes i with observations

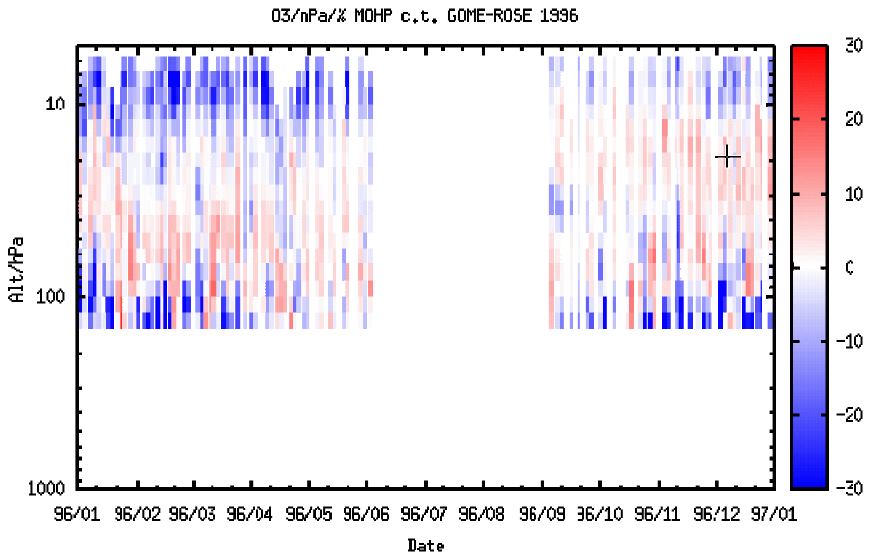
<table>
<tr><td>OMF error statistics for single pressure levels</td><td>Daily accumulated OMF differences for each model grid point:
daily average = $\sum OMF_i$, for all observations i available</td></tr>
<tr><td colspan="2">Models/assimilation</td></tr>
<tr><td>ROSE</td><td>Sensitive to different meteorological data sets

Rejection of observational data which deviates by more than factor 10 from first-guess</td></tr>
<tr><td rowspan="2">HALOE</td><td>Morning and evening observations deteriorate rapidly below approx. 60 hPa (data withheld from comparisons)</td></tr>
<tr><td>For NOX there is an increased scatter above 1 hPa (data withheld from comparisons)</td></tr>
<tr><td>Comparison of ROSE results to HALOE observations for October-March 2003/2004 using two different meteorological driver data

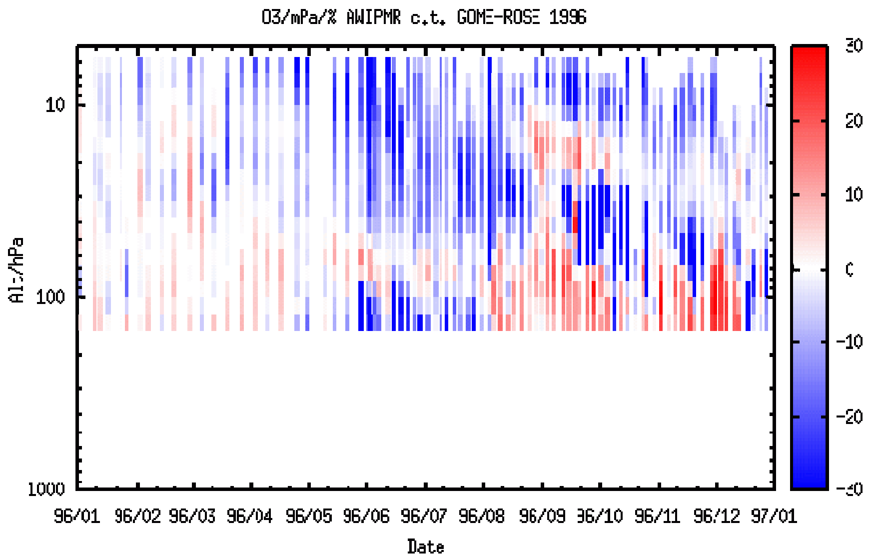
HALOE HCl and NOx were only considered above 56hPa due to poor data quality in lower altitude regions</td><td>Global mean/ppmv, bias/ppmv (ROSE-HALOE) and rms/% results

ROSE/UKMO c.t. HALOE (100-2 hPa)
<table>
<tr><th>obs</th><th>#</th><th>mean</th><th>bias/%</th><th>rms/%</th></tr>
<tr><td>O3</td><td>48776</td><td>5.10</td><td>0.29</td><td>13.71</td></tr>
<tr><td>H2O</td><td>48778</td><td>5.05</td><td>4.29</td><td>9.30</td></tr>
<tr><td>Nox</td><td>41478</td><td>7.79</td><td>0.97</td><td>26.30</td></tr>
<tr><td>CH4</td><td>48576</td><td>4.26</td><td>7.77</td><td>15.19</td></tr>
<tr><td>HCl</td><td>41484</td><td>1.82</td><td>-9.02</td><td>19.61</td></tr>
</table>
ROSE/GME c.t. HALOE (100-2 hPa)
<table>
<tr><th>obs</th><th>#</th><th>mean</th><th>bias/%</th><th>rms/%</th></tr>
<tr><td>O3</td><td>54252</td><td>5.16</td><td>1.64</td><td>8.81</td></tr>
<tr><td>H2O</td><td>54254</td><td>5.09</td><td>5.01</td><td>9.14</td></tr>
<tr><td>Nox</td><td>46137</td><td>7.99</td><td>2.73</td><td>24.86</td></tr>
<tr><td>CH4</td><td>54050</td><td>4.21</td><td>7.49</td><td>13.56</td></tr>
<tr><td>HCl</td><td>46142</td><td>1.92</td><td>-4.28</td><td>15.23</td></tr>
</table></td></tr>
</table>

<table>
<tr>
<td>Comparisons to GAW Ozone Soundings</td>
<td>



Relative differences w.r.t. ozone partial pressure between Hohenpeissenberg (48.02°N, 11.80°E) soundings and GOME-ROSE assimilation results for 1996. Note: only model data above 147hPa (~14km) altitude is used.



Same as above, but for station Neumayer (70.65°S, 8.26°W).

</td>
</tr>
</table>

Table 2.2-3. Validation of individual components of the ROSE products

As mentioned in the table above, HALOE morning and evening observations deteriorate rapidly below approx. 60 hPa. For NOx there is also an increased scatter above 1 hPa. These data has been withheld from comparisons. HALOE is in general well suited for model assessments due to comparable vertical resolution within the stratosphere. Future comparisons will also include ground based ozone soundings. This will allow for a more continuous monitoring with respect to single locations. On the other hand, ozone sondes are only applicable below approx. 10 hPa.

As indicated in Table 2.2-3 assimilation results strongly depend on the quality of meteorological analyses driving the CTM calculations. Therefore, the product quality and applicability (usability) depend also on certain atmospheric conditions, *e.g.* low temperatures allowing PSC formation. The PSC parameterization method is a critical part of chemical model calculations. It depends on assumptions on temperature thresholds for PSC formation, PSC types and microphysical processes involved. ROSE currently employs the Ice-NAT scheme of Chipperfield *et al.* (1999). Future model upgrades foresee a transition to more elaborated Ice-NAT-STS parameterizations.

2.2.4 Validation against specifications and against user requirements

During phase II a second reanalysis of the 1996-2003 GOME/NNORSY time record has been completed making use of ECMWF 6h meteorological data (ERA40 until 2002) and more detailed error analysis. Therefore, the χ^2 correction applied in phase I was skipped, but can be reconsidered in phase III with new error data available. This error data will also help to improve SACADA results (see 1.3.4). Comparing both reanalyses to HALOE observations some improvements are clearly evident (see Figure 2.2-1). For example, the increased RMS error level in 2000 is reduced to average values. Until 2001 there is in general a small reduction of RMS errors compared to the first reanalysis. However, in 2001 statistical deviations from HALOE are now higher. Bias values are still small but seem to increase with time with maximum values in 2003 (4%). With respect to latitude bands the most significant improvements are visible in the tropics.

*Requirements written in italics were not compulsory in Phase 2.

VALIDATION AGAINST SERVICE SPECIFICATIONS & USER REQUIREMENTS			
No limitations/delays for compliance between theoretical and actual service specifications have been indicated by the service provider.			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Parameters (*=GSE-PRO2)	3D-O3R*: 3D gridded fields of synoptic ozone mixing ratios *3D-O3LS*: 3D gridded fields of daily accumulated chemical ozone loss rates as mixing ratios per day* N/A 3D-O3PSC*: 3D gridded fields of synoptic PSC area densities		
Accuracy			
Uncertainty	3D-O3R*: rms < 15%, bias < 0.5% 3D-O3LS*: N/A 3D-O3PSC*: N/A	*< 5%*	3D-O3R*: rms < 10%, bias < 2% 3D-O3LS*: N/A 3D-O3PSC*: N/A
Uncertainty minimum	n.s.	*For O3: Mesosphere: 15% Stratosphere layers: 15% Total column: 5%*	n.s.

Uncertainty target	n.s.	*For O3: Mesosphere: 3%* *Stratosphere layers: 3%* *Total column: 1%*	3D-O3R*: 10% (1 ppmv) 3D-O3LS: N/A 3D-O3PSC: N/A
Spatiotemporal characteristics			
Spatial coverage	Global 1000 to 0.3 hPa	Global	3D global (1000 – 0.3 hPa)
Horizontal resolution	2.5° x 3.7° lat-lon	*2.8°x2.8° for stratosphere*	2.5° x 3.7° lat-lon
Vertical resolution	Vertical 1.3 km	*1 km*	1.3 km
Grid/Projection	Lat-long coordinates on fixed pressure levels	Lat-long	Latitude-longitude coordinates on fixed pressure levels
Temporal coverage	1995-2005	1995-2005. *As long as possible (>20 years per record)*	1996-2003
Temporal resolution	Daily synoptic analysis every 6 h	Daily	Daily synoptic analysis every 6 h
User Interfaces			
PROMOTE Web	n.s.	Complete, operational and up to date	Complete, operational and up to date
ftp	n.s.	n.s.	n.s.
On demand	Email contact	n.s.	Email contact
Data formats and data delivery			
Data access	on demand	Downloadable from PROMOTE Web	on demand
Delivery Mode	Actual base products online (no NRT) depending on data availability, record offline	Online no NRT	no NRT
Delivery frequency	n.s.	When agreed with user. *At the end of every phase*	N/A
Data Format	HDF4, NetCDF	ASCII, HDF, CDF	HDF4, NetCDF

Historical archive	Reanalysis of ERS-2 and ENVISAT data since 1995	n.s.	Reanalysis of ERS-2 GOME data since 1996
Visualization	Quicklooks for single pressure levels (60, 20, 10 hPa)	n.s.	Quicklooks for single pressure levels (60, 20, 10 hPa)
REMARKS No remarks			

Table 2.2-4. Validation against specifications and against user requirements of ROSE Products

2.2.5 ROSE quality assessment and control

*Requirements written in *italics* were not compulsory in Phase 2

QUALITY ASSESSMENT AND CONTROL PROCEDURES				
Service delivery start date: Online delivery of 1996-2003 products until July, 2008				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**N checks/Delivery period**
Quality checks	Continuous monitoring of OMF error residuals for observed species See Table 2.2-3	n.s.	Continuous assessment See Table 2.2-3	Phase 2: Online cjhecks depend on data coverage (avg. 16000 per dday).
Product confidence data	n.s.	n.s.	HALOE, SAGEII	Phase 2: Mean data coverage 30 ozone profiles p.d.
Error bar definition and representation	1 sigma	*Total error; 1 sigma error bar (standard deviation)*	Standard deviation	Phase 2: Monthly data base (approx. 1000 value pairs p.d.)

Representation of missing data	Data coverage and outliers are reported for 3D Ozone profile records	*Filled with higher order regression; cloud and event flags*	Data gaps indicated by high analysis error	Phase 2: Certain periods with reduced coverage: Jan, Mar, Jun 1996; Nov 1999; Feb, Jul 2000; Jan, Feb 2001; Jul 2003 onwards
Documentation of process failure	Convergence of chemical solver is reported	n.s.	Convergence of numerical solver for CTM	Phase 2: Convergence fulfilled; transport time step reduced for ECMWF analysis 2002-2003
Version control mechanisms and representation	Changes are reported, processor version number is increased – this is also indicated in HDF data set	*Number scheme to be defined in S5 Specifications*	GOME/NNORSY V3; ROSE CTM V3; OI/KF V2	Phase 2: OI/KF update

Table 2-2.2-5. Quality assessment and control procedures for ROSE

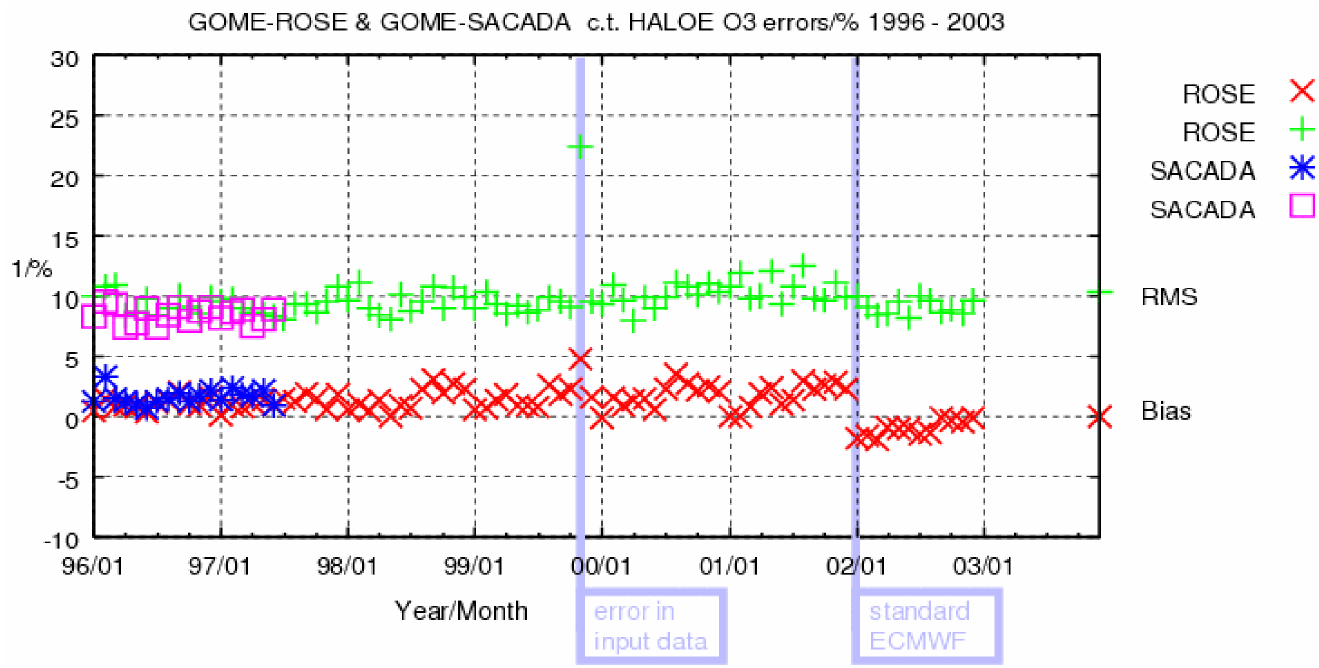


Figure 2.2-1. Global monthly mean results from comparison of GOME/ROSE and GOME/SACADA reanalyses to collocated HALOE observations. Both statistical (rms) and mean deviations (bias) are shown. Note: SACADA results reflect current processing status (not completed). Indicated are two exceptional events: 1. erroneous input data and 2. change from ERA40 to standard ECMWF meteo analyses.

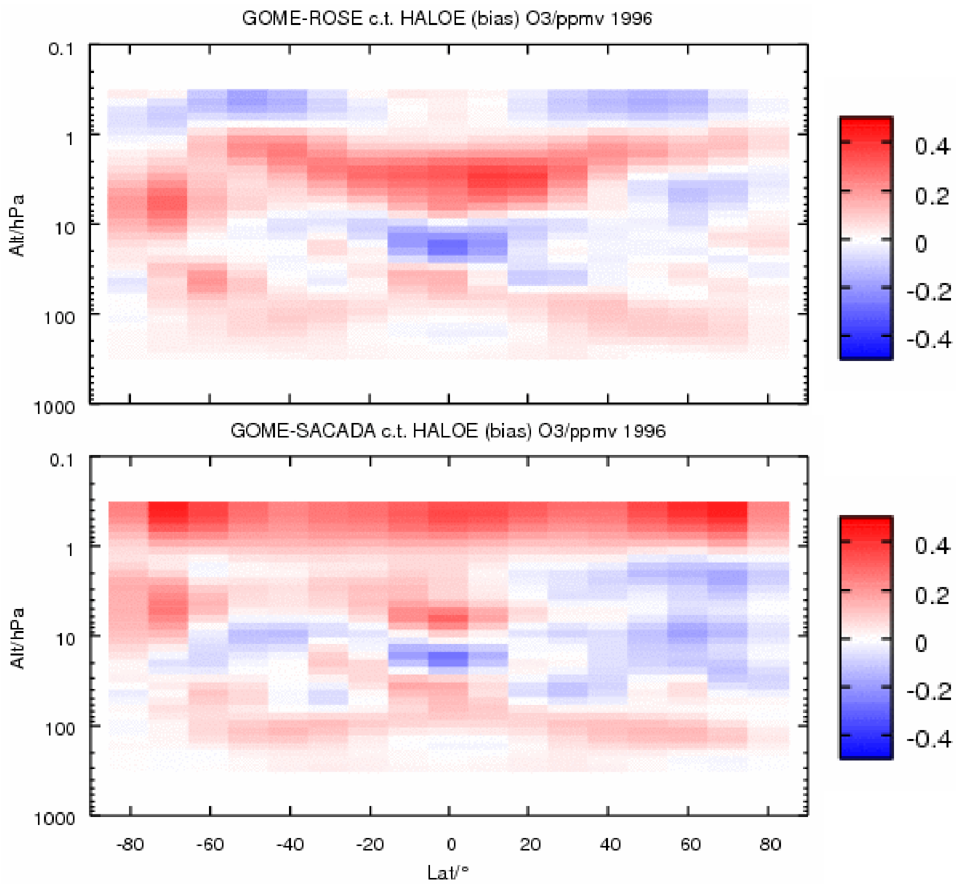


Figure 2.2-2. Global yearly mean results for 1996 from comparison of GOME/ROSE and GOME/SACADA reanalyses to collocated HALOE observations. Shown is the mean deviation between analyses and observations w.r.t. to 10° latitude bins.

2.3 SACADA Products

SACADA (Synoptic Analysis of Chemical constituents by Advanced Data Assimilation) provides long term 3D Records of reactive ozone chemistry. Trace gas observations from ERS-2 GOME/NNORSY, ENVISAL MIPAS, SCIAMACHY, GOMOS, MetOp IASI and GOME-2 trace gas profile and column data are assimilated into SACADA.

SACADA is a 4D-VAR system comparable to BASCOE (see Section 2.3) giving in principle more chemically consistent results than ROSE. Therefore, a transition from ROSE to SACADA is foreseen for project phase 2. Besides stratospheric ozone SACADA will also be used to generate daily active ClOx and NOx compounds for fixed local time.

Service is/will be operational since/after: N/A

Research partners: RIU, BIRA-IASB

Provider(s): DLR

Validation contact: Frank Baier (DLR)

2.3.1 SACADA Product Characterization

PRODUCT CHARACTERISATION	
3D Gridded fields of ozone mixing ratios	
Parameter	Ozone Concentration
Typical range	0 – 10 ppmv
Determination of the typical range (Method, criteria)	maximum simulated mean value for single altitude
Units	ppbv
Standards	-
3D Gridded fields of ClOx for fixed local time	
Parameter	
Typical range	0 – 1 ppbv
Determination of the typical range (Method, criteria)	maximum simulated mean value for single altitude
Units	ppbv
Standards	-
3D Gridded fields of NOx for fixed local time	

Parameter	-
Typical range	0 – 1 ppbv
Determination of the typical range (Method, criteria)	maximum simulated mean value for single altitude
Units	ppbv
Standards	-

Table 2.3-1. Characterization of SACADA products

2.3.2 Validation plan and validation data

VALIDATION PLAN

Evaluation of SACADA performance and products is in an early stage. Extended validation of multi-year data records is foreseen for the end of project phase 3. Additionally a cross-comparison to BASCOE results will take place for the 2003 episode using ESA MIPAS data. Currently results are available for the winter episode 2003/2004 (model version 1.7), also used for ROSE evaluation (see Section 2.2), and derived during operational model runs based on GOME-2 data. Comparisons of model version 1.7 to HALOE and ground based observations are hampered by a strong HCl biased. This has been attributed to missing chlorine reactions with OH and CH2O in the chemistry scheme. Respective reactions have been included during a model upgrade to version 2.0.

VALIDATION DATA	
Ground based observations	
Stations	N/A
***In-situ* observations**	
GAW ozone sondes observations	Availability: GAW 1996-2008 Spatial coverage: n.a. Temporal coverage: approx. one sounding per week Location (coordinates): see GAWSIS station list Accuracy: N/A
Model outputs	
ROSE-GOME	Availability: PROMOTE Spatial coverage: gobal Temporal coverage: 1996-2003 Location (coordinates): -90° South to +90° North Accuracy: <15%
Other EO data	

ENVISAT/GOMOS observations	Availability: Service d'Aéronomie (IPSL-SA) Spatial coverage: global Temporal coverage: 2002 until today Location (coordinates): n.a. Accuracy: 10 – 20% (for night and day measurements)
UARS/HALOE V19 O3 observations	Data availability and access: NASA DAAC Spatial coverage: two latitude bands (max 10° of width) by day Temporal coverage: 1992 - 2005 Location (coordinates): -75° South to +75° North Accuracy: 10%, deteriorates below 20 km altitude

Table 2.3-2. Data used for validation of the SACADA Products

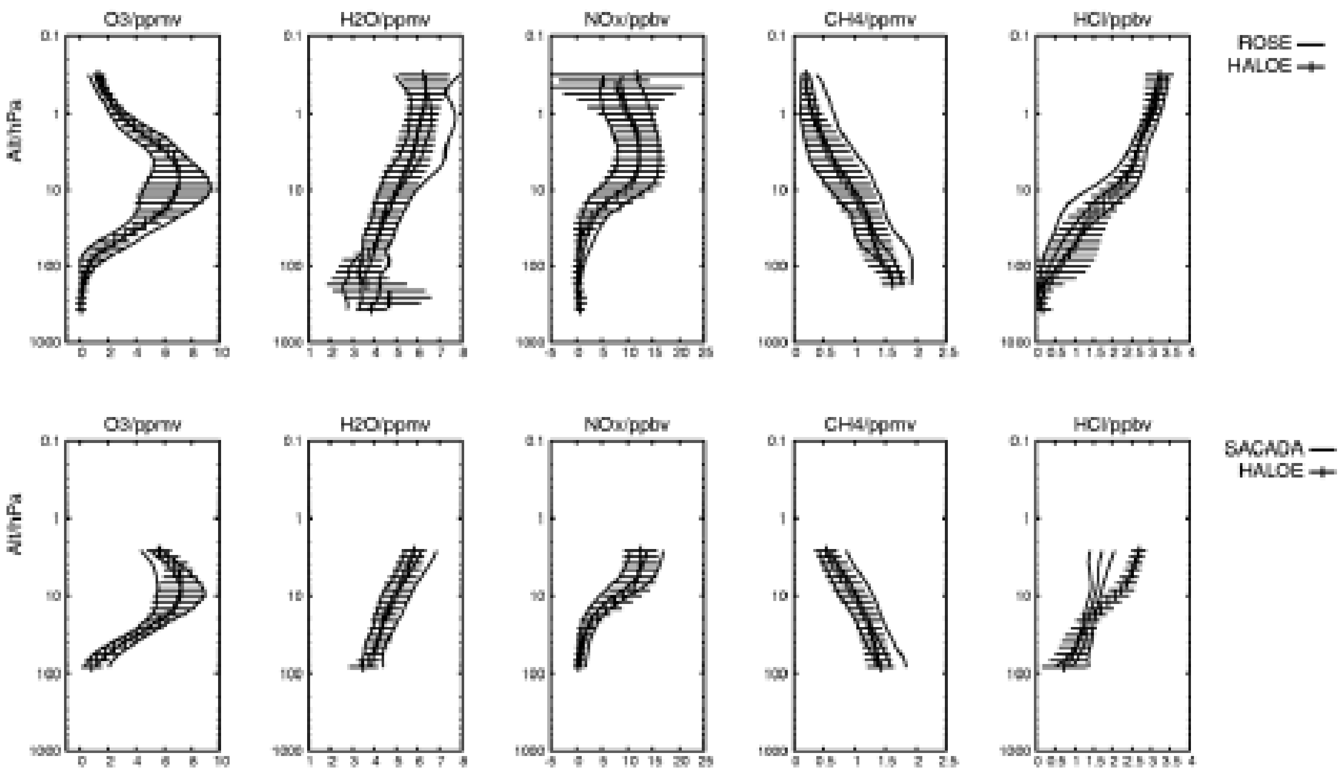


Figure 2.3-1. Global mean results showing a comparison of ROSE (first row) and SACADA (second row) results to respective HALOE observations covering the time period October – March 2003/2004. The indicated scatter (horizontal bars for observations and lines for model analyses) shows the standard deviation from the mean.

2.3.3 Validation of individual components

As mentioned above, current comparisons of SACADA products to independent observations are strongly affected by a model HCl deficit in the upper stratosphere. Because upper stratospheric ozone depends on HCl background concentrations actual comparisons show also a considerable ozone bias. In Table 2.3-3 results for the 100 – 2 hPa altitude regions for October – March 2003/2004 using HALOE observations are included. HALOE HCl and NOx were only considered above 56hPa due to poor data quality in lower altitude regions. The current model set-up applies ECMWF/GME meteo data using GME to calculate 24h forecasts.

Basically, identical validation procedures are foreseen for both SACADA and ROSE results. Because complete ROSE results will be available at the end of project phase 1, they can be used to additionally assess SACADA performance and product quality.

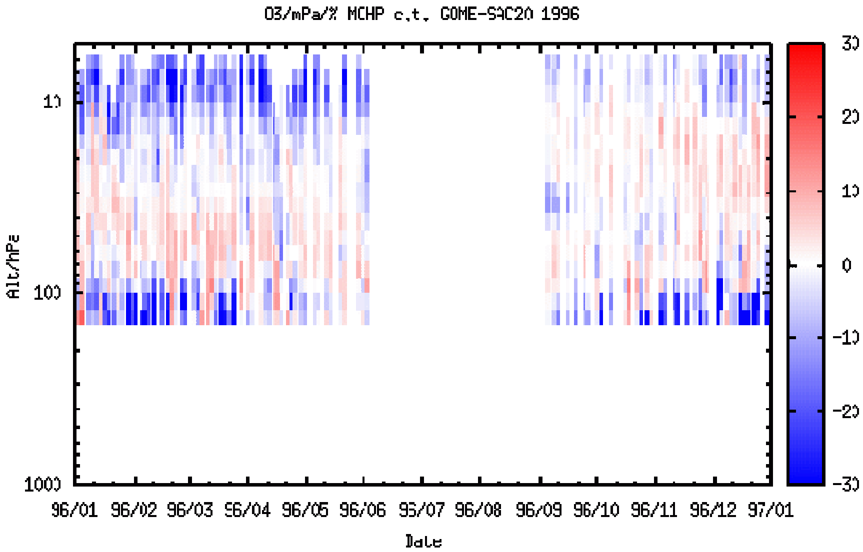
For SACADA products the same chemistry-transport model issues and restrictions as discussed with respect to ROSE are found (see 2.2). In contrast to ROSE, sequential assimilation the 4 D-VAR schemes is more sensitive to model bias. In the case of the identified HCl deficit, this has been demonstrated by deliberately withdrawing the HCl producing reactions in ROSE. In addition, both models showed a strong HCl reduction. This effect was more pronounced in SACADA leading to lower ozone concentrations throughout the upper stratosphere.

VALIDATION OF INDIVIDUAL COMPONENTS	
Accuracy	
Systematic uncertainty	
Random uncertainty	
Quality assessment	
Monitoring of OMF residuals	Daily zonal mean observation minus first-guess (OMF) differences: zonal mean = $\sum$ OMF_i , for all model longitudes i with observations Rejection of observational data which deviates by more than factor 10 from first-guess
OMF error statistics for single pressure levels	Daily accumulated OMF differences for each model grid point: daily average = $\sum$ OMF_i , for all observations i available
MODELS/ASSIMILATION	

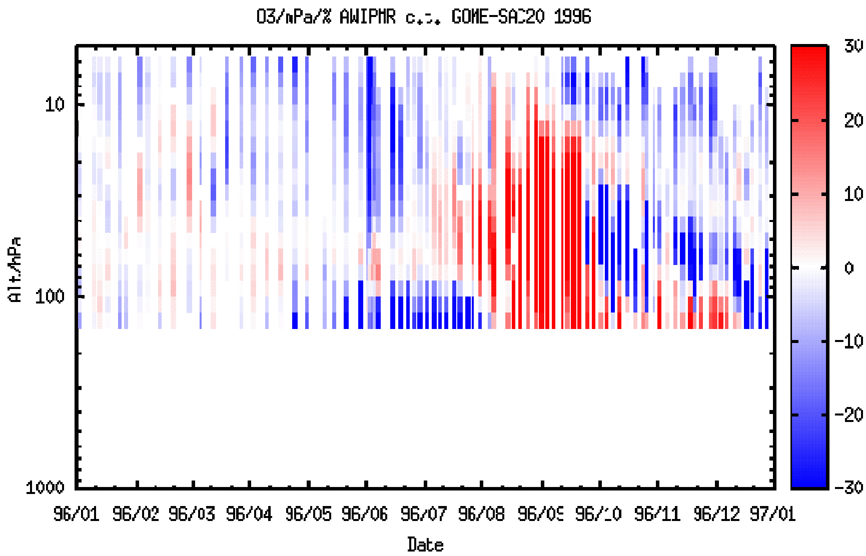
ROSE	ERS-2 GOME/NNORSY assimilated ozone record 1996-2003 Comparisons to daily ozone mixing ratios
BASCOE	ENVISAT MIPAS assimilated ozone record 2002-2004 Comparisons to daily ozone mixing ratios
SACADA	HCl bias due to missing chlorine reactions with OH and CH2O in the chemistry scheme

Comparison to GAW Ozone soundings (WOUDC)

Mean deviation from 69 ozone soundings <5% between 40 and 10 hPa, <10% for other altitudes



Comparison results for Hohenpeissenberg (above) and Neumayer station (below) showing the relativ difference of ozone partial pressure between station and GOME-ROSE reanalysis for 1996.



Same as above, but for Neumayer station, Antarctica (70.65°S, 8.26°W).

Comparison to GOMOS/ENVISAT	N/A
Comparison to UARS/HALOE (NASA)	HCl and NOx were only considered above 56hPa due to poor data quality in lower altitude regions
	SACADA c.t. HALOE (100–2 hPa) obs mean bias/% rms/% O3 65582 4.99 -0.43 13.09 H2O 65584 5.11 4.47 10.00 Nox 55761 6.85 -11.75 24.25 CH4 65452 4.05 6.49 12.45 HCl 55768 1.27 -59.36 75.64 Global mean/ppmv, bias/ppmv (SACADA-HALOE) and rms/% results

Table 2.3-3. Validation of individual components of SACADA products

2.3.4 Validation against specifications and against user requirements

In phase II SACADA has been updated to version 2.0. Among other improvements to the CTM, the number of chemical species and reactions were increased. For example, the OH+ClO -> HCl+O2 reaction was added to increase upper stratospheric HCl values. To allow for the assimilation of ozone columns from the new GOME-2 instrument an additional observation operator has been developed. GOME-2 analysis results are available since late 2007. The offline processing of GOME/NNORSY data has been started recently. Completion of the 1996-2003 period is expected until the end of 2008. First comparisons to BASCOE reanalysis are shown in Figure 2.3-2.

*Requirements written in *italics* were not compulsory in Phase 2.

VALIDATION AGAINST SERVICE SPECIFICATIONS AND USER REQUIREMENTS FOR SACADA PRODUCTS			
No limitations/delays for compliance between theoretical and actual service specifications have been indicated by the service provider.			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Parameters *-GSE-PRO2	3D-O3S: 3D Gridded fields of ozone mixing ratios *3D-Clx: 3D Gridded fields of ClOx for fixed local time* *3D-NOx: 3D Gridded fields of NOx for fixed local time*		
Accuracy	3D-O3S: rms<15%, bias <1% 3D-Clx: rms<25%, bias <1% 3D-NOx: rms<25%,	n.s.	3D-O3S: rms<15%, bias <1% 3D-Clx: N/A 3D-NOx: rms<25%, bias <1%

	bias <1%		
Accuracy minimum	n.s.	*For O3:* *Mesosphere: 15%* *Stratosphere layers: 15%* *Total column: 5%*	n.s.
Accuracy target	n.s.	*For O3:* *Mesosphere: 3%* *Stratosphere layers: 3%* *Total column: 1%*	3D-O3S: rms<10%, bias <1% 3D-Clx: rms<25%, bias <1% 3D-NOx: rms<25%, bias <1%
Spatiotemporal characteristics			
Spatial coverage	3D Global 1000-0.1 hPa	Global	3D Global 1000-0.1 hPa
Horizontal resolution	250 Km (truncated to 2.5°)	*2.8°x2.8°; 50 Km for lower Troposphere*	250 Km (truncated to 2.5°)
Vertical resolution	1.5 Km (lower Stratosphere)	*1 km*	1.5 Km (lower Stratosphere)
Grid/Projection	Interpolated on Lat-long grid from original icosahedron grid on sigma-pressure levels	*Lat-long*	Interpolated on Lat-long grid from original icosahedron grid on sigma-pressure levels
Temporal coverage	1995-2005	*As long as possible (>20 years per record)*	2003-2004
Temporal resolution	Daily synoptic and fixed local time analysis every 6 h	Daily	Daily synoptic and fixed local time analysis every 6 h
User Interfaces			
PROMOTE Web	Complete, operational and up to date	*Complete, operational and up to date*	Complete, operational and up to date
On demand	Email contact	n.s.	Email contact
Data formats and data delivery			
Data availability	1996-2005	n.s.	2003-2004
Data access	n.s.	On demand *Freely downloadable from PROMOTE Web*	On demand

Delivery Mode	Records offline some actual base products online (no NRT)	*Online (no NRT)*	no NRT
Delivery frequency	n.s.	Data agreed with user. *End of Phase 1*	agreed with user
Data Format	HDF4, NetCDF	*ASCII, HDF, CDF*	HDF4, NetCDF
Historical archive	Reanalysis of ERS-2 and ENVISAT since 1995	n.s.	Reanalysis of ERS-2 and ENVISAT since 1995
Visualization	Quicklooks for single pressure levels (60, 20, 10 hPa) in different projections. HDF4, NetCDF.	n.s.	Quicklooks for single pressure levels (60, 20, 10 hPa) in different projections. HDF4, NetCDF.

Table 2.3-4. Validation of SACADA products against specifications and against user requirements

2.3.5 SACADA quality assessment and control

*Requirements written in *italics* were not compulsory in Phase 2.

QUALITY ASSESSMENT AND CONTROL PROCEDURES				
Service delivery start date: Online delivery of 1996-2003 period is ongoing (t.b. finished until Dec, 2008)				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**checks/Delivery period**
Quality checks	Continuous monitoring of OMF error residuals for observed species See Table 2.3-3.	n.s.	Continuous assessment See Table 2.2-3	Phase 2: Online cjhecks depend on data coverage (avg. 16000 p.d.).

Product confidence data	n.s.	n.s.	HALOE, SAGEII	Phase 2: Mean data coverage 30 ozone profiles p.d.
Error bar definition and representation	1 sigma	*Total error; 1 sigma error bar (standard deviation)*	Standard deviation	Phase 2: Monthly data base (approx. 1000 value pairs p.d.)
Representation of missing data	Data coverage and outliers are reported for 3D Ozone profile records	*Filled with higher order regression; cloud and event flags*	Data gaps indicated by high analysis error	Phase 2: Certain periods with reduced coverage: Jan, Mar, Jun 1996; Nov 1999; Feb, Jul 2000; Jan, Feb 2001; Jul 2003 onwards
Documentation of process failure	Convergence of chemical solver is reported	n.s.	convergence of numerical solver for CTM and 4DVAR	n.s.
Version control mechanisms and representation	Changes are reported, processor version number is increased – this is also indicated in HDF data set	*Number scheme to be defined in S5 Specifications*	GOME/NNORSY V3; SACADA 2.0	Phase 2: CTM update

Table 2.3-5. Quality assessment and control procedures for SACADA

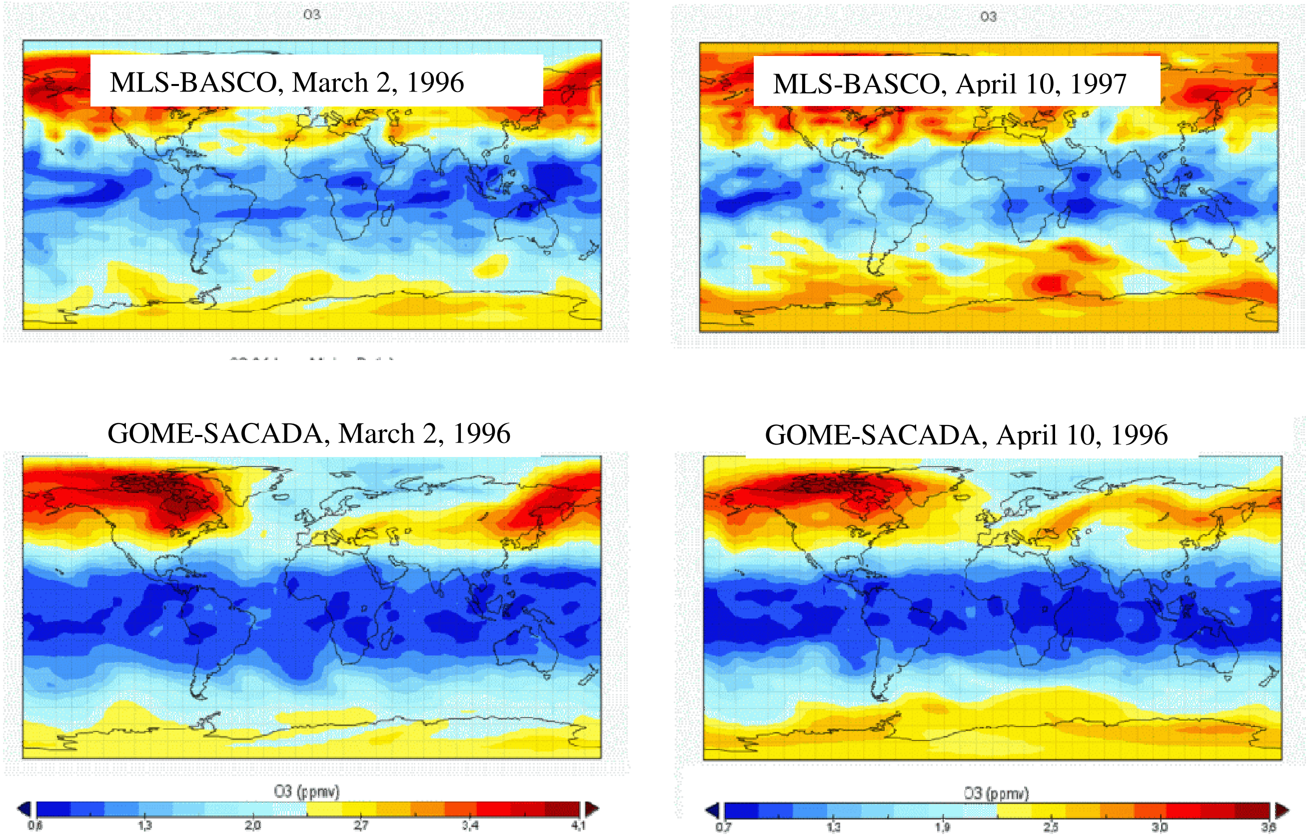


Figure 2.3-2. Ozone mixing ratios derived by MLS-BACOE (above) and GOME-SACADA (below) for the 20 km altitude level. Results illustrate the impact of satellite coverage for two different days. Right top frame: higher ozone levels in the Northern Hemisphere in BASCOE due to missing MLS observations.

2.4 BASCOE Products

BASCOE products consist of vertically resolved global synoptic analysis of stratospheric ozone mixing ratios (3D ozone) and total inorganic chlorine (Cly). Analyses are derived by 4D-Var assimilation of UARS/MLS and MIPAS trace gas observations. To check the consistency of results and analyse model/instrument bias Observation minus First-guess (OMF) residuals are stored along the ozone analysis and its errors. Additionally comparisons of ozone and related trace gases to independent observations (ground based and satellites) are performed.

Service is/will be operational since/after: N/A

Research partners: DLR

Provider(s): BIRA-IASB

Validation contact: Quentin Errera (BIRA-IASB)

2.4.1 BASCOE Product Characterization

PRODUCT CHARACTERISATION	
3D Gridded fields of ozone mixing ratios	
Parameter	Ozone volume mixing ratio (vmr)
Typical range	0-12 ppmv
Determination of the typical range (Method, criteria)	N/A
Units	ppmv
Standards	-
3D Gridded fields of Cly for fixed local time	
Parameter	CLy volume mixing ratio (vmr)
Typical range	0-3.5 ppbv
Determination of the typical range (Method, criteria)	N/A
Units	Ppbv
Standards	-

Table 2.4-1. Characterization of BASCOE Products

2.4.2 Validation plan and validation data

VALIDATION PLAN

Evaluation of BASCOE ozone from MIPAS assimilation, started during phase 1, is now summerized in Errera et al. (2008). The uncertainties of the ozone analyses have been estimated using observations from HALOE and POAM-III. In general, the bias does not exceed ±15% with a standard deviation below 15%. They are exceptions where these values are not valid. At the tropopause, the bias and standard deviation range between +30±30% (Poles) and +45±70% (tropical tropopause). During the 2003 ozone hole, observed values are very low and relatived differences become mainingless. In absolute units, bais and standard deviation are around -3±3 10^{11} molec/cm^3 at 70 hPa (to compared to absolute value 4 10^{12} molec/cm^3 outside ozone hole conditions). During the 2002 Austral Spring, an important disagreement is found between BASCOE and independent observations. It happened that the horizontal resolution of BASCOE (5° lon by 3.75° lat) is too coarse to reproduce accurately the vortex split and, hence, the ozone depletion.

Evaluation of BASCOE ozone from UARS/MLS assimilation has started in phase 2 and is summerized in Viscardy et al, (submitted to JSTARS, under review). The evaluation has been done using independent data from HALOE, ozonesondes and groundbased lidar observations. Outside the South Pole polar vortex and the tropopause region, BASCOE agree well (generally better than 10%) with independent observations, with the tendency by be baised high (e.g. Figure X1). In the polar vortex, BASCOE overestimates the observations, probably due to the use of ERA40 dynamical fields used to drive BASCOE. Moreover, the departure between BASCOE and independent observations increase during the UARS/MLS period. This is partly due to: (1) the decreasing number of observed days by MLS throughout the mission (from ~320 in 1992 to only 68 in 1999) combining with the decrease of data quality after mid-1997 due to the cessation of the radiometer providing temperature and (2) the ERA40 dynamical fields. Finaly, at the tropopause, BASCOE overestimates independent observations (around 50% of disagreement vs o3sondes at 100 hPa, not shown).

Evaluation of BASCOE Cly from MIPAS and UARS/MLS has started in phase 3 where only a qualitative evaluation has been made. The Cly family is sum of the vmr of the following chloring species: 2xCl2O2 + OClO + BrCl + HOCl + ClONO2 + Cl + HCl + ClO + ClNO2 + ClOO. However, taking BASCOE as references, only few of the species have a significant contribution in the total inorganic chlorine: HCl account for almost 100% Cly in the upper stratosphere, the lower mesosphere, more than 90% in the lower stratosphere and more than 50% in the mid-startosphere (and less than 10% around and inside the polar vortex). Adding ClONO2 to HCl and one has almost 100% of Cly except in the upper stratosphere where ClO contribute to 10% and in the polar vortex region where ClONO2 contribute up to 70% at the vortex edge and 30% inside the vortex. The other contribution to Cly in the polar vortex are to the ClOx (ClO+Cl2O2) family. In this situation, validation of the BASCOE Cly product might need independent observervations of HCl, ClONO2 and ClOx.

Errera et al. (2009) have shown that O3 assimilated data can constain the BASCOE HCl in the mid-high stratosphere. However, this constain appear to be weak and thus is only valid in the first year of the MLS mission when the number of operated days is important. Moreover, BASCOE HCl also depend on the used ECMWF dynamical fields ERA-40 or ERA-Interim (Errera et al., 2009). Thus, at this stage, it is not clear if BASCOE HCl come from a pure assimilation or a CTM run. For these reason, BASCOE Cly products are not released.

Data used for the validation of the BASCOE products are summarized in Table 2.4-2 below.

VALIDATION DATA FOR BASCOE PRODUCTS	
Ground based observations	
N/A	N/A
***In-situ* observations**	
Ozone sondes	See Geer *et al.* (2006)
NDACC Ozone sondes	Availability: web Spatial coverage: N/A Temporal coverage: N/A Location (coordinates): -90° South to +90° North Accuracy: 5% between 0 and 20 km; 7% between 20 and 35 km
NDACC Lidar	Availability: web Spatial coverage: N/A Temporal coverage: N/A Location (coordinates): -90° South to +90° North Accuracy: 2% between 20 and 40 km
Other EO Data	
MIPAS	See Geer *et al.* (2006)
TOMS	See Geer *et al.* (2006)
UARS/HALOE V19 O3 observations	Availability: web Spatial coverage: two latitude bands (max 10° of width) by day Temporal coverage: Sep 1991 – Nov 2005 Location (coordinates): -75° South to +75° North Accuracy: >15% below 22 km in the Tropics; 4-12% throughout the rest of the stratosphere (Morris *et al.*, 2002, *JGR*)
UARS/HALOE V19 HCl observations	Availability: NASA DAAC Spatial coverage: two latitude bands (max 10° of width) by day Temporal coverage: Sep 1991 – Nov 2005, approx. 30 profiles per day Location (coordinates): -75° South to +75° North Accuracy: 9-18% (Russell *et al.*, 1996, *JGR*)
POAM-III O3	Availability: web

observations	Spatial coverage: two latitude bands around the Poles Temporal coverage: 1998 – 2005, approx. 30 profiles per day Location (coordinates): -65° to -85° (SH); +55° to +70° (NH) Accuracy: <5% from 13 to 60 km (Randall et al., 2003, *JGR*)

Table 2.4-2. Data used for validation of BASCOE Products

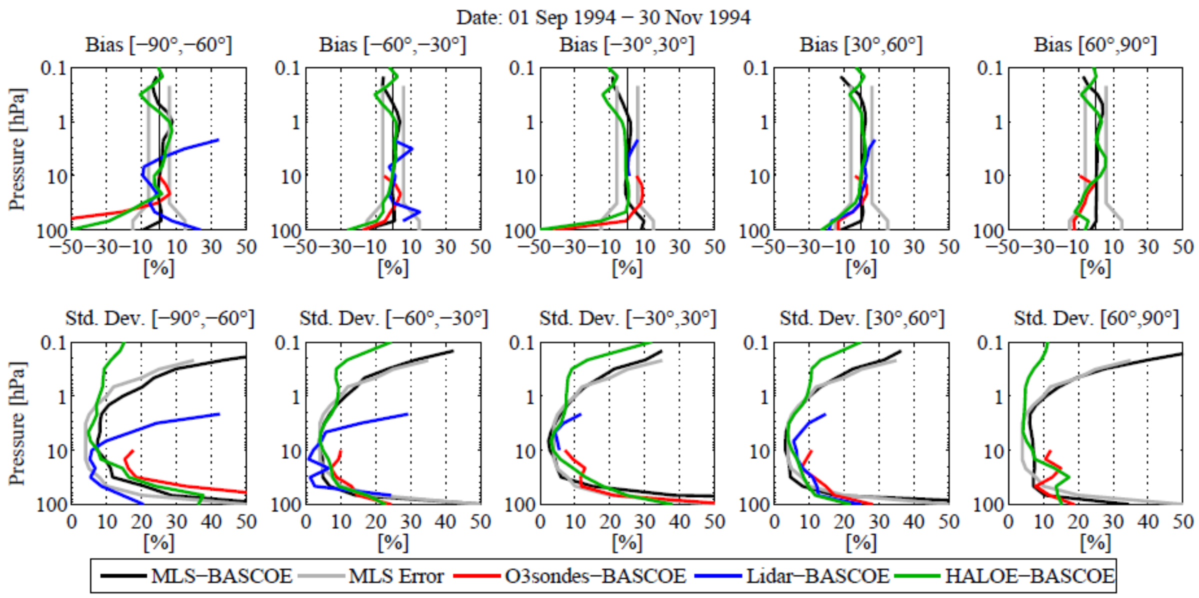


Figure 2.4-1. Mean differences (bias) and standard deviations between observations and BASCOE analyses between September 1, 1994 and November 30, 1994. These observations are MLS (black line), ozonesondes (red line), lidar (blue line) and HALOE (green line). The grey lines represent the estimated MLS bias and precision. The range of latitudes is divided into 5 bands. A positive value of the bias indicates that the analyses are lower than the observations. From Viscardy et al., submitted to JSTARS.

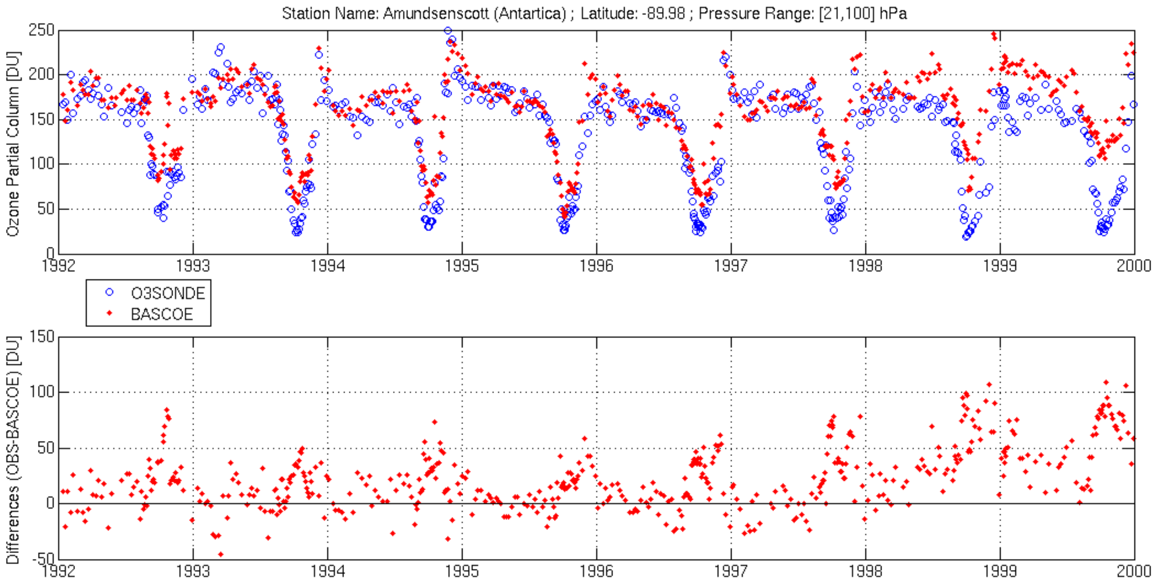


Figure 2.4-2. Comparison between BASCOE Ozone analyses from UARS/MLS assimilation and independent ozonesondes observations at South Pole at 68 hPa for the time period [1992-1999].

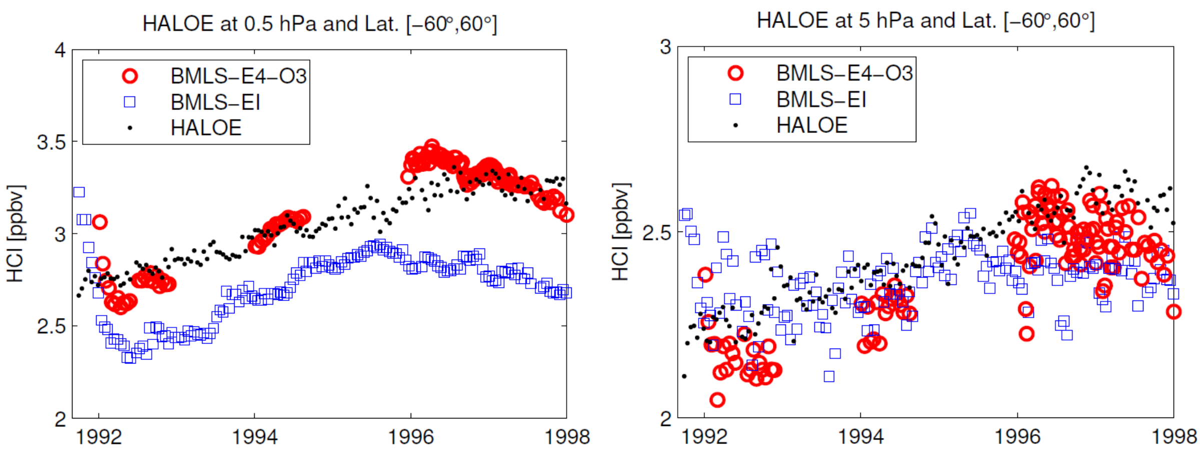


Figure 2.4-3. Time series between September 1991 and December 1998 of HALOE HCl (black dots) averaged over 15 days and between 60°S and 60°N. The red circles correspond to BASCOE analyses based on UARS/MLS assimilation of O3 only using ERA-40 dynamical fields (for several period only) and blue squares correspond to BASCOE analyses of UARS/MLS assimilation (all species) using ERA-Interim.

2.4.3 Validation of individual components

<table>
<tr><td>Estimated uncertainties mean bias (BIAS_OMA) and its standard deviation (STD_BIAS_OMA) based on comparison of BASCOE v4q09 and independent observations (see Fig. 4-1).</td><td>

Pressure	[-90°,-60°]	[-60°,-30°]	[-30°,30°]	[30°,60°]	[60°,90°]
0.46 hPa	-6±9 %	-7±9 %	-11±8 %	-3±11 %	-4±6 %
1 hPa	6±8 %	1.5±9 %	-3±8 %	5±9 %	3.5±5 %
4.6 hPa	3.5±5 %	-2±4 %	-1±4 %	2±4 %	7±4 %
10 hPa	3±8	-1±5 %	-1±4 %	-1±5 %	3±7 %
46 hPa	-6±	-6±9 %	-10±18 %	-10±10 %	-12±14 %
Tropopause	20±29 %	-17±29 %	-42±55 %	21±44 %	13±25 %

</td></tr>
<tr><td>BASCOE Validation against SAGE II</td><td>N/A</td></tr>
</table>

Table 2.4-3 provides a detailed description of the parameters used for the validation as well as a summary of the results obtained after comparing HALOE and BASCOE.

<table>
<tr><th colspan="2">VALIDATION OF INDIVIDUAL COMPONENTS FOR BASCOE PRODUCTS</th></tr>
<tr><td colspan="2">Quality assessment for BASCOE Products</td></tr>
<tr><td>Instrument monitoring</td><td>Independent data sets form non-assimilated instruments (e.g. HALOE) are monitored by BASCOE, i.e. BASCOE state is stored in the observation space of non-assimilated instrument. Our monitoring method follows these rules: (1) at each BASCOE time step (30 min), seek any occurrence of independent data. If any occurrence is found, (2) make a tri-linear interpolation of BASCOE at every location of the profiles (lon, lat, alt) for every observed species (only profiles are considered). This monitoring is done during the first and last 24 hours run of the minimization and is used to calculate the observation minus forecast and analysis, respectively (i.e. OMF and OMA).</td></tr>
<tr><td>OMA, OMF</td><td>Observation Minus Analysis, Observation Minus Forecast:

OMA=(O-A);

OMF=(O-F);

Where: O is the observed vmr, A is the analysis vmr in the observation space (see Instrument monitoring), F is the forecast vmr in the observation space (see Instrument monitoring).</td></tr>
<tr><td>DAY_MEAN_SS_OM</td><td>For each day, each occultation mode (sunset or sunrise) and each pressure</td></tr>
</table>

A, DAY_MEAN_SR_OMA, DAY_STD_SS_OMA, DAY_STD_SR_OMA (Also for _OMF)	layer, the mean and standard deviation between observations and analysis is calculated as: $Mean(OMA) = 100 \times \frac{\sum_{i=1}^{N}(O_i - A_i)}{\sum_{i=1}^{N} O_i}$, in % $STD(OMA) = 100 \times \frac{\sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(O_i - A_i)}}{\sum_{i=1}^{N} O_i}$, in % N being the number of used observations. We use 13 pressure ranges, the boundary being defined as: [0.1, 0.147, 0.316, 0.681, 1.47, 3.16, 6.81, 14.7, 31.6, 68.1, 147, 316, 681, 1000] hPa. This diagnostic is only available for occultation instruments (HALOE, SAGE-II). Obviously, these parameters only consider observation of the same constituent.
DAY_MEAN_LAT_OMA, DAY_MEAN_LAT_OMA, DAY_STD_LAT_OMA, DAY_STD_LAT_OMA (Also for _OMF)	For each day, each latitude band and each pressure layer, the mean and standard deviation between observations and analysis is calculated as: $Mean(OMA) = 100 \times \frac{\sum_{i=1}^{N}(O_i - A_i)}{\sum_{i=1}^{N} O_i}$, in % $STD(OMA) = 100 \times \frac{\sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(O_i - A_i)}}{\sum_{i=1}^{N} O_i}$, in % N being the number of used observations. We use 13 pressure ranges, the boundary being defined as: [0.1, 0.147, 0.316, 0.681, 1.47, 3.16, 6.81, 14.7, 31.6, 68.1, 147, 316, 681, 1000] hPa. We use 5 latitude band defined as: [-90°,-60°], [-60°,-30°], [-30°,30°], [30°,60°], [60°,90°] and [-90°,90°]. Obviously, these parameters only consider observation of the same constituent.
TS_ MEAN_SS_OMA, TS_ MEAN_SR_OMA,	Time series of daily Mean(OMA) and STD(OMA) for sunset or sunrise occultation and for a given pressure range. Note that the pressure range

TS_ STD_SS_OMA, TS_ STD_SR_OMA (Also for _OMF)	should belong to the boundary pressure defined above but more than one layer can be reconsidered. Obviously, these parameters only consider observation of the same constituent.
Z_ MEAN_SS_OMA, Z_MEAN_SR_OMA, Z_STD_SS_OMA, Z_STD_SR_OMA (Also for _OMF)	Profile of the Monthly/Seasonal Mean(OMA) and STD(OMA) for a given occultation mode. Obviously, these parameters only consider observation of the same constituent.
TS_ MEAN_LAT_OMA, TS_ MEAN_LAT_OMA, TS_ STD_LAT_OMA, TS_ STD_LAT_OMA (Also for _OMF)	Time series of daily Mean(OMA) and STD(OMA) a given latitude band and for a given pressure range. Note that the pressure range should belong to the boundary pressure defined above but more than one layer can be reconsidered. Idem for the latitude. Obviously, these parameters only consider observation of the same constituent.
Z_ MEAN_LAT_OMA, Z_MEAN_LAT_OMA, Z_STD_LAT_OMA, Z_STD_LAT_OMA (Also for _OMF)	Profile of the Monthly/Seasonal Mean (OMA) and STD(OMA) for a given latitude band. Note that the given latitude band should belong to those predefined above. Obviously, these parameters only consider observation of the same constituent.
BIAS_OMA (Also for _OMF)	Bias (in %) between analysis and independent observation can be estimates from average the daily mean alogn a given period. It correspond to: BIAS = MEAN(DAY_1_MEAN_*_OMA, …, DAY_N_MEAN_*_OMA) In time, it can consider (1) the whole temporal set of data (global), (2) an annual set of data (yearly), (3) a seasonal set of data (seasonal), (4) a monthly set of data (monthly), … It can aslo consider only sunrise or only sunset or both occultation mode, one latitude band or more, one pressure layer or more, …
STD_BIAS_OMF	Standard deviation (in %) of BIAS parameter: STD = STD(DAY_1_MEAN_*_OMA, …, DAY_N_MEAN_*_OMA)

Models/assimilation	
MIPAS assimilation	BASCOE version v3q33 (phase 1), v4q30 (phase 2)
	BASCOE O3 analyses validation&intercomparison: See Geer *et al.*, 2006

<table>
<tr><td rowspan="2"></td><td>BASCOE H2O analyses intercomparison with ECMWF: see Lahoz et al., 2007</td></tr>
<tr><td>BASCOE analyses of HNO3 and N2O validation wrt FTIR ground-based observation: see Vigoroux et al., 2007</td></tr>
<tr><td>Estimated uncertainties based on mean bias (BIAS_OMA) and its standard deviation (STD_BIAS_OMA) between HALOE and BASCOE v4q30 and between BASCOE v4q30 and POAM-III for O3</td><td>
<table>
<tr><th>Altitude</th><th>Poles[a]</th><th>Mid Latitudes[b]</th><th>Tropics[c]</th><th>2003 Ozone hole[d]</th></tr>
<tr><td>0.5 hPa</td><td>−15±15</td><td>−7±10</td><td>−10±7</td><td>–</td></tr>
<tr><td>10 hPa</td><td>+3±7</td><td>+3±5</td><td>+2±5</td><td>–</td></tr>
<tr><td>70 hPa</td><td>+11±12</td><td>+10±13</td><td>+4±30</td><td>$-3\pm3\times10^{11}$ molec/cm^3</td></tr>
<tr><td>Tropopause[e]</td><td>+30±30</td><td>+40±80</td><td>+45±70</td><td>–</td></tr>
</table>
[a] poleward of 60° N and 60° S ;
[b] 30° N–60° N and 60° S–30° S;
[c] 30° S–30° N;
[d] poleward of 60° S;
[e] 100 hPa at the Tropics, 200 hPa at the Extra-Tropics.
</td></tr>
<tr><td>BASCOE Validation against SAGE II</td><td>N/A</td></tr>
<tr><td rowspan="3">UARS/MLS assimilation</td><td>BASCOE version v4q09 (phase 3)</td></tr>
<tr><td>BASCOE O3 analyses validation&intercomparison: See Viscardy et al., submitted to JSTARS, Errera et al., 2009</td></tr>
<tr><td>BASCOE Cly analyses: see Errera et al., 2009</td></tr>
<tr><td>Estimated uncertainties mean bias (BIAS_OMA) and its standard deviation (STD_BIAS_OMA) based on comparison of BASCOE v4q09 and independent observations (see Fig. 4-1).</td><td>
<table>
<tr><th>Pressure</th><th>[-90°,-60°]</th><th>[-60°,-30°]</th><th>[-30°,30°]</th><th>[30°,60°]</th><th>[60°,90°]</th></tr>
<tr><td>0.46 hPa</td><td>-6±9 %</td><td>-7±9 %</td><td>-11±8 %</td><td>-3±11 %</td><td>-4±6 %</td></tr>
<tr><td>1 hPa</td><td>6±8 %</td><td>1.5±9 %</td><td>-3±8 %</td><td>5±9 %</td><td>3.5±5 %</td></tr>
<tr><td>4.6 hPa</td><td>3.5±5 %</td><td>-2±4 %</td><td>-1±4 %</td><td>2±4 %</td><td>7±4 %</td></tr>
<tr><td>10 hPa</td><td>3±8</td><td>-1±5 %</td><td>-1±4 %</td><td>-1±5 %</td><td>3±7 %</td></tr>
<tr><td>46 hPa</td><td>-6±</td><td>-6±9 %</td><td>-10±18 %</td><td>-10±10 %</td><td>-12±14 %</td></tr>
<tr><td>Tropopause</td><td>20±29 %</td><td>-17±29 %</td><td>-42±55 %</td><td>21±44 %</td><td>13±25 %</td></tr>
</table>
</td></tr>
<tr><td>BASCOE Validation against SAGE II</td><td>N/A</td></tr>
</table>

Table 2.4-3. Validation of individual components of BASCOE Products

2.4.4 Validation against specifications and against user requirements

*Requirements written in *italics* were not compulsory in Phase 2.

VALIDATION AGAINST SERVICE SPECIFICATIONS AND USER REQUIREMENTS FOR BASCOE PRODUCTS			
Indicate limitations/delays for compliance between theoretical and actual service specifications.			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product(s)	-3D Gridded fields of ozone mixing ratios [3D-O3B*] -3D gridded fields of Cly for fixed local time [3D-CLY*]		
Accuracy O_3	RMS [3D-O3B*]<35% Bias [3D- O3B *]<10%	*< 5%*	See Table 2.4-3[1]
Accuracy Cl_y	RMS [3D-CLY*] N/A Bias [3D- CLY*] N/A	-	N/A
Accuracy minimum O_3	n.s.	*For O3:* *Troposphere: 20%* *Mesosphere: 15%* *Stratosphere: 15%* *Total column: 5%*	See Table 2.4-3 (note that the altidude pressure is rather different)
Accuracy minimum Cl_y	n.s.	n.s.	N/A
Accuracy target O_3	-	*For O3:* *Troposphere layers: 3%* *Troposphere column: 5% Mesosphere: 3%* *Stratosphere layers: 3%* *Total column: 1%*	idem above
Accuracy target Cl_y	n.s.	*n.s.*	N/A
Spatial coverage	Global (1000-0.1 hPa)	Global	Global (1000-0.1 hPa)
Horizontal resolution	550(lon)x400(lat) Km^2 truncated to 5°x3.75°	*2.8°x2.8°; 50 Km for lower Troposphere*	550(lon)x400(lat) Km^2 truncated to 5°x3.75°
Vertical resolution	1.5 Km (lower stratosphere) 37 vertical levels	*1 km*	1.5 Km (lower stratosphere) 37 vertical levels
Grid/Projection	Hybrid sigma-p grid	*T42*	Interpolated on latitude-longitude grid on sigma-pressure levels

[1] Here, Standard deviation is given instead of RMS.

Temporal coverage	1992-1999 (UARS/MLS) 2002-2004 (ENVISAT/MIPAS)	1992-1999. *As long as possible; optimal if more than 20 following years*	1992-1999 (UARS/MLS analyses) Jul 2002 - Mar 2004 (21 months, MIPAS analyses)
Temporal resolution	Daily synoptic and fixed local time analysis every 6 hours	*Daily*	Daily
User Interfaces			
PROMOTE Web	Operational, complete and up-to-date	Operational, complete and up-to-date	Operational, incomplete and up-to-date
On demand	n.s.	n.s.	Available
Data formats and data delivery			
Data availability	UARS/MLS: 1992-1999; MIPAS: October 2002 to March 2004	1992-1999. *Long-term records; as long as possible; >20 years*	UARS/MLS: 1992-1999; MIPAS: July 2002 to March 2004
Data access	n.s.	n.s.	online via www
Delivery Mode	Records offline/actual base products online (no NRT)	*Online (no NRT)*	Online
Delivery frequency	On demand	Once per phase	One per phase
Data Format	HDF4	*ASCII, HDF, CDF*	HDF4 (netCDF on request)
Historical archive	Reanalysis available since 1992	n.s.	Phase 1: ENVISAT/MIPAS Oct 2002–Mar 2004 (BASCOE v3q33) Phase 2: ENVISAT/MIPAS Jul 2002-Mar 2004 (BASCOE v4q30) UARS/MLS 1992-1999 (BASCOE

			v4q09)
Visualization	Quicklooks for single pressure levels (60, 20, 10 hPa) in different projections	n.s.	n.a.
REMARKS			
No remarks			

Table 2.4-4. Validation of BASCOE against specifications and against user requirements

2.4.5 Quality assessment and control procedures

*Requirements written in *italics* were not compulsory in Phase 2.

QUALITY ASSESSMENT AND CONTROL PROCEDURES				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**N checks/Delivery period**
Quality checks	Continuous monitoring of OMF error residuals for observed species See Table 2.4-3	n.s.	Yes, OIQC, see Errera et al., 2008	One check per assimilated day
Product confidence data	n.s.	n.s.	n.s.	n.s.
Error bar definition and representation	1 sigma	*Total error; 1 sigma error bar (standard deviation)*	Bias and Std vs indep. obs.	See Table 4-3
Representation of missing data	Data coverage and outliers are reported for 3D Ozone profile records	*Filled with higher order regression; cloud and event flags*	No output missing data. If input missing data, output is from CTM run (no assim.)	n.s.

Documentation of process failure	Convergence of chemical solver is reported	n.s.	N/A	N/A
Version control mechanisms and representation	Changes are reported, processor version number is increased – this is also indicated in HDF data set	*Number scheme to be defined in S5 Specifications*	BASCOE version number provide with analyses	UARS/MLS assim.: v4q09; MIPAS assim.: v4q30

Table 2.4-5. Quality assessment and control procedures for the BASCOE products

2.5 References

2.5.1 Electronic references and online data access paths

This service is briefly described on the promote web site: http://www.gse-promote.org (→ 3D ozone Stratospheric Ozone Profile Record)

BASCOE ozone analyses from MIPAS and UARS/MLS are available through: www.bascoe.oma.be/promote

ROSE/DLR and SACADA are assimilation systems basically used at DLR for the processing of GOME, SCIAMACHY and MIPAS trace gas observations. Background information on the ROSE assimilation service can be found at WDC-RSAT pages: http://wdc.dlr.de/data_products/SERVICES. Access to previous and up-coming PROMOTE results is also provided by WDC-RSAT: http://wdc.dlr.de/data_products/SERVICES/rose/gome_rose_data_o3.php

2.5.2 Bibliographic references

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