



GSE – PROMOTE 2
C6 Validation Report

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TASK: -2-



TITLE:

GMES SERVICE ELEMENT
PROMOTE 2

C6 Validation Report
TOTAL OZONE SERVICE
Version 1




GSE - PROMOTE 2
C6 Validation Report
Total Ozone

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DOCUMENT STATUS SHEET

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DOCUMENT CHANGE RECORD

| Issue | Date | Modified Items / Reason for Change |
|------------------|------------|---|
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| 0.2 | 27.02.2007 | Specifications and SLA Specifications implemented in draft template |
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| Version 2 | | |
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| 1.1 | 20.05.2008 | template updated and distributed |
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| 1.8 | 20.06.2008 | Document edited and ready for final review |

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LIST OF ACRONYMS

| | |
|-----------|---|
| ACC | Anomaly Correlation Coefficient |
| CTM | Chemistry Transport Model |
| DLR | German Aerospace Centre |
| DOAS | Differential Optical Absorption Spectrometry |
| ECMWF | European Centre for Medium-Range Weather Forecasts |
| FRESCO | Fast Retrieval Scheme for Cloud Observables |
| GOME | Global Ozone Monitoring Instrument |
| HDF | Hierarchical data format |
| KNMI | Royal Netherlands Meteorological Institute |
| MEDSUN | Mediterranean sun protection service |
| NRT | Near Real Time |
| OMF | Observation Minus Forecast |
| RIVM | National Institute of Public Health and the Environment |
| S5 | Service Portfolio Specification Document |
| SCIAMACHY | SCanning Imaging Absorption spectroMeter for Atmospheric CartographY |
| SPARC | Stratospheric Processes and their Role in Climate (a WCRP core project) |
| TEMIS | Tropospheric Emission Monitoring Internet Service |
| UV | Ultra Violet |
| 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 TOTAL OZONE SERVICE

1.1 Service summary

PROMOTE 2 products dealing with Ozone records, monitoring and forecast, are provided by two services: the Total Ozone Service and the demonstration Service providing 3D Ozone Records. Figure 1.1-1 shows the structure of the Ozone Services within PROMOTE 2.

Figure 1.1-1 Structure and position of the Total Ozone Service within PROMOTE 2 Ozone

The total ozone service provides NRT ozone observations, forecasts of ozone fields and long-term consistent global total ozone data sets by assimilating the available multi-sensor total ozone satellite dataset into a chemical transport model driven by meteorological analysis.

1.2 NRT Total Ozone Column [GSE-PRO2-TO3-N]


Description: This service provides NRT (i.e. within 3-9 hours) access to GOME, SCIAMACHY and OMI level-2 data . The Total Ozone Column is retrieved from OMI, SCIAMACHY and GOME data by means of DOAS-type algorithms, namely, OMDOAO3 for OMI, TOSOMI for SCIAMACHY and TOGOMI and GOFAP for GOME.

Service is/will be operational since/: 2002

Research partners: none

Provider(s): KNMI

Validation contact: Ronald van der A (KNMI) and Marc Allaart (KNMI)

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1.2.1 Product Characterization

| O₃ column | |
|---|--|
| Parameter | Ozone concentration |
| Typical range | 90-500 DU (above 150 DU outside the Antarctic) |
| Determination of the typical range (Method, criteria) | Analysis of historic data |
| Maximum range | 50-700 DU |
| Units | Dobson units |
| <i>Standards</i> | <i>none</i> |


Table 1.2-1 Characterization of the products of the Total Ozone Service

1.2.2 Validation plan and validation data

Phase 1: The level 2 data from the near-real time algorithm was validated using ground-based observations. This level 2 data is retrieved from GOME and SCIAMACHY observations.

Phase 2: Comparison of OMI collection 3 ozone columns with ground data.

| VALIDATION DATA | |
|---|--|
| Ground based observations | |
| Brewer/Dobson/ DOAS/SAOZ Phase: 1+2 | Data availability and access: Access via WOUDC or NILU databases. Time period depends on station. Spatial coverage and resolution: More than 100 hundred locations over the world. Temporal coverage and resolution: Daily or weekly observations. Location(s) (coordinates): Global distribution of location Accuracy: about 1% |
| In-situ observations | |
| n.a. | |
| EO Data | |

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| | |
|-------------------------|--|
| OMI Phase: 1+2 | Data availability and access: via KNMI Spatial coverage and resolution: Global coverage Temporal coverage and resolution: Daily at 13.30 local time Orbits: all orbits Accuracy: about one percent |
| TOMS/SBUV Phase: 1+2 | Data availability and access: via KNMI Spatial coverage and resolution: Global coverage Temporal coverage and resolution: Daily sampling Orbits: all orbits Accuracy: about one percent |

Table 1.2-2 Data used for the validation of the products of the NRT Total Ozone Column sub-service

1.2.3 Validation of individual components


Phase 1: The level 2 data from the near-real time algorithm was validated using ground-based observations. This level 2 data is retrieved from GOME and SCIAMACHY observations.

The level 2 data quality depends on the quality of the level 1 data and FRESCO results. Therefore, the validation of these components is included.

First results of the validation can be found on the webpage of the ozone service http://www.gse-promote.org/services/ozone_nrt/index.html, the web page of FRESCO <http://www.temis.nl/fresco/> and for level 1 data on the SCIAMACHY validation page <http://www.sciamachy.org/validation/>.

Phase 2: The level 2 data has been compared to ground-based observations around the world. This comparison has been done for the complete period that OMI has made observations to identify possible trends in the results.

| VALIDATION OF INDIVIDUAL COMPONENTS [GSE-PRO2-TO3-N] | |
|---|--|
| Uncertainty estimators | |
| Best estimator: | Bias or Mean offset |
| Error bar | RMS |
| Mean offset | Bias |
| Quality assessment | |
| DOAS quality checks | Range total ozone = [10, 900] Solar zenith angle < 85 degree |
| Level-1 data sanity checks | Existence of spectra check Range satellite height = [700,900] km Range earth radius = [6000,7000] km |

| | | |
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|--|---|
| | Range satellite latitude = [-90.,90.] degree Range satellite longitude = [-180.,180.] degree Range solar zenith angle = [10.,180.] degree Range solar azimuth angle = [-360.,360.] degree Range viewing zenith angle = [-40.,40.] degree Range viewing azimuth angle = [-360.,360.] degree |
| DOAS fitting precision quantification | Convergence check |
| MODELS/ASSIMILATION TOOLS | |
| ECMWF Temperature fields (operational version) | Temperature correction of the ozone cross-sections |
| RETRIEVALS | |
| FRESCO+ Cloud information Version SC-v5 | Correction of the amount of ozone below the clouds Cloud fraction and cloud pressure (see documentation/references on http://www.temis.nl/fresco/) |
| TOSOMI total O ₃ version 0.42 | RMS = 4.9%; collocated ground based data (Brinksma, 2004) Mean offset = -1.5%; collocated ground based data (Brinksma, 2004 and documentation on http://www.gse-promote.org/services/ozone_nrt/index.html) |
| GOME-FD total O ₃ v1.0 | Total ozone columns based on EGOI data (see documentation on http://www.gse-promote.org/services/ozone_nrt/index.html) |

Table 1.2-3 Validation of the individual components of the NRT Total Ozone Column sub-service

1.2.4 Validation against individual components and against user requirements

*Requirements written in *Italics* are not compulsory for Phase 2

| | | | |
|---|--|------------------|---------------|
| VALIDATION AGAINST SERVICE SPECIFICATIONS [GSE-PRO2-TO3-N] | | | |
| [No delays for Phase 2 compliance reported] | | | |
| VALIDATION AGAINST USER REQUIREMENTS [GSE-PRO2-TO3-N] | | | |
| SPECIFICATION | S5 | REQUIRED* | ACTUAL |
| Product 1 | O ₃ column: Ozone column level-2 product based on SCIAMACHY and GOME observations | | |
| Accuracy | ~2% if SZA<75 | - | ~2% |



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| | | | |
|---------------------------------------|---|---|---|
| Accuracy minimum | n.s. | <10% | < 5 % |
| Accuracy target | n.s. | n.s. | 1 % |
| Spatial coverage | Global, swath 2800 km (OMI), 960km (SCIAMACHY), 14 orbits per day | Global | Global [swath 960 km, 14 orbits per day] |
| Horizontal resolution | Mostly 13x24 km, depending on instrument, latitude and viewing angle | 100 x 100 km ² (after provider) <<25x25 km ² | 30 x 80 km |
| Vertical resolution | n.a. | n.a. | n.a. |
| Grid/Projection | n.s. | n.s. | Orbits |
| Temporal coverage | Global in 1 day | n.s. | Global in 1 day |
| Temporal resolution | n.s. | n.s. | n.s. |
| User Interfaces | | | |
| PROMOTE Web | Operational complete and up to date | Operational complete and up to date | Operational, incomplete and up to date |
| ftp | Operational | Operational | Operational |
| Data formats and data delivery | | | |
| Data availability | Operational implementation based on SCIAMACHY measurements since early 2004 | n.s. | Operational implementation based on SCIAMACHY measurements since early 2004 |
| Data access | On line access within few hours after measurement | On line access within few hours after measurement | On line access within few hours after measurement |
| Delivery Mode | NRT | NRT | NRT, 3 to 9 hours after observation, depending on location |
| Delivery frequency | n.s. | n.s. | Per orbit. , 3 to 9 hours after observation |
| Data Format | HDF, ascii | ascii | HDF, ascii |

| | | |
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| | | | |
|--------------------|-------------------------------|------|-------------------------------|
| Historical archive | Ozone column available online | n.s. | Ozone column available online |
| Visualization | GIF Global images | n.s. | GIF Global images |

REMARKS

None

*Requirements written in *Italics* are not compulsory for Phase 2

Table 1.2-4 Validation against specifications and against user requirements of the SCIAMACHY and GOME Ozone column (NRT Total Ozone Column sub-service)


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1.2.5 Quality assessment and control procedures

| Service delivery start date: | | | | |
|---|--|---|---|----------------------------------|
| SPECIFICATIONS | S5 | REQUIRED* | ACTUAL | N checks/Delivery period |
| Quality checks | DOAS Quality Checks, level 1 data sanity tests | n.s. | Phase 1 | For each observations/ per orbit |
| Product confidence interval | n.s. | n.s. | unknown | n.a. |
| Error bar definition and representation | RMS | <i>Total error; 1 sigma error bar per sample</i> | Total error; 1 sigma error bar per sample | For each observations/ per orbit |
| Representation of missing data | Indicated in the browse menus | n.s. | n.a. | n.a. |
| Documentation of process failure | DOAS Quality Checks, level 1 data sanity tests | n.s. | Mayor periods (more than 2 days) are directly communicated by e-mail | No process failure in Phase 2 |
| Version control mechanisms and representation | CVS has been used for software version control. Updates of the software is communicated with a change history document on the web. | <i>Numbering scheme to be defined in the Product Specification Document</i> | CVS Specification of version in Product Specification Document and in header of data | N/A |

*Requirements written in *Italics* are not compulsory for Phase 2

Table 1.2-5 Quality assessment and control procedures for the NRT Total Ozone Column sub-service

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1.3 Total Ozone Forecast

Description: Up to 9 days (medium-range) forecasts of the total ozone distribution. Forecasts are started from ozone analyses based on SCIAMACHY and OMI near-real time ozone columns (See Section 1.2 [GSE-PRO2-TO3-N])

Service is/will be operational since/after: February 2004

Research partners: none

Provider(s): KNMI

Validation contact: R. J. van der A

1.3.1 Product Characterization


| O₃ column forecast | |
|---|---|
| Parameter | 9-day forecast of the total ozone field |
| Typical range | 90-500 DU (above 150 DU outside Antarctica) |
| Determination of the typical range (Method, criteria) | Analysis of historic data |
| Maximum range | 50-700 DU |
| Units | Dobson units |
| <i>Standards</i> | <i>none</i> |

Table 1.3-1 Characterization of the products of the Total Ozone Forecast sub-service

1.3.2 Validation Plan and Validation Data

Phase 1-3: For this product only the forecast abilities will be tested, since the ozone product itself is already validated within the total ozone records. The forecasts will be validated by comparison between forecast for n days with the analysis made with the actual observations. For this the anomaly correlation coefficient as function of time will be analysed.

The ACC is the correlation between the forecast (f) and analysed (a) deviations from climatology (c). The ACC is defined as
$$\frac{(a - c)(f - c)}{(a - c)(f - c)}$$

| | | |
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The ACC can be regarded as a skill score with reference to the climatology.


The ACC is sensitive to similarities in forecasts and analysed patterns, rather than their absolute values. In contrast to RMSE the ACC has a tendency to score large and "good" values during meridional flow situations, small and "bad" values during periods of predominantly zonal flow. This is particular the case in zonal situations when the forecast and observed positions of shallow waves are out of phase. ACC displays a weaker seasonal and annual variability than RMSE.

It has been found empirically that the level ACC=60% corresponds to the limit where the forecast does not exhibit any significant synoptic skill. It can be shown mathematically that ACC=50% corresponds to a categorical forecast for which the RMSE score is equally to a climatological statement.

This ACC will strongly depend on the ACC of the meteorological information from ECMWF used in the forecasts.

| | |
|-----------------------------|---|
| VALIDATION DATA | |
| EO Data | |
| SCIAMACHY Phase: 1+2 | Data availability and access: since August 2002 via KNMI Spatial coverage and resolution: Global coverage Temporal coverage and resolution: Daily at 10.00 local time Orbits: all orbits Accuracy: about one percent |
| OMI Phase: 1+2 | Data availability and access: via KNMI Spatial coverage and resolution: Global coverage Temporal coverage and resolution: Daily at 13.30 local time Orbits: all orbits Accuracy: about one percent |


Table 1.3-2 Data used for the validation of the Total Ozone Forecast sub-service

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1.3.3 Validation of individual components

| VALIDATION OF INDIVIDUAL COMPONENTS [GSE-PRO2-TO3-F] | |
|--|---|
| Uncertainty estimators | |
| Observation minus Forecast | OmF=Observation minus Forecast |
| Error bars | RMS |
| Quality assessment | |
| TM3-DAM forecast minus analysis for 9 days | Forecast (day n) – Analysis (day 0) Anomaly Correlation Coefficient (<i>Eskes et al., ACP, 2, 271, 2002</i>) |
| MODELS/ASSIMILATION TOOLS | |
| ECMFW (Wind, pressure, Temperature) operational version (OD) | Anomaly Correlation Coefficient |
| TM3-DAM (O ₃ Forecast) version 4.12 | Bias (day = n) = Forecast (day n) – Analysis (day 0) Number of days with anomaly correlation > 0.6 (<i>Eskes et al., ACP, 2, 271, 2002</i>) for different regions in the world |
| RETRIEVALS | |
| TOSOMI (O ₃ Column) version 0.42 | See total ozone record. |

Table 1.3-3 Validation of the individual components of the Total Ozone Forecast sub-service

| | | |
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1.3.4 Validation against specifications and against user requirements

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| VALIDATION AGAINST SERVICE SPECIFICATIONS [GSE-PRO2-TO3-F] | | | |
|--|--|--|---|
| No limitations/delays for compliance reported | | | |
| VALIDATION AGAINST USER REQUIREMENTS [GSE-PRO2-TO3-F] | | | |
| SPECIFICATION | S5 | REQUIRED* | ACTUAL |
| Parameters | Daily ozone analysis based on SCIAMACHY observations Ozone forecasts for days 1-9 | | |
| Accuracy | 2D accuracy fields, typically ~3% | - | n.a. Anomaly correlation as function of time is here the only useful parameter |
| Accuracy minimum | n.s. | 5% | n.a. |
| Accuracy target | n.s. | ≤2% | n.a. |
| Spatial coverage | Global | Global | Global |
| Horizontal resolution | 1° Lat. x 1.5° Long. | <i>Minimum: 2.8° Lat. x 2.8° Long.</i> <i>Target: <50 Km for lower troposphere</i> | 1° Lat. x 1.5° Long. |
| Vertical resolution | n.s. | n.s. | 35 layers |
| Grid/Projection | Lat-long, various projections possible | <i>Lat-long, T42</i> | Gridded on 1° x 1.5° grid cells |
| Temporal coverage | 9 days | n.s. | 9 days |
| Temporal resolution | Hourly | Daily | Hourly |
| User Interfaces | | | |
| PROMOTE Web | Operational, complete and up-to-date | Operational, complete and up-to-date | Operational, complete (includes link to NRT for data delivery) and up-to-date |



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| Data formats and data delivery | | | |
|---------------------------------------|--|---|---|
| Data availability | Operational implementation based on SCIAMACHY ozone measurements since February 2004 | As long as possible, better if more than 20 years without gaps are included | Data is available |
| Data access | n.s. | Freely available and downloadable from website | Images available at PROMOTE website. Data is available via FTP. |
| Delivery Mode | NRT; Offline for reanalysis runs | <i>NRT Forecast</i> | NRT Forecast |
| Delivery frequency | Daily | n.s. | Daily |
| Data Format | ASCII, HDF | ASCII, HDF | ASCII, HDF |
| Historical archive | Global ozone analysis and forecasts since August 2002 | n.s. | Global ozone analysis and forecasts since August 2002 |
| Visualization | GIF Images for North and South Hemispheres and globe. | n.s. | GIF Images for North and South Hemispheres and globe. |
| REMARKS | | | |
| No remarks | | | |

*Requirements written in *Italics* are not compulsory for Phase 2

Table 1.3-4 Validation against specifications and against user requirements of the Total Ozone Forecast sub-service



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1.3.5 Quality assessment and control procedures


| Service delivery start date: Phase 1 | | | | |
|---|--|---|--|-------------------------------|
| SPECIFICATION | S5 | REQUIRED* | ACTUAL | N checks/Delivery period ° |
| Quality checks | <p>Routine monitoring of forecast production chain during working hours</p> <p>Overall performance of the ozone forecasting system is studied by a-posteriori comparison of the forecast with the corresponding verifying analyses</p> | n.s. | Routine monitoring of forecast production chain during working hours | once a day (for working days) |
| Product confidence data | n.s. | n.s. | N/A | N/A |
| Error bar definition and representation | RMS | <i>Total error; 1 sigma error bar per sample</i> | Anomaly correlation | n.a. |
| Representation of missing data | n.s. | <i>n.s</i> | n.a. | n.a. |
| Documentation of process failure | n.s. | n.s. | N/A | none |
| Version control mechanisms and representation | n.s. | <i>Numbering scheme to be defined in the Product Specification Document</i> | CVS, Version in Product Specification Document and HDF metadata | N/A |

*Requirements written in *Italics* are not compulsory for Phase 2

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°Between 1st March and 2date of delivery

Table 1.3-5 Quality assessment and control procedures for the final products of the Total Ozone Forecast sub-service.

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1.4 Total Ozone Records

Sub-service description: This service provides long-term daily records of assimilated ozone distributions from OMI, SCIAMACHY, GOME and TOMS.

Service is/will be operational since/after: 2002, but will be complete (prototype) in August 2007

Research partners: none

Provider(s): KNMI

Validation contact: Ronald van der A, Marc Allaart

1.4.1 Product Characterization

| O₃ column | |
|---|---|
| Parameter | Total ozone concentration (assimilated) |
| Typical range | 90-500 DU (above 150 DU outside the Antarctica) |
| Determination of the typical range (Method, criteria) | Analysis of historic data |
| Maximum range | 50-700 DU |
| Units | Dobson units |
| <i>Standards</i> | <i>none</i> |

Table 1.4-1 Characterization of the products of the Total Ozone Records sub-service

1.4.2 Validation plan and validation data

For the total ozone records the OmF (Observation minus Forecast), OmA (Observation minus Analysis), forecast error and fiterror will be analysed, the overlap periods between different satellite instruments will be analysed, and the ozone data will be validated against ground-based data.

Data assimilation parameters

The OmF, OmA and the forecast error will be analysed as function of latitude, longitude, solar zenith angle, viewing angle, cloud fraction, surface albedo and the ozone column amount. Systematic biases will be identified. In addition the χ^2 of the fits will be



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checked. These analyses will be performed at regular time intervals to identify instrument degradation effects.

Overlap period

The overlap periods are important to identify biases between the different instruments. During these periods the ozone values are directly compared to quantify the biases as function of geolocation, cloud parameters, ozone column amounts. The overlap periods are:

22-08-1991 till 06-05-1993 : TOMS-NIMBUS7/TOMS-Meteor3

22-07-1996 till 30-06-2003 : TOMS-EarthProbe/GOME

01-07-2002 till 30-06-2003 : TOMS-EarthProbe/SCIAMACHY

01-07-2002 till 30-06-2003 : GOME/SCIAMACHY


01-10-2004 till today : SCIAMACHY/OMI

The overlap periods will be used to identify instrument degradation if possible

Ground-based data

Ground-based data will be used for the absolute validation of the assimilated fields similar as with the ozone level 2 data.

| VALIDATION DATA | |
|---|--|
| Ground based observations | |
| Brewer/Dobson/ DOAS/SAOZ Phase: 1+2 | <p>Data availability and access: Access via WOUDC or NILU databases. Timeperiod depends on station.</p> <p>Spatial coverage and resolution: More than 100 hundred locations over the world.</p> <p>Temporal coverage and resolution: Daily or weekly observations.</p> <p>Location(s) (coordinates): Global distribution of location</p> <p>Accuracy: about 1 percent</p> |
| EO Data | |
| OMI Phase: 1+2 | <p>Data availability and access: since October 2004 via KNMI</p> <p>Spatial coverage and resolution: Global coverage</p> <p>Temporal coverage and resolution: Daily at 13.30 local time</p> <p>Orbits: all orbits</p> <p>Accuracy: about one percent</p> |
| SCIAMACHY Phase: 1+2 | <p>Data availability and access: since July 2002 via KNMI</p> <p>Spatial coverage and resolution: Global coverage every 6 days</p> <p>Temporal coverage and resolution: Daily at 10.00 local time</p> <p>Orbits: all orbits</p> <p>Accuracy: about one percent</p> |


| | | |
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| | |
|------------------------|--|
| TOMS Phase: 1+2 | Data availability and access: since October 1978 via NASA-DAAC Spatial coverage and resolution: Global coverage Temporal coverage and resolution: Daily Orbits: all orbits Accuracy: about one percent |
|------------------------|--|

Table 1.4-2 Data used for the validation of the Total Ozone Records sub-service

1.4.3 Validation of individual components

| VALIDATION OF INDIVIDUAL COMPONENTS [GSE-PRO2-TO3-R] | |
|--|---|
| Uncertainty estimators | |
| Best estimator: Bias | Global bias between data assimilation results and ground observations |
| RMS | RMS |
| Quality assessment | |
| Ozone | Versus ground observations. As function of latitude, longitude, solar zenith angle, viewing angle, cloud fraction/pressure, total ozone amount, surface albedo. |
| OmF | OmF as function of time, latitude, longitude, solar zenith angle, viewing angle, cloud fraction/pressure, total ozone amount, surface albedo |
| Models | |
| ECMFW (Wind, pressure, Temperature) version | N/A |
| Retrievals | |
| TOMS cloud information version 8 | Cloud fraction and pressure (TOMS algorithm version 8) |
| FRESCO Cloud information, version SC-v5 | Cloud fraction and pressure (Wang et al., 2006) |
| OMI Cloud algorithm OMCLDO2 version 1.0.1 | Cloud fraction and pressure (Joiner et al., 2006) |
| GDP total O ₃ version 4.1 | Total ozone level 2 (Balis, 2003) |
| TOSOMI (O ₃ Column) | RMS = 4.9%; collocated ground based data (Brinksma, 2004) |

| | | |
|---|---|---|
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| | |
|---|--|
| version 0.42 | Mean offset = -1.5%; collocated ground based data (Brinksma, 2004) |
| OMDOAO3 total O ₃ version 1.0.1 | Total ozone level 2 (http://www.knmi.nl/omi/research/product/Ozone/omdoao3.html) |
| TOMS total O ₃ version 8 | Total ozone level 2 (TOMS algorithm version 8) |

Table 1.4-3 Validation of the individual components of the Total Ozone Records sub-service

1.4.4 Validation against specifications and user requirements

*Requirements written in *Italics* are not compulsory for Phase 2

| VALIDATION AGAINST SERVICE SPECIFICATIONS [GSE-PRO2-TO3-R] | | | |
|--|--|--|----------------------|
| No limitations/delays for compliance between theoretical and actual service specifications and requirements reported | | | |
| VALIDATION AGAINST USER REQUIREMENTS [GSE-PRO2-TO3-R] | | | |
| SPECIFICATION | S5 | REQUIRED* | ACTUAL |
| Parameter | 30 Year record of ozone analysis based on ozone observations | | |
| Accuracy | 2D field | n.s. | N/A |
| Accuracy minimum | n.s. | n.s. | n.s. |
| Accuracy target | n.s. | <i>Enough to detect 1% variation trend in 10 years</i> | 1 % |
| Spatial coverage | Global | Global | Global |
| Horizontal resolution | Two dimensional data sets on a 1 degree latitude by 1.5 degree longitude grid. | <25x25 km ² | 1° Lat. x 1.5° Long. |
| Vertical resolution | 35 layers | n.a. | 35 layers |
| Grid/Projection | n.s. | n.s. | 1° Lat. x 1.5° Long. |
| Temporal coverage | 1979-present | n.s. | 1979-present |
| Temporal resolution | 6 hours | daily | daily |
| User Interfaces | | | |

| | | |
|---|---|---|
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| | | | |
|---------------------------------------|---|---|---|
| PROMOTE Web | Operational, complete and up-to-date | n.s. | Operational, incomplete and up-to-date |
| ftp | n.s. | n.s. | not foreseen yet |
| Data formats and data delivery | | | |
| Data availability | All available in 2007 Unique dataset by 2008-9 | 1979-present <i>Single records of more than 20 years</i> | 1979 to present (with gaps) |
| Data access | Through PROMOTE Web Site | <i>Freely available and downloadable from a website</i> | Through PROMOTE Web Site |
| Delivery Mode | Online/offline | Online/offline | Online/offline |
| Delivery frequency | Daily | Daily | Daily |
| Data Format | HDF | HDF | HDF |
| Historical archive | <i>product</i> | <i>product</i> | <i>product</i> |
| Visualization | GIF North, South Hemisphere and Global + IDL | GIF North, South Hemisphere, and Global + IDL | GIF North, South Hemisphere, and Global + IDL |

*Requirements written in *Italics* are not compulsory for Phase 2

Table 1.4-4 Validation against specifications and against user requirements of the Total Ozone Records sub-service

1.4.5 Quality assessment and control procedures

| Service delivery start date: Phase 1 | | | | |
|---|-----------|------------------|-------------------------|-----------------------------------|
| SPECIFICATION | S5 | REQUIRED* | ACTUAL | N checks/Delivery period ° |
| Quality checks | n.s. | n.s. | Visual check of results | N/A |
| Product confidence data | n.s. | n.s. | N/A | N/A |


| | | |
|---|---|---|
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| | | | | |
|---|--|---|---|-------------------------------|
| Error bar definition and representation | n.s. | <i>Total error; 1 sigma error bar per sample</i> | Error field of 1 sigma errors per grid cell | For each grid cell/ daily |
| Representation of missing data | Indicated in the browser | n.s. | Fill value | N/A |
| Documentation of process failure | n.s. | n.s. | N/A | No process failure in Phase 2 |
| Version control mechanisms and representation | CVS used for software version control. Software updates are communicated with a change history document on the Web | <i>Numbering scheme to be defined in the Product Specification Document</i> | CVS, Version in Product Specification Document and HDF metadata | Will be updated when needed |

*Requirements written in *Italics* are not compulsory for Phase 2

°Between 1st March and delivery date.

Table 1.4-5 Quality assessment and control procedures for the final products of the Total Ozone Records sub-service

| | | |
|---|---|---|
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1.5 References

1.5.1 Electronic references and online data access paths

http://www.gse-promote.org/services/ozone_record/index.html

http://www.gse-promote.org/services/ozone_nrt/index.html

http://www.gse-promote.org/services/ozone_forecast/index.html

<http://www.sciamachy.org/validation/>

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

<http://www.knmi.nl/omi/research/product/Ozone/omdoao3.html>

<http://www.knmi.nl/omi/research/product/Cloud/omcldo2.html>

1.5.2 Bibliographic references

Brinksma, E.J., H. Eskes, R. van der A, P. Valks, J.F. de Haan en J.P. Veefkind, Validation of SCIAMACHY Ozone Columns Retrieved with TOSOMI, Second workshop on the Atmospheric Chemistry Validation of Envisat (ACVE-2) SP-562, 3/5/2004-7/5/2004, Frascati, ESA-ESRIN.

Henk Eskes, Peter van Velthoven, and Hennie Kelder, Global ozone forecasting based on ERS-2 GOME observations, *Atmos. Chem. Phys.*, Vol. 2, 271-278, 2002.

Henk Eskes, Peter van Velthoven, Pieter Valks and Hennie Kelder, Assimilation of GOME total ozone satellite observations in a three-dimensional tracer transport model, *Q.J.R.Meteorol.Soc.* 129, 1663, 2003.

H. J. Eskes, R. J. van der A, E. J. Brinksma, J. P. Veefkind, J. F. de Haan, and P. J. M. Valks, Retrieval and validation of ozone columns derived from measurements of SCIAMACHY on Envisat, *Atmos. Chem. Phys. Discuss*, 5, 4429-4475, 2005.

J. Joiner and A.P. Vasilkov, First Results From the OMI Rotational Raman Scattering Cloud Pressure Algorithm, *IEEE Trans. Geo. Rem. Sens.*, 2006, Vol. 44, No. 5, 1272-1282

P. Wang, P. Stammes, N. Fournier, Test and first validation of FRESCO+, *Proceedings of SPIE volume 6362, Remote Sensing 2006*, 11-16, Sep. 2006, Stockholm, Sweden.