# Product Specification Document

# TOSOMI


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## DOCUMENT STATUS SHEET

| Issue | Date | Modified Items / Reason for Change |
|---|---|---|
| 1.0 | 20.01.06 | First Version |
| 1.1 | 12.04.06 | Update from Tosomi version 0.33 to version 0.40 |

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## 1.1 Product description

The Sciamachy total ozone retrieval algorithm TOSOMI (Total Ozone retrieval scheme for SCIAMACHY based on the OMI DOAS algorithm) is an application of the TOGOMI algorithm to SCIAMACHY.

The new GOME algorithm TOGOMI [*Valks and Van Oss*, 2003] is based on the total ozone DOAS (Differential Optical Absorption Spectroscopy) algorithm developed for the OMI instrument [*Veefkind and De Haan*, 2001]. With respect to total ozone column retrieval using the DOAS method, the OMI, SCIAMACHY and GOME instruments are very similar. The main improvements of the new algorithm are:

(i) treatment of the atmospheric temperature sensitivity by using effective ozone cross-sections calculated from ECMWF temperature profiles,

(ii) improvements in the calculation of the air mass factor, using the so-called empirical approach,

(iii) using the Fast Retrieval Scheme for Clouds from the Oxygen A-band (FRESCO) algorithm for the cloud correction,

(iv) a new treatment of Raman scattering in DOAS [*De Haan*, 2003]. This new formulation of DOAS explicitly accounts for the smearing of the solar Fraunhofer lines as well as the atmospheric tracer absorption structures, and

(v) air-mass factors based on semi-spherical polarization-dependent radiative transfer (KNMI DAK model).

The SCIAMACHY total ozone retrieval algorithm TOSOMI combines a Sciamachy level-1 product reading module with the TOGOMI DOAS modules. The Fresco algorithm [*Koelemeijer*, 2001] is applied to the Sciamachy spectra to obtain cloud fraction and cloud top height estimates.

It is important to note that the TOSOMI total ozone product is influenced by the quality of the SCIAMACHY calibration procedure. No additional calibration corrections are applied to the ozone fit window (325-335nm), but a crude correction factor of 1.2 is applied to the radiances in the Fresco window (758-772nm) because especially the cloud fraction retrieval is sensitive to the absolute reflectivity (status October 2003).

The total ozone data is available in the form of ASCII data files (one file per day).

The characteristics of the algorithm are specified in Table below

| | |
|---|---|
| **Product description** | |
| Summary | SCIAMACHY ozone total column |
| **Product properties** | |
| Parameter(s) | Ozone column level-2 product based on SCIAMACHY observations |
| Accuracy | Approx 2% for SZA < 75 degree (to be specified in more detail) |
| Geometric resolution | Mostly 30x60 km, depending on latitude |
| Grid / projection | Orbits |
| Spatial coverage | Global, swath 960km, 14 orbits per day |
| Temporal coverage | Global coverage in approx. 6 days |
| Data format | ascii |
| availability | Operational implementation based on SCIAMACHY measurements. Near-real time data sets available since early 2004. Off-line data sets available from January 2003. |
| **Production process** | |
| Method/algorithm | TOSOMI total ozone retrieval algorithm, combined with FRESCO cloud retrieval. |
| reference | [*Eskes et al.*, 2005],<br>[*Valks et al.*, 2003],<br>[*van Oss et al.*, 2004]<br>[*Veefkind et al.*, 2002] |
| **Quality standards** | |
| Production | Large number of DOAS quality checks, level-1 data sanity checks. |
| Product | DOAS fitting precision quantified. |
| Validation | Intercomparison of the TOSOMI ozone column retrievals with ground-based observations (Brewer, Dobson, DOAS, SAOZ, ozone sondes, lidar etc..) [*Brinksma*, 2004], with GOME ozone retrievals and with data assimilation [*Eskes*, 2005]. |
| **Input data** | |

| | |
|---|---|
| EO data | SCI_NL_1P |
| Other data | none |
| **Optional or other specific properties (if applicable)** | |
| Historical archive | All data is archived. |
| Visualization standards | Images in gif format provided of global distribution. |

## 1.2 Product format specification

The KNMI total ozone product is available in the form of two files:

- A header file describes authors, software version and the list of SCIAMACHY level 1c input files.
- A data file. The format is explained below.Each line in the ascii data file is one retrieval.

The specification of the fields in the data file:

Product Specification Table (ASCII) TOSOMI ozone product

| Dataset name | Data type | Position | Unit | Description |
|---|---|---|---|---|
| Date | string | 1-8 | - | Date in format (YYYYMMDD) |
| Time | string | 9-19 | - | UTC time in format (_hhmmss.sss) |
| Longitude 1 | integer | 18-26 | 0.01 degree | Longitude of corner point 1 of the ground pixel |
| Latitude 1 | integer | 27-33 | 0.01 degree | Latitude of corner point 1 of the ground pixel |
| Longitude 2 | integer | 34-40 | 0.01 degree | Longitude of corner point 2 of the ground pixel |
| Latitude 2 | integer | 41-47 | 0.01 degree | Latitude of corner point 2 of the ground pixel |
| Longitude 3 | integer | 48-54 | 0.01 degree | Longitude of corner point 3 of the ground pixel |
| Latitude 3 | integer | 55-61 | 0.01 degree | Latitude of corner point 3 of the ground pixel |
| Longitude 4 | integer | 62-68 | 0.01 degree | Longitude of corner point 4 of the ground pixel |
| Latitude 4 | integer | 69-75 | 0.01 degree | Latitude of corner point 4 of the ground pixel |
| Longitude 5 | integer | 76-82 | 0.01 degree | Longitude of center coordinate of ground pixel |
| Latitude 5 | integer | 83-89 | 0.01 degree | Latitude of center coordinate of the ground pixel |
| Pixel subtype | integer | 90-92 | - | StateID ( for backscan-pixels: stateID + 50 ) * |
| Total ozone column | integer | 93-97 | 0.1 DU | total vertical ozone column |
| Error | integer | 98-102 | 0.1 DU | (minimum) error in the ozone column |
| Raw ozone column | integer | 103-107 | 0.1 DU | vertical ozone column above cloud-top |
| Slant ozone column | integer | 108-113 | 0.1 DU | total slant ozone column |
| SZA | integer | 114-118 | 0.01 degree | solar zenith angle at the Earth?s surface |
| VZA | integer | 119-124 | 0.01 degree | viewing zenith angle at the Earth?s surface |
| cloud fraction | integer | 125-128 | % | cloud-fraction as derived with FRESCO |
| cloud-top pressure | integer | 129-133 | mb | cloud top pressure as derived with FRESCO |
| Radiance weight cld. | integer | 134-137 | % | radiance weight of cloudy part of pixel |
| AMF | float | 138-144 | - | clear-sky AMF |
| AMF-cloud | float | 145-151 | - | cloudy AMF (cloud-albedo=0.8) |
| Ghost column | integer | 148-151 | DU | ghost ozone column below the cloud |

* *A decription of the states for nominal operations can be found on the web-site : http://atmos.af.op.dlr.de/projects/scops/states_description/states_description_actual.html*

## 1.3 Software release history

Current release is version 0.40 of the Sciamachy DOAS total ozone retrieval software "TOSOMI".

The TOSOMI implementation is based on the GOME software "TOGOMI" by Pieter Valks, the OMI DOAS ozone column retrieval "OmiO3Doas" by Pepijn Veefkind, on the Fresco algorithm version SC-v3, and on the Sciamachy Level-1c file read software (Ronald van der A).

Operational processing is based on version 0.32, 0.33 and 0.40 of the algorithm. Earlier versions were all development versions, and have not been used to create data sets for public use. The main change between version 0.33 and 0.32 is an upgrade of the Fresco algorithm (from Nicolas Fournier) which improves the cloud retrieval especially over deserts.

The main changes in version 0.40 are:
1) The use of high-resolution Bass-Paur ozone cross sections which replace the GOME flight model cross sections that were used in versions 0.32 and 0.33. As a result the ozone values are on average about three percent higher than in version 0.33.
2) An added correction for the mismatch between the detector readout time and time at which the geometrical information is reported.

Below is a detailed list of implementation changes made to the TOSOMI code in all updates.

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**version notes, tosomi v0.40** (April 2006)

- Cross sections: GOME Flight Model 98 cross sections are replaced by effective cross sections based on Bass-Paur high resolution data. Bass, A.M., and Paur, R.J., Proc. Quadrennial Ozone Symp., Chalkidiki, Greece, Eds. C. Zefros and A. Ghazi. 1986.

- Obsolete Cabannes correction factors removed in ComputeAmfModule.f90, line 252

- Added cycle command in "main.f90"
  if (SciaPixelOut%amfQa < 0 ) cycle
  This to skip the current observation in case the AMF is undefined,
  e.g. because input parameters are out of range

- sciaReadModule.f90
  Added correction to compensate for the mismatch between the detector readout time and the time at which the geometrical information is provided.
  l 373, 374: definition of parameters
  l 609-643 : implements the correction for the vza at satellite "dVzaSat"
  For the evaluation of "isBackScan" the longitude/latitude information and scanmirror angle is needed. The calculations for this have been moved up (l 504-553).

- "writeOutputModule" header line updated

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**version notes, tosomi v0.33** (August 2005)

- The NASA toolbox has been replaced by a toolbox simulator module for portability reasons.
- The spectral reflectivity data base for the FRESCO algorithm is upgraded to a 0.25 degree resolution map (by Nicolas Fournier)
- FrescoModule.f90, line 1585: Small bug fix in FRESCO
- sciaArrayDimsModule, line 21: Maximum number of SCIAMACHY pixels has been increased
- sciaFrescoInterface, line 262: Radiometric calibration fudge factor is changed from 1.25 to 1.2 for the FRESCO algorithm
- terrainHeightModule, line 12: The terrain height map resolution has increased to 0.25 degree
- toolkitSimulator: This is a new module
- A few error messages have been replaced by warnings

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**version notes, tosomi v0.32**

- The centre coordinates (longitude) of the pixels had a problem near the date line. This coordinates was simply taken from the level-1 file and copied to the output file.
- For pixels on the date line, the longitude is now recomputed based on the pixel corner coordinates: sciaPixel%longitude(5) = sum(sciaPixel%longitude(1:4))*0.25
- sciaReadModule.f90: lines 597-619
- writeOutputModule.f90: new output format (units 0.1 DU)

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**version notes, tosomi v0.31**

- A spherical geometrical air-mass factor is introduced to reduce solar-zenith angle dependent interpolation errors in determining the air-mass factor. The input air-mass factor tables are updated and contain

AMF(Empyrical,DAK)/AMF(Geometric,spherical)
instead of
AMF(Empyrical,DAK)/AMF(Geometric,plane parallel)

- computeAmfModule.f90: The call to "computeAmfGeo" is replaced by "computeAmfGeoSpherical". A new subroutine "computeAmfGeoSpherical" is added.

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**version notes, tosomi v0.3**

- Version 0.3 contains new lookup tables based on semi-spherical DAK (Johan de Haan).

These tables replace the old ones:
data/AmfClear_325_335.h4
data/AmfCloudy_325_335.h4
The old plane-parallel lookup tables are still available as
data/AmfClear_325_335_PP.h4
data/AmfCloudy_325_335_PP.h4

- readSciaModule.f90: The lookup table angles are defined at the Earth's surface.

line 473: dAtmosphereHeight = 0.0d0

- sciaFrescoInterface.f90:

line 261:
```
! RONALD'S FUDGE FACTOR
! The extra factor 1.25 accounts for problems with the
! radiometric calibration of Sciamachy
erad(i)=1.25*erad(i)
```
line 266:
```
if ( firstcall ) then
  print*,'sciaFrescoInterface WARNING: ',&
      'scaling factor 1.25 applied to account for calibration errors'
end if
```

- sciaFrescoInterface.f90: A larger radiance error improves the Fresco performance, factor 0.005->0.05, line 261: errerad(i)=erad(i)*0.05

- writeOutputModule.f90: A 7-line header is added to the data file, with processor version + authors

- dataModule.f90: fields "product" and "soft_version" added to "SciaL1RadGenType"

- "bin/sciadto.opf"
contains extra field "SZA_MAX" set to 85.0 degree
"getOpfModule.f90"
reads the variable "opfData%szaMax"
"dataModule.f90"
variable "opfData%szaMax" added

"main.f90"
implements check on the solar zenith angle - "szaMax"

- "sciaUtilityModule.f90"
  extra subroutines "asin_" and "acos_" are defined to avoid NaNs due to over/underflow of the argument. These alternative routines are used in the angle manipulation subroutines.

- "frescoModule.f90"
  Extra output flag value "xflag=5" introduced to intercept errors in "gaussjf" related to singular matrices. Numerical recipes subroutine now passes it's error by the variable "istatus"

- "sciaFrescoInterface.f90": An extra variable has been added to "acceptFrescoRetrieval" to account for the new Fresco error warning.

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**version notes, tosomi v0.25**

- Code added to correct the angles in the Scia level-1c files: "sun_zen_ang" and "sun_azi_ang" are specified at top-of-atmosphere instead of at-satellite (as the other coordinates are).
- sciaUtilityModule.f90: subroutine added: "RecoverSolarAnglesAtSat"
- dataModule.f90: logical :: correctAnglesToaSat
- sciaReadModule.f90: lines 502-514: optional call to "RecoverSolarAnglesAtSat"
- sciaFrescoInterface.f90:
  lines 276-288: optional call to "RecoverSolarAnglesAtSat"
  extra input var: "opfData"
- getOpfModule.f90: line 333: read "correctAnglesToaSat", line 129 initialisation
- file "sciadto.opf" in directory "bin": definition of "L1_CORRECT_ANGLES"

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**version notes, tosomi v0.24**

- Bug fix in angle calculation; sciaReadModule.f90:
  wrong: relAzi = abs( real( dVzaToa(i)-dSzaToa(i), 4) )
  correct: relAzi = abs( real( dVaaToa(i)-dSaaToa(i), 4) )
- Bug fix, sciaReadModule.f90:
  "QuadratureFraction" undefined, replaced by real*8 "dQuadratureFraction"
  declaration of "QuadratureFraction" removed

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**version notes, tosomi v0.23**

- New definition of "subType" identifier:

(changes in sciaReadModule.f90, writeOutputModule.f90, main.f90)
subType = stateID (forward scan)
subType = stateID + 50 (backscan)

- Extra variable "scanMirrorAngle"

(changes in dataModule.f90, sciaReadModule.f90, writeOutputModule.f90)

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**version notes, tosomi v0.22**

- src/sciaReadModule.f90:

longitude calculation changed
line 466: if ( dLonSat < 0.) dLonSat = dlonSat + 360.
line 585: if ( sciaPixel%longitude(i) < 0.)
sciaPixel%longitude(i) = sciaPixel%longitude(i) + 360.
line 591: if ( sciaPixel%longitude(5) < 0.)
sciaPixel%longitude(5) = sciaPixel%longitude(5) + 360.

- src/sciaReadModule.f90:

new way of calculating dVzaSat (improved averaging)
lines 503-523: if ( abs(dVaaSat(2)-dVaaSat(1)) < 90. ) then ...

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**version notes, tosomi v0.21, changes since version 0.2:**

- src/Makefile: new library paths for IRIX
- src/writeOutputModule.f90: write format statement changed
- src/sciaReadModule.f90: status check "Check validity of cloud data" relaxed from "status == 0" to "status >= 0"
- src/main.f90:

- Extra check on number of nadir pixels
- After call to SciaExtractEarthRadiance:
stop replaced by cycle
- After ComputeScd
stop replaced by cycle

- install-tosomi: Slatec library not used - path removed

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**version notes, tosomi v0.2, changes since version 0.1:**

- how_to_run documentation adapted
- install-tosomi file created
- readscial1c library and modules of 14-08-2003 or newer are required
- makefile has been adapted so that it can be used on SGI-IRIX and linux
- frescoModule.f90:

subroutine "spline_int1"
array sizes adapted to real array size

subroutine "readfile":
parameter definitions rewritten, intent in/out
subroutine "writeout":
format statement on one line

- modules getOpfModule.f90 , computeScdModule.f90 and main.f90
boolean-variable == .true. exchanged by just the boolean-variable
(IRIX compiler issue)
- New AMF lookup tables added (generated by Pieter Valks):
files "AmfClear_325_335.h4" and "AmfCloudy_325_335.h4"
- Pixel time bug fix in "sciaReadModule"
int_time = real(Level1data%..%intg_time)/16.0
- "writeOutputModule": New output definition
- Print statements that were used for testing are removed

## 1.4 Implementation details

See TOSOMI algorithm document (TEM/AD3/001)

## 1.5 List of known issues

The validation exercise shows a good overall agreement between TOSOMI, GOME and ground-based total ozone measurements. One persistent feature is an offset of roughly -1.5% with respect to GOME retrievals and ground-based observations reported for TOSOMI version 0.33 [*Eskes et al.*, 2005]. This feature may be partly attributed to issues in the radiometric calibration of the SCIAMACHY measurements. Ozone columns in version 0.40, which uses Bass Paur cross sections, is about 3% higher than ozone values in version 0.33, corresponding to an offset of about +1.5% with respect to ground-based observations. Note that such differences reflect uncertainties in presently available ozone cross sections.

## 1.6 Data quality assessment

See TOSOMI algorithm document (TEM/AD3/001) and [*Eskes et al.*, 2005]

## 1.7 References

Eskes, H. J., 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.

Valks, P., and R. van Oss, TOGOMI Algorithm Theoretical Basis Document, Issue 1.2, TOGOMI/KNMI/ATBD/001, KNMI/ESA, November 2003, http://www.gse-promote.org/services/ozone nr t/togomi ATBD v1.21.pdf.

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Veefkind, J.P. and J.F. de Haan, OMI Algorithm Theoretical Basis Document, Barthia, P.K (ed), Volume II - Chapter 3, DOAS Total Ozone Algorithm, ATBD-OMI-02, Version 2.0, August 2002 http://www.knmi.nl/omi/documents/data/OMI ATBD Volume 2 V2.pdf, 2002.