



**Product Specification  
Document  
TOSOMI**

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**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

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<b>Product description</b>	
Summary	SCIAMACHY ozone total column
<b>Product properties</b>	
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.
<b>Production process</b>	
Method/algorithm	TOSOMI total ozone retrieval algorithm, combined with FRESCO cloud retrieval.
reference	[Eskes <i>et al.</i> , 2005], [Valks <i>et al.</i> , 2003], [van Oss <i>et al.</i> , 2004] [Veeffkind <i>et al.</i> , 2002]
<b>Quality standards</b>	
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].
<b>Input data</b>	

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EO data	SCI_NL_1P
Other data	none
<b>Optional or other specific properties (if applicable)</b>	
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:

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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 description 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](http://atmos.af.op.dlr.de/projects/scops/states_description/states_description_actual.html)*

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### 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 Veeffkind, 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).

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- "writeOutputModule" header line updated

#### **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

#### **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:  

$$\text{sciaPixel\%longitude}(5) = \text{sum}(\text{sciaPixel\%longitude}(1:4)) * 0.25$$
- sciaReadModule.f90: lines 597-619
- writeOutputModule.f90: new output format (units 0.1 DU)

#### **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




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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.

### 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

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"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.

#### 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"

#### version notes, tosomi v0.24

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

#### version notes, tosomi v0.23

- New definition of "subType" identifier:

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(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)

#### 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 ...

#### 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

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

- how\_to\_run documentation adapted
- install-tosomi file created
- readsciallc 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

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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

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## 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.
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