TITLE:

Product Specification Document

Tropospheric NO_2

Authors :

R.J. van der A (KNMI)
H.J. Eskes (KNMI)

DOCUMENT STATUS SHEET

Issue	Date	Modified Items / Reason for Change
0.9	19.01.06	First Version

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1. GLOBAL TROPOSPHERIC NO2 SERVICE

1.1 Product description

The retrieval of NO2 will be based on a combined retrieval/modeling approach which has been developed recently. A chemistry-transport model, driven by high-quality meteorological fields, will provide best-guess profiles of NO2, based on the latest emission inventories, atmospheric transport, photochemistry, lightning modeling and wet/dry removal processes.

These model forecast fields will be collocated with the GOME/SCIAMACHY observations, and the radiative transfer modeling in the retrieval will be performed based on the model trace gas profile and temperature profiles. The modelled stratospheric NO2 distribution will be employed to derive a tropospheric column by subtracting the modelled (assimilated) stratosphere from the measured column. The retrieval is coupled to cloud top height and cloud fraction retrievals derived from the GOME/SCIAMACHY data, and the retrieval will be coupled to high quality albedo maps.

Product description	
Summary	Daily tropospheric NO2 columns (level 2)
Product properties	
Parameter(s)	Total column of NO2 Tropospheric column of NO2 Error on the tropospheric column of NO2
Accuracy	Specified as parameter Detailed analysis in Boersma et al. (2004)
Geometric resolution	60 x 30 km^2 (ENVISAT) except for high latitudes
Grid / projection	Orbit geometry
Spatial coverage	Swath 960 km, 14 orbits per day, i.e. global coverage in approx. 1 week

Temporal coverage	Daily
Data format	HDF
availability	Operational service in TEMIS (http://www.temis.nl/) and in PROMOTE (http://www.gse-promote.org/)
Production process	
Method/algorithm	SCD retrieval of NO2 with GwinDOAS Tropospheric VCD retrieval of NO2 using data assimilation Atmospheric model TM4, radiative transfer model DAK, and FRESCO cloud parameters are used
Model / assimilation	Data assimilation using TM4
reference	none
Quality standards	
Production	Detailed error calculation, error checking and output range control
Product	- Comparison ground observation within ACVE validation campaign - Intercomparison regional High-resolution model CHIMERE
validation	See algorithm document TEM/AD1/001
Input data	
EO data	SCI_NL_1P, GOME lv1c (all calibration option on) Combined TOMS-GOME albedo climatology
Other data (static)	Meteorological data of ECMWF GTOPO30 (topology database) Emission databases (EDGAR, etc)
Optional or other specific properties (if applicable)	
Historical archive	GOME (ERS-2) : 1996-2003

	SCIAMACHY (Envisat) : 2003-today
Offline/NRT	NRT (within max. 1 day)
Visualization standards	Images available.
Ongoing improvement	Improved model
Level 3 product	Monthly mean maps (0.25 degree) available

1.2 Product format specification

TEMIS columnar NO_2 will be made available in HDF4. The HDF files will contain NO_2 data for one day, and are organised as follows:

- SDS global attributes, containing information on the file.
- Vdata, i.e. the actual data

The SDS global attributes (meta data) is described in more detail in the following table:

Product Specification Table : SDS global attributes

Attribute name	Type	Description
Version	string	Version number of the software used for generating the data.
Author	string	Name of the person responsible for the data.
Affiliation	string	Affiliation of the author
Email	string	E-mail address of the author
Data_created_by	string	The assimilation code that produced the fields.
Field_column	integer	A brief description of the content of the field
Field_std	integer	A brief description of the error of the field
Units	string	The units of the fields
Note	string	A brief description how the arrays are stored in the file SDS Global Attributes Name Value

The Vdata contain the data product, and consists of one generic and 3 repeating data fields:

- Pressure grid (the generic field)
- NO2_ymmddttt (contains the main NO2 retrieval data for one SCIAMACHY state)
- GEO_ ymmddttt (contains all geometric data associated with the retrievals in this state)
- ANC_ ymmddttt (contains all ancillary data associated with the retrievals in this state)

The Vdata contains only one generic pressure grid field. This table defines the pressure grid at which the averaging kernel is provided. The Vdata table attribute also provides the recipe to convert the level constants, *a_lev*, *b_lev*, and surface pressure *p_surf* into the hybrid level pressures p (in Pascal). The equation is:

$$p = a\_lev + p\_surf \cdot b\_lev$$

and the variable *p_surf* is stored in NO2_ymmddttt: the surface pressure is provided for each individual SCIAMACHY pixel.

The VData may contain as many as 120 (maximum number of SCIAMACHY states in one day – 15 orbits times 8 states) pieces of NO2_ymmddttt, GEO_ymmddttt and ANC_ymmddttt. The array NO2_ymmddttt is accompanied by a VData Table Attribute that contains the name of the state, and the start- and end time (year, month, day, hour, minutes, and seconds) as follows:

Name	Value
track_identifier	30101071
start_time	2003, 1, 1, 7, 5, 59
end_time	2003, 1, 1, 7, 35, 3

The main data table is NO2_ymmddttt and it contains 15 fields. They are summarized below and commented on.

Product Specification Table : HDF - Data Fields

Name	Type	Range	Description
date	char*8		Date of SCIAMACHY retrieval (yyyymmdd) e.g. 20030101 for 1 Jan. 2003
time	char*8		Time of SCIAMACHY retrieval (hhmmsshu) e.g. 07055900 for 7:05'59"00
lon	real	[0.0 – 360.0]	Centre longitude of pixel [degree]
lat	real	[-90.0 – 90.0]	Centre latitude of pixel [degree]
vcd	real	[0.0 – 500.0]	Retrieved total vertical column density [10^{15} molec. cm^{-2}]
sigvcd	real	[0.0 –1e3]	Error in the total vertical column density [10^{15} molec. cm^{-2}]
vcdtrop	real	[-5.0 – 5e2]	Retrieved tropospheric vertical column density [10^{15} molec. cm^{-2}]
sigvcdt	real	[0.0 –1e3]	Error in the tropospheric vertical column density [10^{15} molec. cm^{-2}]
vcdstrat	real	[0.0 – 6.0]	Retrieved stratospheric vertical column density [10^{15} molec. cm^{-2}]
sigvcds	real	-	Error in the stratospheric vertical column density [10^{15} molec. cm^{-2}]
fltrop	integer	[-1,0]	Flag that indicates whether tropospheric retrieval was meaningful, 0 =yes, -1 = no.
psurf	float	-	Surface pressure of the pixel (in Pa)
sigvcdak	float	-	Error in total vertical column density when averaging kernel information is used in 10^{15} molec. cm^{-2} (without profile error contribution)
sigvcdtak	float	-	Error in tropospheric vertical column density when averaging kernel information is used in 10^{15} molec. cm^{-2} (without profile error contribution)
kernel	float	-	Averaging kernel vector, corresponding to the kernel values at the pressure levels as defined above

Product Specification Table : HDF - Geolocation Fields

Name	Type	Range	Description
sza	real	[0.0 – 85.0]	Satellite solar zenith angle
vza	real	[0.0 – 32.0]	Satellite viewing zenith angle
raa	real	[0.0 – 360.0]	Satellite relative azimuth angle
ssc	real	[0,3]	SCIAMACHY subset counter 90 = forward scan, 3 = backscan)
loncorn	4*real	[0.0 – 360.0]	Longitudes of the four corners of the pixel
latcorn	4*real	[-90.0 – 90.0]	Latitudes of the four corners of the pixel

Additional retrieval data is provided by the ancillary data table ANC_ymmddttt, and it contains 10 columns:

Product Specification Table : HDF – Ancillary Data

Name	Type	Range	Description
scd	real	[0.0 – 100.0]	Slant column density, in 10^{15} molec. cm^{-2} (from IASB, derived for 220 K)
amf	real	[2.0 – 15.0]	Total air mass factor used to compute vcd (=scd/amf)
amftrop	real	[0.1 – 15.0]	Tropospheric air mass factor used to compute vcdtrop (=[scdstr-scd]/amftrop)
amfgeo	real	[2.0 – 25.0]	Geometrical air mass factor
scdstr	real	[1.0 – 8.0]	Stratospheric slant column density (amfgeo*vcdstrat)
clfrac	real	[-1, 0.0-1.0]	Cloud fraction from FRESCO, -1 = snow or ice covered
cltpress	real	[1.05e5 – 1.3e4]	Cloud top pressure from FRESCO, 1.3e4 corresponds to tropopause cloud
albclr	real	[0.0 – 1.0]	Surface albedo for clear part of the pixel from TOMS/GOME database
crfrac	integer	[0.0-100.0]	Cloud radiance fraction, i.e. percentage of the light coming from cloudy part of the scene
ltropo	integer	[18-22]	TM3 pressure level in which tropopause occurs
ghostcol	float	-	Vertical column between surface and cloud level derived from TM3 (10^{15} molec. cm^{-2})

Monthly mean data of NO2 is available in ASCII-TOMS format and ESRI-ASCII grid format.

1.3 Software release history

Current version: TM4NO2A, version 1.1.1

Version 1.1.1 16 August 2005

Changes:
General:

- Added: ass_dimension.f90 (voor alle modules gelijk)
- Added: ass_modisalbedo (extra albedo map based on MODIS observations)
- ass_err_retr: extra check, undefined for amftroptotal < 0.1
- ass_amflut: improved reading, extra checks
- ass_Hx: small improvements:
    - ltropo at centre of pixel
    - cloudpres = min(surfpres,cloudpres)
    - extra parameter checks
    - NO2ErrEstimate call only when amftroptotal >= 0.1

In ass_Hx.f90:

- grouping of commands for more logical structure
- extra checks added to avoid division by zero and unphysical results
- error estimate routine is now only called when the tropospheric AMF > 0.1 (see line 450)
- line 210: ltropopause = Ltropo(ixc,iyc)
- line 234: cloudpres = min(surfpres,cloudpres)
  cloudpres = max(cloudpres,130.)

Bug fix, ass_amflut.f90, line 180:

- added initialisation of sds_index (= 0)

Bug fix, ass_obsread_sciano2.f90, line 435:

- if (ipix > obsTrack%count) then
  call tau2date(obsTrack%pixelTMTime(obsTrack%count+1),idate6)

Bug fix, assim.f90, line 384:

old:
no2pcf(i,j,l) = no2pcf(1,j,l) (j not defined)
new:
no2pcf(i,1,l) = no2pcf(1,1,l)
no2pcf(i,jm,l) = no2pcf(1,jm,l)

In ass_oi_subr.f90 (Small changes):

- checks on negative concentrations and division by zero, see variable "subcolumnLimit"

- lines 30, 172, 450, 606
- Print statement removed: "ERROR, small qfc value", line 175
- 3D array "qfcmat" removed - no longer needed - in subr Bx.

Version 1.1 July 2004

Changes since version 1.04:

- Update to parallel version of TM4 (9 July) performed by replacing the following files with OPENMP prepared files from Ernst Meijer:
  chemistry.f90
  chemistry_par.f90
  convection.f90
  marked_tracers.f90
  photolysis.f90
  slopes.f90
  tracer.f90
  makefile

- The fillowing lines have been added to the script "assimNO2.csh":
  limit stacksize unlimited
  setenv OMP_NUM_THREADS 4

Version 1.04 June 2004

- Update from TM3 to TM4
- New AMF lookup table included (HDF format)

1.4 Implementation details

See tropospheric NO2 algorithm document TEM/AD1/001

1.5 List of known issues

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1.6 Data quality assessment

See tropospheric NO2 algorithm document TEM/AD1/001