3. SCIAMACHY LIMB-NADIR MATCHING (LNM) TROPOSPHERIC NO_2 PRODUCT OF THE AIR QUALITY MONITORING SERVICE

3.1 Product Specification of the SCIAMACHY Limb-Nadir Matching (LNM) tropospheric NO_2 Product of the Air Quality Monitoring Service

One area of uncertainty in the determination of the tropospheric column concentration from solar backscatter nadir measurements is the error of 10% to 20% introduced by estimating the stratospheric column concentration (Boersma et al. 2004). To improve on this topic, it is required to use the measured stratospheric column above the ground scene of interest. SCIAMACHY with its limb-nadir matching measurement mode (Bovensmann et al. 1999) is providing radiances from the same volume of air in limb and nadir geometry since 2002. The spectrometer continuously alternates between limb-and nadir observation geometry. The viewing angles for the acquisition of limb spectra are tuned in such a way that the tangent points are as close as possible over a region, which is covered by a nadir state measured 7 minutes later. This enables to infer vertical stratospheric concentration profiles (von Savigny et al. 2004) directly over the region of the nadir measurement. Integrating these profiles from the tropopause upwards yields the measured stratospheric *VCD* above the target area. The total column concentration is derived from the collocated nadir measurement. The tropospheric column is then - very briefly speaking - determined as the difference between the total and the stratospheric column.

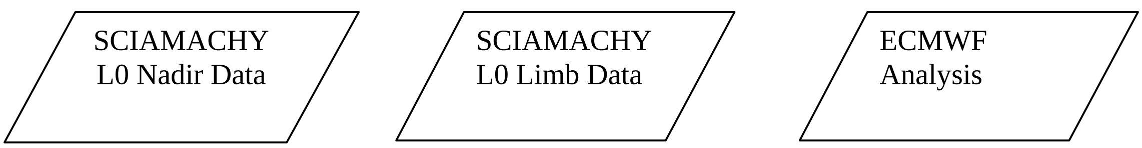
The method described here is unique in the sense that the information on the stratospheric content is directly taken from the co-located limb measurement and no other assumptions (longitudinal homogeneity) or an estimate of the stratospheric column from a model or from data assimilation are necessary.

Product description	
Summary	Daily tropospheric NO_2 column concentration
Product properties	
Parameter(s)	Tropospheric Column NO_2 Total column NO_2 Stratospheric Profile NO_2 Stratospheric Column NO_2
Accuracy	TBD
Geometric resolution	60 x 30 km^2
Grid / projection	Orbit geometry
Spatial coverage	Swath 960 km, 14 orbits per day, i.e. global coverage within 6 days at the equator, (4 days over Europe)
Temporal coverage	Daily
Data format	TBD
availability	Science demonstrator existing, Semi-operational off-line service planned for 2005 Planned service for international campaigns by End 2004
Production process	

Method/algorithm	total SCD with IUP-DOAS, stratospheric profile with optimal estimation, AMF by radiative transfer calculations and use of LUT
Model / assimilation	Direct retrieval, no model needed to estimate the stratospheric content
reference	Sierk, B., A. Richter, A. Rozanov, Ch. von Savigny, A.M. Schmoltner, M. Buchwitz, H. Bovensmann, and J.P. Burrows, Retrieval and Monitoring of atmospheric trace gas concentrations in nadir and limb geometry using the space-borne SCIAMACHY instrument, presented at the “5th International Symposium on Advanced Environmental Monitoring", submitted to “Environmental Monitoring and Assessment”, 2004 Savigny, C. v., A. Rozanov, H. Bovensmann, K.-U. Eichmann, S. Noel, V. V. Rozanov, B.-M. Sinnhuber, M. Weber, and J. P. Burrows, The ozone hole break-up in September 2002 as seen by SCIAMACHY on ENVISAT, J. Atmos. Sci., in press, 2004 Richter, A., and J.P. Burrows, *Tropospheric NO_2 from GOME measurements*, Adv. Space Res., 29, 1673-1683, 2002
Quality standards	
Production	Quality checks to identify outliers
Product validation	Case study validation ongoing Large scale validation planned
Input data	
EO data	SCI_NL_1P
Other data (static)	trop. AMF database, ECMWF for tropopause determination
Optional or other specific properties (if applicable)	
Historical archive	SCIAMACHY (ENVISAT): 2002 – today can be processed
Offline/NRT	Global: offline Specific Campaigns for selected regions: NRT
Visualization standards	Through GIF, TIFF etc.
Simultaneous input	All input data are simultaneous from the same platform and the same orbit with the exception of the ECMWF data for tropopause determination
Ongoing improvement	AMF calculation are currently updated based on ongoing research
Level 3 product	Daily gridded maps and monthly mean maps will be developed
Underlying primary user requirement(s)	
Key requirement	Speciation for trop. NO2
Originator(s)	meteorological users, chemical data assimilation service

Table 3.1-1: Characteristics of tropospheric NO2 LNM product

3.2 System Overview



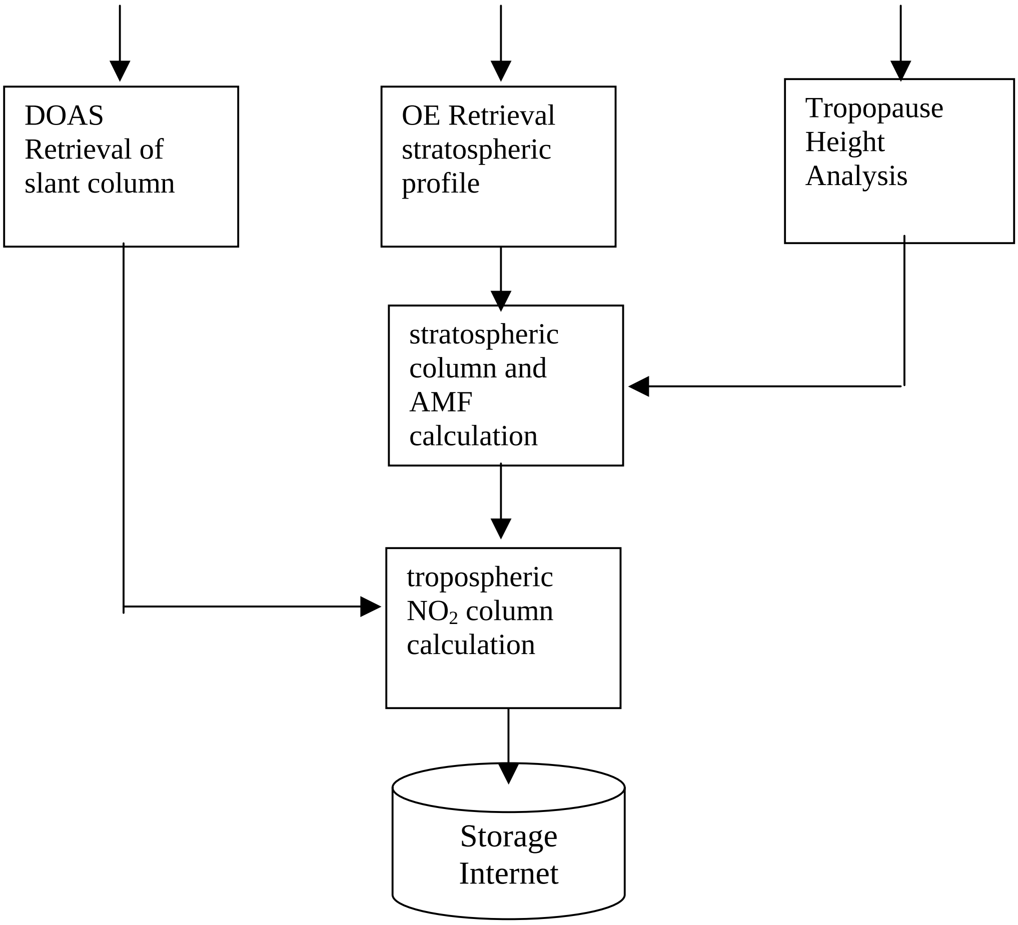


Figure 3.2-1: Overview of SCIAMACHY trop. NO_2 LNM process

The retrieval system can be broken down into four major steps:

1. retrieval of the total NO_2 slant column density (SCD) by DOAS fitting

2. retrieval of the stratospheric profile by an optimal estimation retrieval scheme

3. stratospheric column calculation: calculation of tropopause height from ECMWF data, integration of the stratospheric profile to a stratospheric column and calculation of the stratospheric AMF to convert stratospheric VCD to stratospheric SCD

4. calculation of the tropospheric SCD and VCD

As the DOAS analysis of the nadir spectra yields the total *SCD*s for the ground scene pixels, the stratospheric *VCD* has to be mapped to nadir observation geometry by transforming it to a corresponding stratospheric *SCD*. With AMF_{strat} denoting the stratospheric component of the airmass factor, we can form the difference

$$SCD_{trop} = SCD_{total,\ nadir} - VCD_{strat,\ limb} \times AMF_{strat,\ limb}$$

to obtain the tropospheric slant column density $SCD_{trop.}$

In the computation of AMF_{strat}, once more the measured profiles derived from limb observation is used. This is done by running a RTM calculation with CDI, using the inferred stratospheric NO_2 profiles as input information. In this way, AMF_{strat} is calculated for all nadir measurements considering the observation geometry (given by SZA and line-of-sight (LOS) of the measurement) and the chosen wavelength window for the DOAS analysis of the nadir spectra. The stratospheric *VCD* is scaled by AMF_{strat}, and subtracted from the total *SCD*. The resulting slant tropospheric column can then be transformed into VCD_{trop} by an estimate of the tropospheric airmass factor AMF_{trop}. The latter is again obtained from an RTM calculation, in which assumptions on the tropospheric absorber profile and other factors have to introduced.

Number	Origin	Short name	Description	Backup
1	EO	SCI_NL_1P	SCIAMACHY earthshine radiances and solar irradiance	n.a.
2	ECMWF	Met. Fields	Fields of Meteorological Parameters	n.a.

Table 3.2-1: Input data of the trop. NO2 LNM service

Number	type	Process name
1	preprocessing	SCIAMACHY data preparation incl. cloud processing
2	retrieval	total SCD from SCIAMACHY nadir measurements
3	retrieval	stratospheric profile from SCIAMACHY limb measurements
4	pre-processing	stratospheric column and AMF calculation: integrate stratospheric profile to stratospheric column and calculate the stratospheric AMF by using the measured stratospheric profiles
5	retrieval	tropospheric NO_2 column derivation
6	Post processing	Quality check (fit error, outliers etc.)

Table 3.2-2: Sub-processes of the trop. NO2 LNM service

Number	Short name	description	Key features
1	trop. NO_2 column	tropospheric NO_2 column concentration from SCIAMACHY Limb-Nadir Matching (LNM)	
2	strat. NO_2 column	stratospheric NO_2 column concentration from SCIAMACHY Limb Measurements	
3	strat. NO_2 profile	stratospheric NO_2 profile from SCIAMACHY Limb Measurements	
4	total NO_2 column	total NO_2 column from SCIAMACHY limb and nadir	

		measurements	

Table 3.2-3: Output of the trop. NO2 LNM service

Technical requirements

External interface(s)

SCIAMACHY L1 data is available via ESAs DDS satellite link. The historic data is only available after reprocessing of the year 2002 and parts of 2003 data by the ENVISAT ground segment. ECMWF data is routinely available. The stratospheric and tropospheric data can be made available by the IUP standard web interface (troposphere: http://www.doas-bremen.de/doas/no2_contrace.htm, stratosphere/clouds: http://www.iup.physik.uni-bremen.de/scia-arc/)

Verification and quality control

For internal quality control the fit errors are checked and outliers will be identified. Overall data quality needs to be assured by continuous validation of the data set.

Hardware

Currently the algorithms are running on PC's (IUP-DOAS, trop. VCD) and Workstations (profile retrieval, AMF calculation).

Software

The current algorithm suite is able to process 1 day of global data within 2 hours. Currently the most resource consuming step is the profile retrieval, which currently needs approx. 1 hour processing time on an IMB P690 (32 CPUs, 64 GB RAM) for 1 day of global data. Further reductions in processing time can be expected from algorithm optimisations.

Short description for process 1: SCIAMACHY data preparation

In a pre-processing step, the relevant L1 data is extracted w.r.t. geolocation, relevant spectral windows and cloud filtering.

Short description for process 2: DOAS total slant column retrieval

The NO_2 total slant column is retrieved by a least-squares fit of the DOAS equation, which is derived from Beer's law, to the reflectances I_j measured by the detector pixel j and normalized to the corresponding extraterrestrial intensity I_{0j}:

$$ln\left(\frac{I_{0j}}{I_j}\right) = \sum_n SCD_{nj} \cdot \sigma_{nj} + P(\lambda_j)$$

The *SCD*s retrieved in the above outlined analysis represent the effective amount of molecules encountered by photons along their average propagation path. The fit parameters determined in the least-squares analysis are the slant column densities (SCD_n) for each trace gas *n* absorbing in the spectral window and the coefficients of a polynomial P in wavelength λ. The latter accounts for attenuation processes owing to Rayleigh and Mie scattering, which are assumed to be smooth and slowly varying in the considered spectral interval. The retrieval of each trace gas using the above equation requires knowledge of the individual molecular absorption cross sections σ_n, which have been measured in laboratory calibration measurements using the SCIAMACHY instrument [Bogumil et al., 2003].

Short description for process 3: stratospheric profile retrieval

Vertical profiles of NO_2 were retrieved employing an information operator approach [Rozanov, 2003] based on spectral fitting in the spectral range 420 to 450 nm. A forward modeling was performed using the CDI radiative transfer model [Rozanov et al., 2001]. Weighting functions were calculated in single scattering approximation. The vertical profiles are retrieved between 15 and 40 km at altitude levels coinciding with measurement tangent heights. First validation of SCIAMACHY NO_2 profiles with HALOE shows that good profiles can be retrieved from SCIAMACHY limb measurements. In addition first comparisons with data from balloon experiments were performed, demonstrating the good accuracy even in the lower stratosphere . Taking the preliminary status of the validation of NO_2 profiles into account, the error can currently be estimated to be typically 15%.

Short description for process 4: stratospheric column calculation

To calculate from the stratospheric profile the stratospheric column, first the tropopause height needs to be determined. The tropopause height is computed from meteorological model data provided by the European Center for Medium Range Weather Forecast (ECMWF). These data comprise three-dimensional model calculations of pressure and temperature on a latitude/longitude grid of 1° resolution and 60 height levels up to about 60 km. From these data, tropopause heights can be computed using either a temperature gradient or a PV criterion is applied. With this scheme, a global tropopause map is computed from the ECMWF data. The tropopause height yields the lower boundary for the numerical integration of the corresponding NO_2 limb profiles, and thus the stratospheric vertical column density.

To convert the stratospheric vertical column (VCD) into a stratospheric slant column (SCD), the stratospheric AMF needs to be calculated. In the computation of AMF_{strat}, one can once more make use of the distribution profiles derived from limb observation. This is done by running a RTM calculation with CDI, using the inferred stratospheric NO_2 profiles as input information, and setting the NO_2 concentration in the height layers below the tropopause to zero. In this way, AMF_{strat} is calculated for all nadir measurements considering the observation geometry (given by SZA and line-of-sight (LOS) of the measurement) and the chosen wavelength window for the DOAS analysis of the nadir spectra

Short description for process 5: derivation of tropospheric NO2 concentration

The stratospheric SCD is subtracted from the total *SCD*. The resulting slant tropospheric column can then be transformed into VCD_{trop} by an estimate of the tropospheric airmass factor AMF_{trop}. The latter is again obtained from an RTM calculation, in which assumptions on the tropospheric absorber profile and other parameters like aerosol and albedo have to be taken into account. It has been shown, that the uncertainties introduced by imperfect knowledge on albedo, cloud fraction and aerosol loading, are the dominating error contributions (Boersam et al. 2004, Richter et al. 2002) and needs to be carefully controlled.

Short description for process 6: quality check

In a post processing step, the quality of the intermediate and the end result will be checked, including the analysis of fit residuals and retrieval analytics. An error budget will be provided with the data.

References

Boersma, K.F., Eskes, H.K., and E.J. Brinksma, Error analysis of NO_2 retrieval from space, J. Geophys. Res., 109, D04311, doi:10.1029/2003JD003962, 2004

Bogumil, K., J. Orphal, T. Homann, S. Voigt, P.Spietz, O.C. Fleischmann, A. Vogel, M. Hartmann, H. Bovensmann, J. Frerik and J.P. Burrows, "Measurements of Molecular Absorption Spectra with the SCIAMACHY Pre-Flight Model: Instrument Characterization and Reference Data for Atmospheric Remote-Sensing in the 230-2380 nm Region", J. . Photochem. Photobiol. A., 157, 167-184, 2003

Bovensmann, H., J. P. Burrows, M. Buchwitz, J. Frerick, S. Noël, V. V. Rozanov, K. V. Chance, and A. P. G. Goede, *SCIAMACHY: Mission Objectives and Measurement Modes*, J. Atmos. Sci., 56, 127 - 150, 1999.

Richter, A., and J.P. Burrows, *Tropospheric* NO_2 *from GOME measurements*, Adv. Space Res., 29, 1673-1683, 2002

Rozanov, A., Rozanov V., and V., Burrows, J.P., *Numerical RTM for a spherical planetary atmosphere: combined differential-integral approach involving the Picard iterative approximation*, JQSRT, Vol. 69, p. 513-534, 2001.

Rozanov, A., Modeling of radiative transfer through a spherical planetary atmosphere: Application to atmospheric trace gases retrieval from occultation- and limb-measurements in UV-Vis-NIR, Logos Verlag Berlin, ISBN 3-8325-0138-X, ISSN 1615-6862, 2003

Rodgers, C.D., Characterization and error analysis of profiles retrieved from remote sounding measurements, J. Geophys. Res., 95, pp. 5587-5595, 1990

Savigny, C. v., A. Rozanov, H. Bovensmann, K.-U. Eichmann, S. Noel, V. V. Rozanov, B.-M. Sinnhuber, M. Weber, and J. P. Burrows, The ozone hole break-up in September 2002 as seen by SCIAMACHY on ENVISAT, J. Atmos. Sci., in press, 2004.

Sierk, B., A. Richter, A. Rozanov, Ch. von Savigny, A.M. Schmoltner, M. Buchwitz, H. Bovensmann, and J.P. Burrows, Retrieval and Monitoring of atmospheric trace gas concentrations in nadir and limb geometry using the space-borne SCIAMACHY instrument, presented at the “5th International Symposium on Advanced Environmental Monitoring", submitted to “Environmental Monitoring and Assessment”, 2004