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Evolution product of water vapour total columns retrieved from UV/vis satellite observations using the advanced AMF (A^3) algorithm

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1 INTRODUCTION

Water vapour (H_2O) is a key component of the Earth atmosphere and has a strong impact on the Earth's radiative balance. Satellite observations offer the unique opportunity to study the spatial and temporal variability of H_2O on a global scale.

The operational DLR H_2O total column product of GOME, SCIAMACHY and GOME-2 is retrieved using the absorptions of H_2O and of molecular oxygen (O_2) in the spectral range from 614-683.2 nm [Wagner 2003, Grossi et al. 2015]. This algorithm is robust and easy to implement and is almost independent of external data sets. However the operational retrieval also has its limitation:

1. The differences in vertical profiles of H_2O and O_2 can lead to large errors for individual observations
2. Several post-corrections complicate a detailed error analysis
3. The retrieval does not explicitly account for the impact of strong absorptions on the effective light path and terrain height variations.

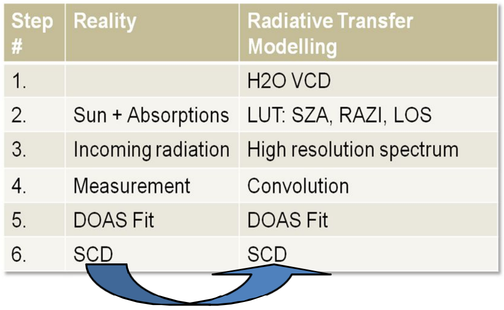
In order to overcome these limitations, a new advanced AMF algorithm (A^3) for H_2O has been developed in the framework of the ESA project 'GOME-Evolution' based on a look-up-table (LUT) approach. The LUT is built as described in section 2. The input to the LUT are the H_2O slant column densities (SCDs) as derived from the DOAS analysis as well as information about the cloud properties (derived from the same satellite observations) and the observation geometry. The output is the corresponding H_2O VCD. The LUT is computed for all relevant atmospheric scenarios and observation geometries using the Radiative Transfer Model (RTM) LIDORT [Spurr 2008].

2 A^3 LUT-BASED WATER VAPOUR RETRIEVAL ALGORITHM

2.1 General idea

The LUT used for the A^3 water vapor product is built based on RTM simulations. The H_2O VCD as a function of SCD is given in the LUT. The H_2O VCD can be derived from the LUT by comparing the SCD retrieved from satellite measurements with those in the LUT. The generation of the LUT is based on the RTM simulations of high resolution spectra with different H_2O VCDs and for different sun and measurement geometries. The reason of using the high resolution spectra is to properly account for the saturation-effect of H_2O absorption in the DOAS fit. The saturation-effect is due to the impact of strong atmospheric absorptions on the effective light path and due to the effect of the instrumental slit function on the highly resolved absorption lines of H_2O (and O_2). Due to the saturation effect the H_2O SCDs retrieved from the spectra using DOAS fits are significantly smaller than the true H_2O SCDs (see Fig. 1). In order to keep the DOAS slant column fit, which is fast and is performed at the spectral resolution of the satellite instrument, the A^3 algorithm relies on constructing the LUT by simulating satellite measurement. First the high resolution spectra are convoluted with the instrument slit function. Second, the convoluted spectra are analysed in the same way as the measurement spectra are treated. The flow chart of the algorithm is shown in Table 1.

Table 1 flow chat of the A^3 retrieval algorithm



Step #	Reality	Radiative Transfer Modelling
1.		H2O VCD
2.	Sun + Absorptions	LUT: SZA, RAZI, LOS
3.	Incoming radiation	High resolution spectrum
4.	Measurement	Convolution
5.	DOAS Fit	DOAS Fit
6.	SCD	SCD

As computation time does not allow calculating all spectra at a spectral resolution of 2pm, the high-resolution spectra are determined in analogy to the correlated-k method [Buchwitz et al 2000]. First, radiances are calculated for different values of the H_2O cross section (covering the whole range of cross section values in the spectral range of interest). As a result a function of the radiance depending on the cross section is obtained. Second, an absorption spectrum is calculated by interpolating this function to the wavelength dependent H_2O cross section. As within the width of the wavelength window the effect of Rayliegh scattering cannot be neglected, each of the quantities is calculated for 2 distinct wavelengths (625 and 665 nm), between which the intensities are then interpolated.

For the high resolution spectrum the initial LUT is used for a given viewing geometry (SZA, RAZI, LOS, Albedo, Terrain height) and is then treated as a function F interpolating between the values of the cross-section and wavelength for the given viewing geometry. This immediately yields the required radiance spectrum.

The final LUT of the Evolution product does not contain the high resolution spectra, but the DOAS fit yields the corresponding H_2O SCDs of the convoluted high resolution spectrum.

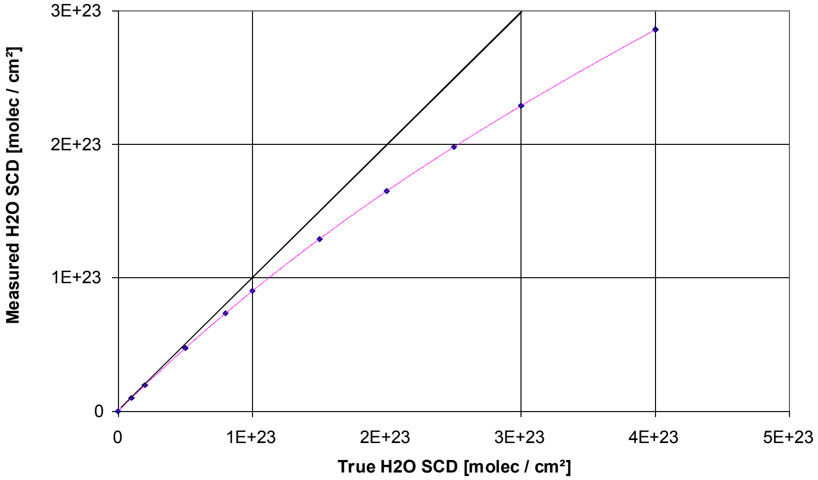


Figure 1 Dependence of the retrieved H_2O SCD on the true H_2O SCD for a typical viewing geometry.

2.2 Generation of the LUT

2.2.1 Radiative Transfer Computations

The intensities at 625 and 665nm are simulated using the linearized discrete ordinate radiative transfer model LIDORT for 10 H_2O xs values for each scenario at DLR. The scenarios are shown in Table 2. The dependence of the intensities as function of the xs F(xs) is acquired. Considering the wavelength dependence of Rayleigh scattering, the intensities are simulated at 625nm and 665nm. One example of the simulated intensities is shown in Fig. 2.

Table 2 Scenarios for RTM simulation of intensities

Quantity	Range, Stepsize	numbers
A-priori H_2O VCD (above sea level) (10^{21} molecules cm^{-2})	1.68, 2.78, 4.58, 7.55, 12.4, 20.5, 33.8, 55.8, 92, 152, 250, 412	12

Albedo	0.03 0.05 0.10 0.15 0.20 0.40. 0.60 0.80 1.00	9
SZA	25-85°, 5° steps	13
RAZI	0-180°, 45° steps	5
LOS	0-55°,3.44° steps	16
Terrain Height and cloud height	0, 0.5, 1, 2, 3, 4, 6, 8, 12	9
Wavelength	625nm; 665nm	2
Cross-section	equidistant	10
Total:		20217600

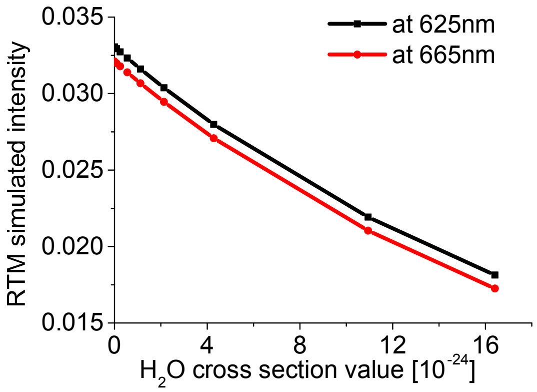


Figure 2 Example of the intensities simulated by the RTM at 625nm and 665nm for 10 H_2O xs values for one scenario.

Following the approach of [Buchwitz et al 2000 and references therein] magnitude sorted cross-section values were binned in a way, that the sum of all cross-section values in each bin yields the same value. The number of bins needs to represent the dependence of the intensity values on the cross-section without introducing large interpolation errors. However, as the dependence of the intensity as well as of the AMF (as shown in Fig. 3) is smooth with respect to the cross-section values until an effective optical depth of unity is reached, a number of bins of 10 was found to be suitable.

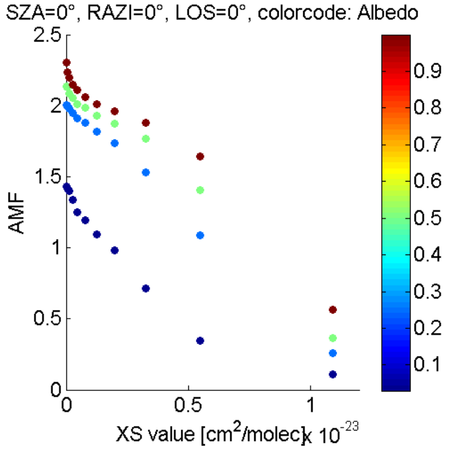


Figure 3: Simulated AMF for a water vapour VCD of 2.5x10^{23} molec/cm^2 and a scale height of 2km as function of the cross-section, using the RTM simulations, for a nadir pixel. The colorbar indicates the surface albedo.

An unknown parameter for the retrieval of the water vapour VCD is the exact profile shape. Dominantly, it is governed by the temperature profile of air and the relative humidity. According to the Magnus-equation (or Clausius Claypeyron), an upper limit or the water vapour content at a given height and temperature is obtained. The typical water vapour scale height is in the order of 2km [e.g. Wagner et al., 2013], which was also observed from radio sondes [Otarola et al 2011]. This is also the scale height which was assumed for the current, operational water vapour product.

In order to simplify the treatment of clouds, the VCD in the LUT is the VCD from sea level. However, the radiative transfer calculations were done for the respective viewing geometry in which in a certain height (terrain height or cloud top height) the light was blocked from penetrating deeper into the atmosphere (by the ground or by a simplified Lambertian cloud).

Therefore the VCD from the LUT needs to be corrected for the terrain height T by a simple subtraction of the part of the vertical column between sea level height and terrain height. This is also valid for negative terrain heights.

The water vapour profile is assumed to have an exponential shape with a scale height S:

$$c(h) = a_0 e^{-\frac{h}{S}}$$

And accordingly the total VCD

$$\mathrm{VCD}_0 = \int_0^\infty c(h)\,\mathrm{d}h$$

the real VCD is then calculated by subtracting the VCD within 0 - T:

$$VCD_T = \int_0^T c(h)\,\mathrm{d}h = VCD_0\left(1 - e^{-\frac{T}{S}}\right)$$

$$VCD = VCD_0 - VCD_T = VCD_0 e^{-\frac{T}{S}}$$

2.2.2 Calculation of high resolution spectra and treatment of clouds

The intensities at 625nm and 665nm as the function of the cross section values (F_{625}(xs) and F_{665}(xs) are acquired from the RTM simulations for the 10 cross section values for the individual scenarios. Then the high-resolution spectra I(λ) are constructed from the two F(xs) and the high-resolution H_2O xs(λ) by interpolations:

$$I\,(\lambda) = \frac{665-\lambda}{40} \times F_{625}\big(xs(\lambda)\big) + \frac{\lambda-625}{40} \times F_{665}\big(xs(\lambda)\big)$$

The A^3 water vapour product relies on cloud properties (effective cloud fraction and cloud pressure) retrieved using FRESCO [Koelemeijer et al 2001]. Since the Lambertian surface with the surface albedo of 0.8 is assumed in the FRESCO cloud product, the same Lambertian cloud model is used for the generation of the LUT. In order to explicitly consider the cloud effect, clouds are included in the calculations of the high resolution spectra. The intensities simulated by the RTM for an albedo of 0.8 (F(xs, albedo=0.8)) represent the cloudy scenarios. Therefore the high-resolution spectra I_{cloud}(λ) for a satellite pixel fully covered by clouds can be calculated based on the F(xs, albedo=0.8). The spectra for a satellite pixel partially covered by clouds is calculated by combing the spectra from the clear part (I_{clear} (λ)) and the cloudy part (I_{cloud}(λ)) based on the independent pixel approximation:

$$I_{sum}\,(\lambda) = (1-CF) \times I_{clear}(\lambda) + CF \times I_{cloud}(\lambda)$$

Here CF is the effective cloud fraction. Then the I_{sum}(λ) is convolved with the instrumental slit function (Gaussian shape of 0.5nm FWHM for GOME-2) and sampled at 0.1nm to get I_{conv}(λ).

2.2.3 DOAS fits to retrieve H_2O SCD

The linear fit is applied to the logarithm of I_{conv}(λ) to retrieve the H_2O SCD in the spectral range from 614-683.2nm. A polynomial of 5th degree and the H_2O cross section convolved with the instrumental slit function are included in the fits.

2.2.4 Final LUT dimensions

The final LUT of the A^3 product contains the following dimensions

1. H_2O VCD (above the ground)
2. A-priori H_2O VCD (above sea level)
3. CF
4. Cloud height
5. SZA
6. RAZI
7. LOS
8. Surface albedo
9. Terrain height
10. H_2O SCD

For each measurement, the corresponding H_2O VCD is retrieved by comparing the measured H_2O SCD with the H_2O SCD in the LUT.

2.3 Implementation of the LUT in retrievals of real measurements

The use of AMF is well established for the retrieval of trace gases like NO_2 and HCHO; the AMF (and thereby the VCD) can be directly gained from online RTM simulations or interpolation of a LUT. However, for H_2O, the situation is more complex as the AMF depends also on the VCD.

Thus, a two-step procedure has to be applied:

For a given scene (viewing geometry, cloud properties, surface albedo & terrain height), both the H_2O SCD and true VCD (above ground) are interpolated from the LUT yielding a relation between true VCD and the measured SCD (see blue crosses in Fig. 4). This step can be done for a complete orbit within one interpolation call and is fast.

For each satellite ground pixel, the final VCD (green line in Fig. 4) is derived by interpolating VCD = f(SCD) to the measured SCD (red line in Fig. 4). As f is different for each scene, this has to be done within a loop. Therefore the AMF is not explicitly used in the conversion of SCD to VCD but implicitly used.

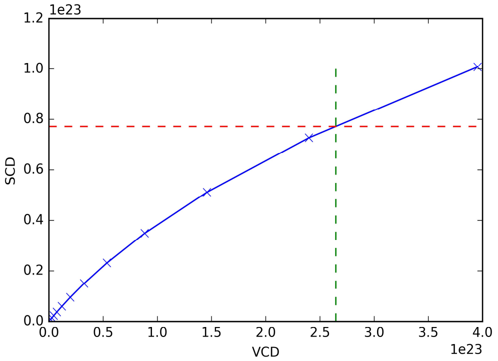


Figure 4 Illustration of the LUT interpolation procedure. This example for CF=0.25, CH=8.6 km, elevation = 0.1 km.

The input quantities for the retrieval of the H_2O VCDs from the GOME-2 observations using the A^3 LUT are listed in Table 3.

Table 3: Dynamic input information needed in the evolution product.

Name/Data	Symbol	Unit	Source
Effective cloud fraction	f_c	---	FRESCO
Cloud height	Z_{ct}	km	calculated from FRESCO cloud pressure
H_2O SCD		molec/cm^2	MPIC DOAS retrieval (same settings as in GDP)
SZA, RAZI, LOS			GOME-2 level 1

Measurement time and geo-location			GOME-2 level 1
Surface albedo			Merged Koelemeijer/Grzegorski (see Grossi et al., AMT, 2015, page 1116, for details)
Terrain height		km	GTOPO30, downscaled to 0.1° horizontal resolution

2.4 Error analysis

2.4.1 Verification of the algorithm

The new LUT AMF approach was tested by applying it also to the measured O_2 absorption. For that purpose a new LUT for the O_2 absorption at 630 nm was calculated in the same way as for the H_2O absorption at 650 nm. Then the O_2 VCD was derived from the measured O_2 SCD at 630 nm by combining the O_2 LUT with cloud information (cloud fraction and cloud height) derived from the FRESCO algorithm. It was found that the derived O_2 VCD as almost independent from cloud fraction and cloud height, although completely different O_2 absorption bands are used by the FRESCO algorithm and our DOAS analysis. From this finding two important conclusions could be derived:

a) The FRESCO cloud properties are perfectly suited for application to our new LUT approach.

b) Our new LUT approach works almost perfectly: the LUT is consistently read out and applied to the derived DOAS results and the cloud products are correctly assigned to the corresponding entries of the LUT.

2.4.2 Validation of the H_2O products

A first inspection of the new H_2O results showed that the global distribution of the H_2O VCD is in general consistent with existing data sets. However, it was also found that the derived results strongly depended on the cloud properties. A validation study clearly indicated that acceptable results are only obtained for medium cloud fractions and medium cloud heights. After several tests, in particular the test described in section 2.4.1, it turned out that the most probable reason for the deviations is a non-perfect assumption of the H_2O vertical profile for the construction of the LUT. Here an exponential profile with a scale height of 2 km was assumed. The validation results indicated that the chosen value for the scale height of 2 km is probably too large. Moreover, the choice of a constant scale for the whole globe might not be fully appropriate.

This issue will be addressed by investigating the spatio-temporal variability of atmospheric H_2O profiles from radio sonde measurements and atmospheric model simulations. After an improved value (or climatology) of the H_2O profile is determined, the LUT will be recalculated and again applied to the satellite measurements.

3. PRODUCT DATA FIELD DESCRIPTION

The listed parameters to be stored as the result of the data processing of the H_2O A^3 product will be provided in HDF5 format. The following information listed in Table 4 is included in for each pixel. Files are organized as the respective GOME-2 level 1 files, i.e. one file per orbit.

Table 4: List of output parameters for the A^3 product

Group	Field Name	Unit	Description
H2O	**TCWV**	kg/m^2	Total column water vapor
auxiliary	**cloud_fraction**	---	
	cloud_height	km	
geolocation	**center_lat**	degree	Latitudes of the pixel center
	center_lon	degree	Longitudes of the pixel center
	sza_sat	degree	Solar zenith angle
	vza_sat	degree	Viewing zenith angle
	razi_sat	degree	Relative azimuth angle all angles at satellite
time	**time**	seconds	Seconds since 1 Jan 2000, 0:00 UTC

4. AUXILIARY INFORMATION NEEDS

Table 5: Static auxiliary information needed in the evolution product.

Name/Data	Symbol	Unit	Source	Pre-process needs	Comments
Instrument slit function	*SF*	---	Slit function provided by wavelength/detector Or Kurucz Fit	---	---
High-resolution reference solar spectrum	E_s	W $m^{-2}nm^{-1}$	Chance and Kurucz [2010]	---	---
Digital elevation map	Z_s	km	Same DEM for all L2 products	---	---
Albedo map			Koelemeijer/Grzegorski		see Grossi et al., AMT, 2015, page 1116, for details

5. ABBREVIATIONS AND ACRONYMS

A list of abbreviations and acronyms which are used throughout this document is given below:

A^3	Advanced AMF Algorithm
AMF	Air Mass Factor
ATBD	Algorithm Theoretical Basis Document
CF	effective Cloud Fraction
DLR	German Aerospace Center (Oberpfaffenhofen)
DOAS	Differential Optical Absorption Spectroscopy
ESA	European Space Agency
FRESCO	Fast REtrieval Scheme for Clouds from the Oxygen *A*-band
FWHM	Full Width at Half Maximum
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
GOME-2A	GOME-2/MetOp-A
GOME-2B	GOME-2/MetOp-B
GTOPO30	Global 30 Arc-Second Elevation
H_2O	Water Vapour
LIDORT	LInearized Discrete Ordinate Radiative Transfer
LOS	Line Of Sight
LUT	Look Up Table
MetOp	Meteorological Operational

MPIC	*Max Planck Institute for Chemistry (Mainz)*
O_2	molecular oxygen
RAZI	relative azimuth angle between the sun and the viewing direction of the instrument
RTM	Radiative Transfer Model
SCD	Slant Column Density
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CartograpHY
SZA	Solar Zenith Angle
TCWV	Total Column Water Vapour
VCD	Vertical Column Density
xs	cross section

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