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Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring:

WP2 Initial report on measurement uncertainty gap analysis

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1. Introduction and Overview

The ECV/instrument combinations discussed in the following sections were chosen because the technique and data analysis is mature enough for these ECVs to be likely candidates for data streams of reference quality. The development of reference quality measurement capabilities and uncertainty quantification is built on the efforts previously made by groups and networks such as GRUAN, NDACC, TCCON and ACTRIS-EARLINET.

Copious measurements made under the umbrella of these high quality global networks require only relatively little effort to ensure traceability and robust uncertainty estimation, and our aim is to improve our understanding of the fundamental measurement uncertainties of these selected ECV/instrument combinations and to further develop these existing data products so they can be of reference quality. The analysis algorithm and uncertainty characterisation is undertaken by the respective instrument experts within the relevant consortium in consultation with the wider scientific community. A brief background about the measurement technique & instrumentation, the measurement procedure & analysis algorithm and the method to calculate the measurement uncertainties is provided in Section 2. The known gaps in the uncertainty assessment for each of the investigated ECV/instrument combination are listed in a table in Section 3.

2. Measurement Technique and Uncertainty Quantification

2.1 Aerosol, water vapour, ozone and temperature profiles measured by lidar

2.1.1 Lidar commonalities

Lidars (lidar is the acronym for light detection and ranging) are the primary instruments to provide height resolved information in the atmosphere. The measurement principle is based on the optical analogon of the radar, where the elapsed time between emission of a laser pulse and the reception time from the target, in combination with the received signal intensity provides range-resolved information. The interaction of the laser beam with the atmosphere is complex: A variety of scattering and absorption phenomena take place simultaneously, both elastic (i.e. at the same wavelength as the emitted laser beam that excites the processes, in particular Mie and Rayleigh scattering, including multiple scattering) as well as inelastic (i.e. at a different wavelength: vibrational and rotational Raman, fluorescence). Therefore, the application drives the set-up of the lidar in order to optimise the sensitivity for the subject at hand.

In the context of this project, the lidars provide quantitative properties in a traceable way, for which the uncertainty budgets will be determined (e.g. Immler, 2010).

2.1.2 Aerosol lidar

Measurement technique and instrumentation
Aerosol lidars are the primary instruments to provide height resolved information about the presence of aerosols, and to a certain extent clouds. Two instrument types provide quantitative aerosol optical information:

- Aerosol Raman Lidar (**AERL**), that uses inelastically (Raman) scattered laser light by nitrogen molecules in addition to the elastically scattered laser light by molecules and particles, and

- High-Spectral Resolution Lidar (**HSRL**) that separates the molecular signal from the signal that is dominated by the particle scattering by using narrow band filtering techniques.

Both instrument types provide the optical aerosol extinction coefficient (indicated by α_{aer} in units of m^{-1}) and the backscatter coefficient (indicated by $ß_{aer}$ in units of $Sr^{-1}.m^{-1}$). The ratio of α_{aer} and $ß_{aer}$ gives the so-called lidar ratio S (in units of Sr) that is an intensive parameter, i.e. particle specific and independent of the quantity of the particles. The lidar ratio therefore provides important information about the aerosol species, although the lidar ratio alone is not sufficient for a full speciation. Additional information about the aerosol species and microphysical properties such as effective size can be obtained by measurements at additional wavelengths of both α_{aer} and $ß_{aer}$. Backscatter lidars and ceilometers are not considered in this context as they do not provide quantitative information that meet the criteria for reference data of optical aerosol properties.

Measurement procedure and analysis algorithm
A formalism has been developed in the framework of NDACC and EARLINET that will be investigated.

Uncertainty quantification
The description will take the following uncertainties into account: measurement uncertainty (including noise (background, detector noise), systematic uncertainties (e.g. non-linearities, overlap effects), wavelength tuning uncertainties, spectral width) and analysis uncertainties (including range resolution (smoothing, vertical resolution settings, calibration constants (backscatter profile), density profile (pressure), rayleigh correction, temperature profile correction, wavelength dependence, multiple scattering).

2.1.3 Water vapour lidar

Measurement technique and instrumentation
To make lidar measurements specifically sensitive to water vapour, use is made of the spectroscopic properties of water vapour. Two instrument types provide this information:

- Water Vapour Raman lidar (**WVRL**), that uses inelastically (Raman) scattered laser light by water vapour molecules in addition to the inelastically (Raman) scattered laser light by nitrogen molecules. The ratio of the two lidar signals is directly proportional to the water vapour mixing ratio (specific humidity, q in units of g/kg). Calibration to an external source is necessary.
- Water Vapour Differential absorption lidar (**WVDIAL**) uses a set of two lidar signals from elastically scattered laser light, where the laser wavelengths are tuned to the water vapour absorption spectrum. The tuning is such that one wavelength is absorbed more than the other. The ratio of the signals thus contains information about the water vapour concentration profile. Since the laser wavelengths and water vapour absorption cross-sections are known, no further external calibration is needed. The water vapour concentration is expressed in units of mol/m^3.

Measurement procedure and analysis algorithm
The treatment of uncertainty in lidar retrievals depends on the choice of the theoretical equations used as well as their implementation to the real world, i.e., after considering all the caveats associated with the design, setup, and operation of an actual lidar instrument. To retrieve a number density profile in the troposphere or stratosphere using, we start from the same initial theoretical model, namely the Lidar Equation (e.g., Hinkley, 1976). This equation in its most

compressed form describes the emission of light by a laser source, its backscatter at altitude *z*, its extinction and scattering along its path up and back, and its collection back on a detector.

Uncertainty quantification
A formalism that will be incorporated here has been developed in the framework of NDACC. The uncertainty description will take the following uncertainties into account: measurement uncertainties (including noise (background, detector noise), systematic uncertainties (e.g. non-linearities, overlap effects), wavelength tuning errors, spectral width) and analysis errors (including range resolution (smoothing, vertical resolution settings), calibration constants, density profile (pressure), Rayleigh correction, temperature profile correction, wavelength dependence, multiple scattering, vertical resolution, aerosol correction (wavelength dependent and inhomogeneity differential effects)).

2.1.4 Ozone lidar

Measurement technique and instrumentation
To make lidar measurements specifically sensitive to ozone, use is made of spectroscopic properties of ozone, in particular, absorption. Ozone Differential Absorption Lidar (**O3DIAL**) uses a set of two lidar signals from elastically scattered laser light, where the laser wavelengths are tuned to the ozone absorption spectrum. The tuning is such that one wavelength is absorbed more than the other. The ratio of the signals thus contains information about the ozone concentration profile. Since the laser wavelengths and ozone absorption cross-sections are known, no further external calibration is needed. The ozone concentration is expressed in units of mol/m^3.

Measurement procedure and analysis algorithm
Here we will follow the same procedure as outlined under 2.1.3.

Uncertainty quantification
A formalism that will be incorporated here has been developed within the framework of NDACC. The uncertainty description will take the following uncertainties into account: measurement uncertainties (including noise (background, detector noise), systematic uncertainties (e.g. non-linearities, overlap effects), wavelength tuning uncertainties, spectral width) and analysis uncertainties (including Range resolution (smoothing, vertical resolution settings), calibration constants (backscatter profile), density profile (pressure), Rayleigh correction, temperature profile correction, wavelength dependence, wavelength tuning uncertainties, spectral width, multiple scattering, aerosol correction (wavelength dependent and inhomogeneity differential effects)).

2.1.5 Temperature lidar

Measurement technique and instrumentation
To make the lidar measurements specifically sensitive to temperature, two instrument types provide this information:

- Temperature dependence of pure rotational Raman scattering (**PRRTL**). Here, use is made of the shift in population density, and therefore scattering intensity, in pure-rotational Raman lines excited in nitrogen. Higher orders (at a larger wavelength shift from the central (laser) line are preferred as temperature increases while the lower wavelength shifts will become more sparsely populated. The ratio between the ‘low-shift’ and ‘high-shift’ wavelength band therefore contains information about the atmospheric temperature. Since this is a relative effect, the temperature needs to be calibrated against an external source.

- The Rayleigh-Mie lidar technique (**RMTL**). The temperature profile is computed from the density profile assuming that the atmosphere obeys the perfect gas law and is in hydrostatic equilibrium and in the absence of aerosols. The constant mixing ratio of the major atmospheric constituents (nitrogen, oxygen and argon) and the negligible value of the water vapour mixing ratio justify the choice of a constant value for the air mean molecular weight.

Measurement procedure and analysis algorithm
Here we will follow the same procedure as outlined under 2.1.3.

Uncertainty quantification
The uncertainty description will take the following uncertainties into account: measurement uncertainties (including noise (background, detector noise), Systematic uncertainties (e.g. non-linearities, overlap effects), wavelength tuning uncertainties, spectral width) and analysis uncertainties (including range resolution (smoothing, vertical resolution settings), calibration uncertainties, density profile (pressure), wavelength dependence, spectral bandwidth, wavelength tuning uncertainties, multiple scattering, aerosol correction (wavelength dependent and inhomogeneity differential effects)).

2.2 Temperature and H_2O profiles measured by microwave radiometers

2.2.1 Measurement technique and instrumentation

Atmospheric temperature and humidity profiles can be inferred by ground-based microwave radiometer (MWR) observations. Ground-based MWR is an instrument calibrated to measure the natural down-welling thermal emission from the Earth's atmosphere. The quantity measured by a MWR is atmospheric radiance ($W/(m^2\cdot sr\cdot Hz)$), which is usually converted into brightness temperature (Tb) to adopt the units of Kelvin.

The most common MWR commercial units operate in the 20-60 GHz frequency (0.5 to 1.5 cm wavelength) range, in which atmospheric thermal emission comes from atmospheric gases (primarily oxygen and water vapour) and hydrometeors (mainly liquid water particles, while ice emission is negligible). In this range the scattering contribution is generally negligible unless under moderate to heavy precipitation conditions.

Thus, the down-welling atmospheric radiance in the 20-60 GHz range depends upon the atmospheric temperature, humidity and liquid cloud conditions. Thus MWR Tb observations at selected frequency channels are used to infer atmospheric temperature and humidity profiles as well as information on the vertically-integrated total column water vapour (TCWV) and liquid water (TCLW).

With careful design, a MWR can make continuous observations (time scales of seconds to minutes) in a long-term unattended mode in nearly all weather conditions.

2.2.2 Measurement procedure and analysis algorithm

MWR receivers output a detector voltage which is related to brightness temperature through a set of parameters which are determined by the radiometer calibration. The radiometer calibration is performed by letting the receivers observe at least two targets at known different temperatures (warm/cold), ideally covering a large temperature range. This 2-point calibration typically exploits two high emissivity targets (approximating black body): the cold calibration point is obtained by cooling the target with liquid nitrogen (LN2), while the warm calibration point is obtained by heating or keeping the other target at ambient temperature. The 2-point calibration allows to determine two calibration parameters, being the detector gain and the receiver noise temperature. An advanced calibration method is the 4-point calibration which uses additional power injected by a noise diode located within the MWR electronics. The noise is injected during the calibration process to generate two additional calibration points. The four calibration points are then used to determine four calibration parameters being the detector gain, the receiver noise temperature, the receiver non-linearity, and the noise diode temperature. Another method, called tipping curve calibration, exploits observations at different elevation angles to extrapolate a cold calibration point from the microwave cosmic background radiation. The tipping curve calibration method relies on the linear relationship between air mass and atmospheric opacity under the assumption of horizontally homogeneous conditions. Thus, the tipping curve calibration method is only applicable to semi-transparent channels (typically 20-35 GHz channels only).

Calibrated brightness temperature at several frequency channels (typically ten to thirty) are then processed to infer the atmospheric properties, i.e. TCWV, TCLW, temperature and humidity profiles. This requires a retrieval model, which transforms the measured radiative quantities (Tb) into thermodynamic atmospheric quantities (TCWV, TCLW, temperature and humidity profiles). Retrieval models are generally based on the theory of microwave radiative transfer through the atmospheric medium. However, the inverse problem is ill-posed and a rigorous mathematical solution does not exist. Therefore, the MWR measurements are to be considered as constraints and need to be coupled with supplementary sources of information to reduce the domain of solutions. Supplementary information can be provided by a priori information obtained from past data (i.e. radiosonde ascents) or from the output of numerical meteorological models.

Typically, synthetic Tb derived via radiative transfer calculations from representative long-term radiosonde data sets for the specific geographic region are used to derive statistical algorithms via regression or neural network techniques. Alternatively, optimal estimation methods (OEM) solve the inverse problem in a physically consistent way, optimally coupling MWR observations with a priori background knowledge accounting for their uncertainty characteristics. OEM are currently only applied in post-processing on a research level.

The MWR measurement traceability needs to be enforced in the calibration procedure (transfer from raw voltages to Tb). This implies the use of certified black-body targets and temperature sensors (measuring the target temperature). Commercial black-body targets have reached a mature state, but the manufacturer's data are usually limited (e.g. 18 GHz is a typical maximum frequency even if the target is used above that frequency). Despite many realizations of microwave brightness temperature standards exist in the form of heated or cooled calibration targets, none are currently maintained as a national standard by a National Measurement Institute (NMI). Metrology applicable to microwave remote sensing radiometry is currently under development, including Tb standards. It is expected that SI-traceable Tb calibration for black-body targets and transfer standards in the form of calibrated black-body targets will be available in the next few years.

2.2.3 Uncertainty quantification

Commercial MWR make use of statistical algorithms (regression or neural networks) to estimate temperature and humidity profiles as well as TCWV and TCLW. Regression or neural network techniques are fast to apply in real time but do not provide uncertainty profile estimates for an individual measurement. Thus, MWR retrieval uncertainty is often estimated as within the agreement with respect to atmospheric profiles measured by nearly simultaneous and colocated radiosonde ascents. In this regard, the open literature reports consistent results for root-mean-square difference with respect to radiosonde measurements:

- Temperature profile ~0.5 K - 2.0 K (increasing almost linearly with height from near the surface to mid-troposphere);
- Humidity profile ~0.5-1.5 g/m^3 (increasing from the surface to mid-troposphere, decreasing above);
- TCWV ~1 kg/m^2.

Since common radiosondes do not measure cloud liquid, the uncertainty of TCLW is estimated through the analysis of simulated data within 20-30 g/m^2.

However, a proper uncertainty quantification of MWR retrievals shall result from the propagation of the uncertainty in calibration (transfer from raw voltages to Tb) and the uncertainty in the retrieval (transfer from Tb to atmospheric variables).

For current MWR technology the noise level at 1 s integration time is of the order of few tenths of a Kelvin. Conversely, the uncertainties on the absolute calibration are larger, due to the uncertainties on the detector non-linearity and at the calibration points. The latter arise from uncertainties in the target emissivity and the temperature measurement of the targets. The main contribution to the calibration uncertainty results from uncertainties at the cold calibration point. The calibration uncertainties depend on the applied calibration techniques. For example, the uncertainty of the LN2 calibration is estimated to be in the order of 1 K, while the uncertainty of the tipping curve calibration is estimated within 0.5 K, when conditions are such to be applicable.

Retrieval uncertainty stems from the uncertainties in the a priori information (first guess), in the absorption model, and in the solution of the inverse problem. The uncertainty in the a priori information is estimated from the set of supplementary information available, e.g. from the variability of a past long-term record data set. The uncertainty in the absorption model results from the combination of the uncertainties in the microwave absorption of water vapour, oxygen, and liquid water. The major uncertainties are related to the absorption of supercooled water, water vapour, and oxygen at relative transparent frequencies. The uncertainty arising from the solution of the inverse problem can be estimated by propagating the instrument uncertainty through the inverse method equations.

A convenient way to estimate the total uncertainty is to use OEM. OEM have the advantage to associate a dynamical error characterization to the retrieved atmospheric variables. In fact, OEM not only provide the optimal estimate of the retrieved quantities, but also an estimate of their uncertainty, effectively accounting for both the calibration and retrieval uncertainties. Different realizations of OEM, such as the so-called Integrated Profiling Technique (IPT) and the one-dimentional variational retrieval (1-DVAR), have already demonstrated the capability to provide TCWV, TCLW, temperature and humidity profiles with the associated dynamical uncertainties.

2.3 CH_4, CO_2, O_3, and H_2O columns and profiles measured by FTS

2.3.1. Measurement technique and instrumentation

For all species, the technique is the same: it is the remote-sensing of the total column abundance of the species and, if possible, also information about its vertical distribution in the atmosphere, using ground-based solar absorption spectrometry in the infrared spectral range, with a Fourier-transform infrared spectrometer of the Michelson interferometer type (FTIR).

Ozone and H_2O vapour are measured in the mid-infrared region of the spectrum as part of the NDACC network. CH_4 and CO_2 can be measured in both the mid- and near-infrared region of the spectrum, in the NDACC and TCCON networks, respectively. Nevertheless, CO_2 is a standard product of the TCCON network rather than the NDACC network; therefore, in GAIA-CLIM, we will not discuss the NDACC CO_2 measurements and focus on the TCCON CO_2 measurements only.

In the data user guide of the NORS project a detailed description of the FTIR measurement technique and instrument is provided (http://nors.aeronomie.be/projectdir/PDF/NORS_D4.2_DUG.pdf).

2.3.2. Measurement procedure and analysis algorithm

The data user guide of the NORS project also provides information on the FTIR measurement procedure & analysis algorithm (http://nors.aeronomie.be/projectdir/PDF/NORS_D4.2_DUG.pdf).

2.3.3. Uncertainty quantification

In the NORS report of uncertainty budgets, a description of the FTIR uncertainties for O_3 and CH_4 and the way they are evaluated at present and the limitations hereof can be found (http://nors.aeronomie.be/projectdir/PDF/NORS_D4.3_UB.pdf). For H_2O, the description of the evaluation of the uncertainty budget can be found in Schneider et al. (2012).

For TCCON CO_2 and CH_4, the following table lists the sources of uncertainty:

Source of uncertainty	xCO_2		xCH_4	
GGG Version	2012	2014	2012	2014
Laser mis-sampling	0-0.25%	<0.025%	0-0.25%	<0.025%
Detector non-linearity	0.03 %	0.03 %		0.05 %
Optical misalignment	0.10 %	0.10 %		
A priori profile shape	0.06 %	0.06 %	0.05 %	0.05 %
In Situ Calibration	0.1% (Np=16)	0.07% (Np=32)	0.45% (Np=9)	1.04% (Np=26)
Atmospheric a priori temperature	0.04 %	0.04 %		0.05 %
Atmospheric a priori pressure	0.06 %	0.06 %		0.04 %
Surface Pressure		0.04 %		0.04 %
Mainly solar photon noise (N=number of spectra averaged)	0.25N-0.5%	0.25N-0.5%	0.3N-0.5%	0.3N-0.5%

from https://tccon-wiki.caltech.edu/

2.4 Total column ozone measured by UV/visible spectroscopy

2.4.1 Measurement technique and instrumentation

UV/visible spectroscopy is a measurement technique used to determine the amount of atmospheric trace gas species, such as ozone, by analysing zenith-sky spectra at large solar zenith angle (SZA). For the analysis of total column ozone, the absorption features of ozone and other relevant trace gases are fitted in the Chappuis bands within a wavelength window of 450-550 nm using a nonlinear least-squares fitting algorithm. This wavelength range avoids contamination by the strongest water vapour (H_2O) and O_4 absorption bands while allowing for a good ozone retrieval. Because the light source is the sun and the sun is low on the horizon at large SZA, this allows for a long light path through the atmosphere and the depth of the absorption of the trace gas of interest is used to determine the amount of trace gas measured along the slant paths the sunlight travels through the atmosphere before arriving at the detector. Hence, the product of the spectral analysis are the slant column densities (SCDs), which are then converted into vertical column densities (VCDs) using so-called air mass factors (AMFs) derived by radiative transfer (RT) calculations from locally measured or climatological ozone and air density profiles.

The instrumentation consists of (1) the receiving optics (telescope) to collect the light and guide it into the spectrometer, (2) a grating spectrometer to separate the radiation into the different wavelengths and to re-image them onto a detector, and (3) a detector to convert the spectrum into a signal which is then read out and transferred to the control computer.

2.4.2 Measurement procedure and analysis algorithm

Protocols for measurement procedures, data analysis and quality assessment are defined as part of the activities of the NDACC UV-visible spectroscopy working group. To ensure the availability of long-term high-quality data sets within the network, homogenisation of the data sets is vital including clear recommendations for the analysis settings, the absorption cross-sections used and the input parameters for the RT calculations (see NDACC UV-vis working group report, http://ndacc-uvvis-wg.aeronomie.be/tools/NDACC_UVVIS-WG_O3settings_v2.pdf).

As part of the analysis procedure, all spectra are corrected for their dark current and offset contributions. Each “to-be-analysed” spectrum is then ratioed with a so-called “reference” spectrum to remove the strong Fraunhofer bands and, if relevant, some instrumental artefacts. This “ratio” spectrum is then fitted with the absorption cross-sections of the absorbers relevant for the wavelength range chosen for the analysis. For total column retrievals from zenith-sky UV-visible spectra the recommended wavelength range is 450-550 nm and absorption cross-sections for ozone, NO_2, H_2O and O_4 are used as well as a Ring cross-section to correct for the filling in of the Fraunhofer bands (Ring effect), a polynomial term to filter out broadband atmospheric attenuation and an offset term to deal with straylight in the spectrometer.

The ozone amount in the reference spectrum is determined using the Langley plot method and added back to the SCD. The measured SCD is then divided by the AMF to calculate the VCD in molecules/cm^2 which is then converted into Dobson Units. The NDACC UV-visible spectroscopy working group recommends the use of a generic look-up table of ozone AMFs which has been developed at BIRA-IASB (see NDACC UV-vis working group report) and accounts for the latitudinal and seasonal dependencies of the ozone vertical profiles. The NDACC recommendation is furthermore to average all retrieved vertical columns of ozone between 86^{o} and 91^{o} SZA. This range minimizes measurement uncertainties due to slant column fitting and AMF calculation and provides stratospheric ozone measurements with limited sensitivity to tropospheric ozone and clouds.

2.4.3 Uncertainty quantification

The uncertainty budget of the measurements is obtained by considering uncertainty sources affecting the determination of 1) the differential slant column densities (DSCD), 2) the residual amount in the reference spectrum, and 3) the AMF.

1) Uncertainties in the DSCDs evaluated within the fitting procedure are uncertainties caused by instrumental imperfections such as resolution change, etaloning and other non-linearities of the detector, stray-light, and polarisation effects, as well as uncertainties in the Ring effect, unknown absorbers, and the wavelengths dependency of the AMF. Such errors are mostly random in nature and therefore can be estimated statistically from the least-squares fit procedure. Fitting errors derived from the least-squares analysis typically result in unrealistically small uncertainties and often underestimate the measurement uncertainty by a factor of two. Results from intercomparisons exercises (e.g. Van Roozendael et al., 1998, Vandaele et al., 2005, Roscoe et al., 2010) show that state-of-the-art instruments hardly agree to better than a few percent, even when standardised analysis procedures are used. This indicates that the actual accuracy on the DSCDs is limited by uncontrolled instrumental and/or analysis factors. Based on experience and results from intercomparison campaigns, an uncertainty of approximately 3% is typically used for the ozone DSCDs. This uncertainty adds to systematic uncertainties in ozone absorption cross sections in the Chappuis bands and in their (very small) temperature dependence which is also of the order of 3% in our spectral range (Orphal, 2003).

2) The accuracy in the determination of the residual amount of ozone in the reference spectrum is determined by the method used to derive the vertical column at the time of the reference spectrum acquisition. If the Langley plot approach is used, the contribution from this uncertainty source to the total uncertainty budget is potentially small, of the order of 1%.

3) Sources of uncertainty in the ozone AMF calculations are the choice of the ozone profiles, the choice of the aerosol extinction profiles, clouds, albedo and the actual radiative transfer model used for the calculations. Hendrick et al. (2011) found that the uncertainty in the calculated AMFs based on uncertainties in the ozone profiles is around 1% and the aerosol profiles around 0.6%. They also found that AMFs calculated for cloudy conditions are systematically larger than AMFs calculated for non-cloudy conditions with the difference in the 86^{o} – 91^{o} SZA range being approx. 3.3 %. The typically small impact of clouds on zenith-sky ozone UV-vis measurements at twilight is due to the fact that the mean scattering layer is generally located at higher altitude than that of the clouds. The impact of surface albedo on the ozone AMF calculations and the actual model used for the calculations are two more sources in the uncertainty and within the 86^{o} – 91^{o} SZA range, both are about 0.7%.

In summary, Hendrick et al. (2011) conclude that the precision in the total column ozone measurements is 4.7% to which the largest contribution is coming from the AMF and from the uncertainty in the SCD estimated to be 3% at twilight (including the impact of unknown instrumental and systematic misfit effects) and that the total accuracy, important for comparison with other instruments, is 5.9 %.

2.5 Tropospheric ozone measured by MAX-DOAS and Pandora

2.5.1 Measurement technique and instrumentation

As detailed in Section 2.4, UV/visible spectroscopy is a measurement technique used to determine the amount of atmospheric trace gases, such as ozone, by analysing zenith-sky spectra. More recently an addition to this technique, the so-called MAX-DOAS method, is used to also retrieve the tropospheric components of trace gases such as ozone or NO_2. The MAX-DOAS measurement technique has been described in detail in e.g. Hoenninger et al. (2004) and Wittrock et al. (2004).

In brief, measurements of skylight spectra are made at several elevation angles between the horizon and zenith to retrieve the amount of the tropospheric trace gas of interest and to separate the tropospheric component from the stratospheric one (Roscoe et al., 2010 and references within). Because the path to the last scattering point is confined to lower altitudes at elevations close to the horizon, measurements at several elevations down almost to the horizon yield also information about the vertical profile of the absorber within the troposphere.

Although their appearance can vary widely (see Fig 3, Piters et al., 2012), MAX-DOAS instruments usually consist of (1) the receiving optics including the scanning mechanism to collect the light and to guide it into the spectrometer, (2) a grating spectrometer to separate the radiation into the different wavelengths and to re-image them onto a detector, and (3) a detector to convert the spectrum into a signal which is then read out and transferred to the control computer. Some MAX-DOAS instruments are also capable of automatically measuring at different azimuth settings. The number of MAX-DOAS instruments deployed worldwide has grown considerably in recent years. This increasing use of MAX-DOAS instruments for observations of tropospheric trace gases, together with the diversity of their designs and operational protocols, definitely creates a need for a more unified and formal approach to the measurement set-up and analysis procedure (Roscoe et al., 2010).

One of the recently developed UV/visible spectrometers to measure trace gas profiles is the Pandora Spectrometer. It was originally developed by NASA's Goddard Space Flight Center (Herman et al., 2009, Tzorziu et al., 2012) and was first deployed in 2006. The Pandora direct sun observations are used to measure column values of ozone and NO_2 as well as other trace gasses. By scanning the sky from the horizon to zenith profile information of ozone and NO2 can be obtained using the MAX-DOAS technique. While the Pandora column observations have already been used relatively extensively in the recent validation activities, the development and characterization of the profile observations is under development (J. Herman, NASA, personal communication).

2.5.2 Measurement procedure and analysis algorithm

The accuracy of the elevation angle seen by the MAX-DOAS instruments is of great importance, as air mass factors change considerably with small changes in elevation when within one or two degrees of the horizon. Hence a proper calibration of the elevation angles is crucial for the interpretation of the MAX-DOAS measurements and the instruments are often aligned using an external reference surface set to horizontal using a spirit level. Depending on the uniformity of the observed trace gas, the choice of the elevation angles and viewing direction can have an impact on the observed trace gas amount.

The underlying spectral analysis technique is similar to what is described in Section 2.4 and the MAX-DOAS measurements usually contain zenith-sky spectra measured as part of each scan sequence, since each scan sequence usually contains one spectrum measured at an elevation angle of 90^o (looking straight up into the zenith). The basic principle behind the MAX-DOAS analysis is in short: Since the light paths through the stratosphere looking at low elevation angles as well as at the zenith are almost identical, and if spectrum measured at low elevation angles is divided by a zenith sky spectrum, the result of the subsequent spectral analysis is only sensitive to the tropospheric absorber amount.

The actual spectral analysis is then performed as described in Section 2.4 with the relevant absorption cross sections being fitted over a chosen wavelength range using a nonlinear least-squares fitting algorithm. Uniformity in wavelength range and absorption cross sections for the fitting procedure is vital if measurements made with different instruments and at different locations are expected to be of comparable quality.

From the resulting MAX-DOAS slant columns the tropospheric column amounts and some information on vertical profiles can be derived. Several different retrieval methods have been developed to convert MAX-DOAS slant column densities to vertical column densities and onward to vertical profiles (see Piters et al., 2012 and references within). The number of degrees of freedom for MAX-DOAS profile retrievals is typically between 2 and 3, depending on clouds and aerosols and on the profile shape itself.

2.5.3 Uncertainty quantification

An estimate of the measurement uncertainty forms an important ingredient in the profile retrieval algorithm. One procedure is described in Vlemmix et al. (2011) where the uncertainty is determined for each measurement parameter from its temporal variation. Measurement time series of the various parameters and elevations are first put on the same time grid, using linear interpolation between the times of measurement. A one-hour running average is then applied to the measurements and the variations of the raw measurements with respect to these averaged measurements are used to determine the RMS. This procedure yields a measure for uncertainty that is generally larger than if the uncertainty estimate would be based on the residual of the DOAS fit and combined with the uncertainty estimates of the absorber cross sections and the vertical temperature profile. The latter and alternative approach would give, however, a more accurate uncertainty estimate for individual differential slant column observations valid for tropospheric trace gases which are more uniformly distributed and of a temporally slower changing nature. Certain environmental conditions such as scattered clouds can lead to a significant increase in the uncertainty estimate of the measurements.

2.6 Total Column Water Vapour measured by GNSS

2.6.1 Measurement technique and instrumentation

The terms Total Column Water Vapour, Integrated Precipitable Water, Precipitable Water Vapour, Precipitable Water and Integrated Water Vapour (hereafter referred to as IWV) represent different synonyms of the same atmospheric parameter used in scientific literature, i.e. water that is contained in a column of unit cross section extending all of the way from the earth's surface to the "top" of the atmosphere, measured in units of [kg/m^3] or in [mm]. The idea of using GNSS observations for retrieving a numeric value of IWV at a site is rather old. It dates back to 1992, while Bevis et al. (1992) published a description of the method. The implementation of the method has been described in numerous articles and textbooks since. The method is based on measuring the GNSS-signal propagation delays in the atmosphere between the GNSS-satellite and the GNSS-receiver.

For high quality IWV measurements only double-frequency geodetic grade instruments can be used and the installation must follow technical requirements and recommendations documented by the International GNSS Service (hereafter referred to as IGS-service and by Shoji et al., 2012.

The receiver “can see” the satellites in a visibility cone determined by the antenna’s cut-off angle (usually 10 degrees or less). The orbits and satellite clock parameters are determined and offered by the IGS-service. So we can expect a precise navigation result for each measurement epoch. In practice we get always a difference between the observed and estimated/calculated values (the residuals). This “noise” (i.e. difference from analytically calculated and observed values of measured parameters) gives an important input for the IWV analysis. The main task is to eliminate everything from the measured “noisy” signal that can be modelled or found analytically. The result is a true value for the parameter we search and uncertainties from approximations and contribution of environmental effects very difficult (or impossible) to model.

There exist also non-atmospheric contributors to the uncertainty budget like Geometric Dilution of Precision (GDOP), multipath and earth quakes (Hoffmann-Wellenhof et al., 1992).

The first step for getting IWV is finding a value for the Zenith Total Delay (ZTD) – a summarized delay of all visible satellites’ slant delays mapped to a vertical at the position of GNSS-receiver’s antenna. The mapping of slant delays to zenith is done by using a mapping function, for example (Niell, 1996).

ZTD values for IGS sites are offered as one of the final products of the IGS-service. Alternatively, they can be calculated for any geographic site by using special geodetic software (Bernese, GIPSY/OASIS, GAMIT/GLOBK, or something equivalent). After having a value for ZTD (separable into hydrostatic and wet components), the hydrostatic component of ZTD - Zenith Hydrostatic Delay (ZHD in mm) can be derived by Saastamoinen (1972) model using ground meteorological measurements as input parameters.

The difference, ZTD-ZHD=ZWD (Zenith Wet Delay). The value of IWV can be obtained from ZWD by using a conversion factor. This conversion factor depends on several known atmospheric constants and the mean temperature of the atmosphere. A mean temperature of the atmosphere (Tm) is defined by weighting the temperature profile with the profile of the wet refractivity above the site.

The dedicated reader can find detailed descriptions by Elgered et al. (2004), User Manual (Bernese), 2007 and Herring et al. (2009).

2.6.2 Measurement procedure and analysis algorithm

The data analysis starts with collecting/archiving the data (GNSS-data together with meteorological data), managing the data formats and obtaining the necessary information for GNSS-data processing (IGS-orbits, clock corrections). Optionally (if not relying on approximation formulas only), the user may need data for the mid-temperature of the atmosphere (either from radiosonde measurements, from ERA databases or NWP models), atmospheric and oceanic load, earthquakes and everything that may have an impact on measurement quality.

Simplified workflow for the full process is explained in Figure 1. In general, for IWV we need GNSS-data (observations, precise orbits) and ground meteorological data at the measurement site. For traceability it is necessary to have metadata records also (i.e. information about the data itself, including the conditions of the measurements, instrumental maintenance, etc.). Additionally, it should be documented how the data are processed and the uncertainties estimated (software and settings).

Deriving IWV from GNSS-measurements needs geodetic data processing software, mentioned in Section 2.6.1. However common and well-documented, the quality of the results depends not only on the meteorological or technical conditions, but also on the user's skills to implement the methods and numerous tuning options the software offers. Additionally there exist two different methods for GNSS-data processing – Precise Point Positioning (PPP) and Double Differencing (DD). The choice between the methods is done according to the user's (the data analyst's) preferences and technical constraints. Both methods have their pros and cons.

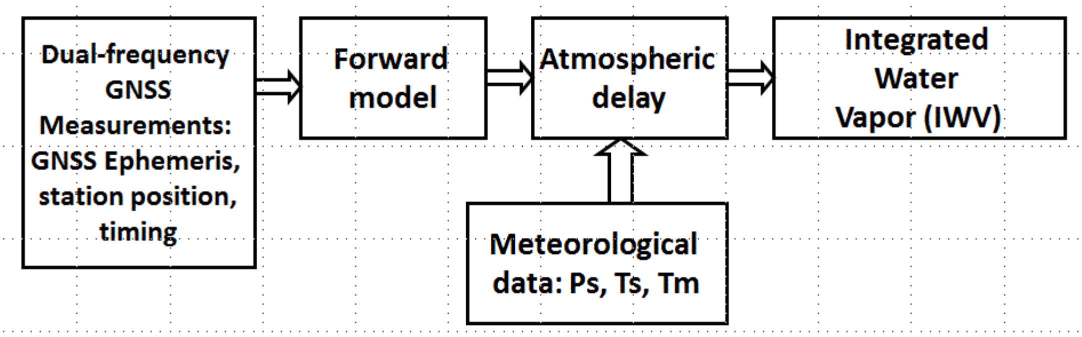

Figure 1 The workflow for IWV. Meteorological data - ground pressure (Ps), temperature (Ts) at the site and a mean temperature of the atmosphere (Tm).

The analysis algorithms can be chosen and tuned during data processing, which is described in the User Manuals of the geodetic software (User Manual (Bernese), 2007, Herring et al., 2009). Requirements for the instrumentation are documented in Shoji et al. (2012).

2.6.3 Uncertainty quantification

Detailed description of calculating the uncertainties for meteorological measurements is given in Immler et al. (2010) and elaborated for climate applications by Ning (2012). These descriptions are the basis for calculating GNSS-IWV uncertainties for GRUAN sites (and could be recommended as best practices).

It is noted and illustrated in Ning (2012), that uncertainties of ZTD and ground pressure dominate the GNSS-IPW uncertainty budget. Ground pressure uncertainty can be handled with using well-calibrated and serviced pressure sensors. ZTD uncertainty is affected by many factors and remains mostly impossible to handle by changing/tuning technical and numerical means. The only way that can be done is to make as good as possible installations and to follow the best practices suggested by the geodetic communities. It is also noticed, that the uncertainties depend on GNSS antenna's cut-off angle (Ning and Elgered, 2012) and this fact needs to be remembered while making IWV trend analysis calculations.

Because of practical considerations it is suggested in Ning (2012) that ZTD uncertainty value for IWV uncertainty estimation would be taken 4 mm.

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