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To cite this version:
F. Mavromatakis, C. A. Gueymard, Y. Franghiadakis. Improved total atmospheric water vapour amount determination from near-infrared filter measurements with sun photometers. Atmospheric Chemistry and Physics Discussions, European Geosciences Union, 2007, 7 (3), pp.6113-6141. hal-00302750

HAL Id: hal-00302750
https://hal.archives-ouvertes.fr/hal-00302750

Submitted on 8 May 2007

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Improved total atmospheric water vapour amount determination from near-infrared filter measurements with sun photometers

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Received: 14 March 2007 – Accepted: 26 April 2007 – Published: 8 May 2007

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Abstract

In this work we explore the effect of the contribution of the solar spectrum to the recorded signal in wavelengths outside the typical 940-nm filter’s bandwidth. We use gaussian-shaped filters as well as actual filter transmission curves to study the implications imposed by the non-zero out-of-band contribution to the coefficients used to derive precipitable water from the measured water vapour band transmittance. The moderate-resolution SMARTS radiative transfer code is used to predict the incident spectrum outside the filter bandpass for different atmospheres, solar geometries and aerosol optical depths. The high-resolution LBLRTM radiative transfer code is used to calculate the water vapour transmittance in the 940 nm band. The absolute level of the out-of-band transmittance has been chosen to range from $10^{-6}$ to $10^{-4}$, and typical response curves of commercially available silicon photodiodes are included into the calculations. It is shown that if the out-of-band transmittance effect is neglected, as is generally the case, then the derived columnar water vapour is systematically underestimated by a few percents. The actual error depends on the specific out-of-band transmittance, optical air mass of observation and water vapour amount. We apply published parameterized transmittance functions to determine the filter coefficients. We also introduce an improved, three-parameter, fitting function that can describe the theoretical data accurately, with significantly less residual effects than with the existing functions. Further investigations will use experimental data from field campaigns to validate these findings.

1 Introduction

Water vapour is a key constituent of the atmosphere, particularly in the lower layers of the troposphere. It determines in part cloudiness and rainfall, and therefore needs to be known accurately for meteorological and climatological purposes, including weather forecasts and energy budget studies. Being very variable on daily, intraseasonal (Chen
et al., 1996) and seasonal time scales, its measurement has been the subject of continuous improvements over the last decades. Recent studies (Ross and Elliot, 1996; Elliot and Angell, 1997) have shown that an increasing trend in water vapour is discernible on a continental scale, which is of concern because of the interaction between water vapour, atmospheric heating/cooling, and various feedbacks linked to the hydrological cycle as a whole. This observation is of great significance considering the implications of the current global climate change. For this reason, any trend in water vapour must be monitored closely and regionally with appropriate instrumentation.

Radiosonde sites are numerous and provide the longest historical record, but are usually launched only twice a day. Recent ground-based instrumentation include GPS receivers and microwave radiometers, which are gaining acceptance in the community. In some cases, ground-based data are assimilated with spaceborne retrievals to generate gridded datasets (Randel et al., 1996). Sun photometers constitute the only ground-based optical alternative to these measurements. They require a visible sun’s disc, which is used both for calibration and radiometric determination of the optical depth of water vapour and of another variable atmospheric constituent, namely the aerosols. Under cloudless skies, aerosols and water vapour are the two major sources of extinction in the shortwave spectrum, and their time variations are generally uncorrelated (Holben, 1990). It is therefore convenient that they can be retrieved simultaneously from a single instrument. Some countries developed water vapour measurement networks using a combination of GPS receivers and sun photometers (Bokoye et al., 2003; Morland et al., 2006). International sun photometer networks, such as AERONET (Holben et al., 1998) and the Global Atmosphere Watch¹ (GAW) also exist for combined aerosol and water vapour measurement, totaling hundreds of sites worldwide. A handy feature of sun photometers is that they are portable, and therefore can be embarked either on terrestrial vehicles for in-situ ground truthing (Bruegge et al., 1990) or regional assessment, or on airborne platforms for profiling or radiative closure experiments (Livingston et al., 2003).

¹http://www.wmo.int/web/arep/gaw/gaw_home.html
Although various techniques exist to determine water vapour from multiwavelength sun photometers, the most common is based on single-filter measurements in the 940-nm water vapour absorption band, the strongest one below the 1100-nm limit of silicon detectors. The technique, which has matured over the years (Bruegge et al., 1992; Ingold et al., 2000; Michalsky et al., 1995; Schmid et al., 1996, 2001; Thome et al., 1992), combines the experimental determination of band-averaged water vapour transmittance with preliminary theoretical calculations of the same to derive the desired total amount of water vapour along a vertical atmospheric column. Refinements to this technique are proposed here, by investigating and quantifying the effects caused by the combination of imperfect filter out-of-band (OOB) rejection, varying solar zenith angle, water vapour and aerosols, and non-zero site elevation, on the derivation of water vapour.

This contribution is aimed at improving the determination of precipitable water by eliminating various sources of systematic or random errors that have been generally overlooked so far.

2 The method

Sun photometers use filters, in carefully chosen wavelength bands, in order to determine aerosol optical depths and columnar water vapour. Manufacturers quote, among other characteristics, the blocking of their filters. Ideally, each filter’s transmittance should be less than this number for all out-of-band wavelengths listed in its datasheet.

In this work we study the effect of the out-of-band transmittance on the filter coefficients used to determine the amount of precipitable water in the atmosphere. In addition, interference filters may display significant leaks at wavelengths well away from their nominal in-band range (e.g. Schmid et al., 1998), which adds to the problem.

Assume that $T_F(\lambda)$ and $T_D(\lambda)$ are the wavelength-dependent responses of the filter and detector used to record the incoming photons, respectively. The incident photons may be of any wavelength, whereas the response of a silicon photodiode is limited
to the range ∼300–1100 nm. In this waveband, water vapour absorption is strongest around 940 nm. The methodology detailed below uses filter measurements in this absorption band to obtain the total water vapour amount in a vertical column that would extend from the ground to the limit of the atmosphere. This amount is usually expressed as the equivalent depth of condensed water, and referred to as precipitable water (PW).

The extraterrestrial solar spectrum is described by a function $I_o(\lambda)$, the shortwave range (e.g. 300–4000 nm) of which is only of concern here. There exists a number of references in the literature that describe the extraterrestrial solar spectrum. The recent spectrum of Gueymard (2004) is adopted here. It is used in the SMARTS radiative code package\(^2\) (Gueymard, 2001), and is also available directly from http://rredc.nrel.gov/solar/spectra/am0/special.html#newgueymard. In what follows, all calculations are limited to the range defined by the optical characteristics of the detector/filter system, including its out-of-band (OOB) contribution.

The average atmospheric transmittance, $T$, weighted by the detector/filter system’s response is given by

$$T = \frac{\int I_o(\lambda) T_F(\lambda) T_D(\lambda) e^{-m\tau_\lambda} d\lambda}{\int I_o(\lambda) T_F(\lambda) T_D(\lambda) d\lambda}$$

(1)

where $m$ is the optical air mass and $\tau_\lambda$ stands for the total optical depth, including all major sources of extinction (Rayleigh, ozone, mixed gases, trace gases, aerosols and water vapour). The solar spectrum finally recorded by the device is described by the function $I(\lambda)$ and its relation to the extraterrestrial solar flux is given by

$$I(l1) = I_o(\lambda) e^{-m\tau_\lambda}$$

(2)

$I(\lambda)$ can be predicted by radiative models or codes (such as SMARTS) for a user-defined set of input parameters describing either ideal or realistic atmospheric conditions.

\(^2\)available from http://rredc.nrel.gov/solar/models/_SMARTS/
Because of the lack of complete OOB rejection in practice, two areas of integration are defined. The first characterizes the waveband where the small but finite OOB response of the filter contributes to the recorded signal. Since the response of the filter in the range of, e.g. 300–910 nm and 960–1100 nm is not zero, it is clear that a low level signal will leak in and contribute to the final one. The actual intensity of this parasitic signal depends upon the OOB blocking. The worse the blocking, the higher its contribution to the recorded signal and the larger the uncertainty in the derived quantities. The second integral covers the waveband where the filter’s transmittance is above a certain limit (e.g. $10^{-6}$ or $10^{-4}$). Typically, this waveband ranges from 910 to 960 nm. Consequently, we may further process Eq. (1), for the specific water absorption band, as

$$T = \frac{\int_{\text{in}} I_0 T_F T_D e^{-m_{\tau_w}} d\lambda + \int_{\text{out}} I_0 T_F T_D e^{-m_{\tau_w}} d\lambda}{\int_{\text{in}} I_0 T_F T_D d\lambda + \int_{\text{out}} I_0 T_F T_D d\lambda}$$  \hspace{1cm} (3)$$

The terms “in” and “out” refer to the inband and OOB integration limits, respectively. Assuming that absorption by gases other than water vapour and ozone is negligible in the waveband 910–960 nm, the left term in the numerator of Eq. (4) can be written as $e^{-m_{\tau_R}}e^{-m_{\tau_{O3}}}e^{-m_{\tau_{aer}}}\int_{\text{in}} I_0 T_F T_D e^{-\tau_{w\lambda}} d\lambda$, while the right one can be simplified into $\int_{\text{out}} I T_F T_D d\lambda$. Note that four specific and distinct optical masses ($m_{\tau_R}$, $m_{\tau_{O3}}$, $m_{\tau_{aer}}$, and $m_{\tau_w}$) are now considered for each extinction process, rather than just the more conventional air mass, which was used in Eqs. (1–3) for conciseness.

The integrated water vapour transmittance finally reads,

$$T_w = \frac{\int_{\text{in}} I_0 T_F T_D e^{-m_{\tau_{w\lambda}}} d\lambda}{\int_{\text{in}} I_0 T_F T_D d\lambda + \int_{\text{out}} I_0 T_F T_D d\lambda}$$

$$+ e^{m_{\tau_R}}e^{m_{\tau_{O3}}}e^{m_{\tau_{aer}}}\int_{\text{out}} I T_F T_D d\lambda$$ \hspace{1cm} (4)$$

where $T_w = T e^{m_{\tau_{R}}}e^{m_{\tau_{O3}}}e^{m_{\tau_{aer}}}$, and $\tau_{w\lambda}$ denotes the spectral water vapour optical
depth. The optical depths $\tau_R$, $\tau_{O_3}$, and $\tau_{aer}$ can be assumed constant over the filter’s bandwidth or calculated as a weighted average.

The above four integrals are calculated numerically for any combination of atmospheric profile, geometry and aerosol conditions. Thus, for any given OOB transmittance a total of $6(\text{atmos}) \times 12(\text{aerosol}) \times 42(\text{airmass}) = 3024$ data points are calculated and fitted with appropriate software to a simpler function of the main driving variable, $W = m_w W$, which represents the total water vapour amount integrated along the slant column. We use the fit program “GaussFit”, originally designed to perform astrometry on data from the Hubble Space Telescope, as a robust estimator (HST AST, 2001).

All 3024 rows of data can be fitted simultaneously to any transmittance function, or 12 different fits can be performed, each with 252 rows of data. We preferred the second approach because it allows to monitor the change in coefficient values as a function of $\tau_{aer}$. Whenever fitting coefficients are quoted in the following, they are derived as the mean of the twelve values mentioned above, while the quoted errors are the standard deviations based on these values. Consequently, the errors are mainly coupled to the variation in the aerosol contribution due to the OOB leakage rather than to the goodness of the fit. When the OOB response is ideally zero, the errors are indeed representative of the goodness of the fit. The error analysis that has been done (see Sect. 3.2) considers that the absolute error in each individual optical depth is 0.01. This may be achieved in practice for Rayleigh scattering and ozone absorption. For aerosol absorption however, this is a rather conservative estimate, if we keep into account the sources that may contribute to it (e.g. Shaw, 1976; Schmid and Wehrli, 1995; Reagan et al., 1986; Schmid et al., 1998). Larger errors would simply improve the $\chi^2$ values even more.

For any of the ideal atmospheres mentioned in Table 1, the water vapour transmittance is calculated with the high-resolution (line-by-line) radiative transfer code LBLRTM$^3$ v10.3, while the absorbed solar spectrum $I(\lambda)$, outside the filter’s bandpass, as well as the optical depths due to Rayleigh, ozone and aerosol extinction are calcu-

\[3 \text{http://www.rtweb.aer.com/} \]
lated with the moderate-resolution code SMARTS v2.9.5. The LBLRTM code utilizes the HITRAN 2000 spectroscopic database with certain updates from 04/2001 for calculations in the water vapour band around 940 nm, as well as “mt_ckd v1.3” for the continuum data (Mlawer et al., 2003). The RFM code has also been used to study the OOB effect. This code was originally developed at the department of Atmospheric, Oceanic and Planetary Physics of the University of Oxford. The results are qualitatively similar to those obtained with LBLRTM. In the following, the quoted results are based on the LBLRTM code. Our calculations assume a flat OOB filter response with the following possible values in units of $10^{-6}$: 1, 5, 10, 25, 50, 75, and 100.

The ideal spectral irradiance incident on the filter is calculated for zenith angles ranging from 0 to 82 degrees, with 2-degree steps. The water vapour optical mass ($m_w$), as all the other optical masses, is calculated by SMARTS as a function of the sun’s zenith angle. The atmosphere models adopted in the calculations are the midlatitude summer (MLS), midlatitude winter (MLW), U.S. Standard Atmosphere (USSA), tropical (TRO), sub-arctic summer (SAS) and sub-arctic winter (SAW). The aerosol properties are defined by a Rural aerosol model (Shettle and Fenn, 1979), which is one of the default models implemented in SMARTS. The aerosol optical depth at 1000 nm (also known as the Ångström’s turbidity coefficient $\beta$, a conventional measure of aerosol extinction), is varied logarithmically from 0.015 to 0.405 in 12 steps. The adopted conditions are summarized in Table 1.

3 Results

3.1 Gaussian filters

The above method is implemented first for a gaussian filter centered at 940 nm and characterized by a full width at half maximum (FWHM) of 10 nm. The resulting transmittances (actually the negative part of their natural logarithm) are fitted with functions

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4http://www-atm.physics.ox.ac.uk/RFM
of the form “$A + B \cdot W^C$” (Model 1) and “$B \cdot W^C$” (Model 2). Model 1 is a modified version of the function proposed by Thome et al. (1992) and similar to that used by (Ingold et al., 2000), while Model 2 is the simpler function most commonly used (e.g. Bruegge et al., 1992; Schmid et al., 2001). Figure 1 shows the variation of the coefficients $A$, $B$, and $C$, for Model 1 (left) and coefficients $B$ and $C$ for Model 2 (right) as a function of the OOB response. The coefficients of the parametrized transmittance for the ideal case are assigned, arbitrarily, an OOB response of $10^{-7}$ in order to display the plot in logarithmic scale. It can be seen that the variation in almost all coefficients is $\sim$2%, but it is more for coefficient $A$ of Model 1. Note that the derived filter coefficients slightly depend upon the code used to perform the appropriate calculations (e.g. Ingold et al., 2000). Our own results, obtained with both the LBLRTM and RFM codes for the same exact atmospheric conditions, support this finding.

The same procedure is repeated for a filter with a FWHM of 15 nm. The variations here are much smaller, especially for Model 2. In the case of Model 1, the variation in coefficients $B$ and $C$ is less than 1%. However, coefficient $A$ displays again the largest variation ($\sim$8%). Broadband filters like this hypothetical one allow for stronger signals to be recorded than with 10 nm FWHM filters, and, consequently, are less affected by the OOB contribution. Our numerous simulations show that filters with FWHM narrower than 10-nm are increasingly affected by the OOB effect. The latter is therefore anticorrelated with FWHM.

The large variations in coefficient $A$ of Model 1 as a function of the OOB response are attributed to (i) the simple functional form adopted to represent $T_w = f(w)$; and (ii) the large range of $W$ covered by the adopted conditions. This quantity ranges here from $\sim$0.4 up to $\sim$30 cm, where the latter corresponds to the TRO atmospheric profile, which is characterized by the largest columnar water vapour of all model atmospheres. The optical depth for OOB responses of $1 \times 10^{-6}$ and $75 \times 10^{-6}$ is plotted in Fig. 2 as a function of $W$. The two curves are similar in shape (little variation in $B$ and $C$) but at higher $W$ values, the two curves begin to diverge. The fitting program optimally varies coefficient ($A$) to reduce the $\chi^2$. 
3.2 Aerosol Robotic Network filters

Apart from ideal gaussian filters, we also consider data from typical filters used in the AERosol RObotic NETwork (AERONET; Holben et al., 1998). Two filter transmittance curves have been made available to us. One of these filters was used recently in Crete, Greece at the FORTH site. The second filter is representative of those used at AERONET sites in the continental U.S. We first apply the proposed scheme to the filter used in Crete with Model 2, which is the currently accepted model by AERONET. For an ideal OOB transmittance of zero, we obtain $B=0.713$ and $C=0.587$. For the same filter, AERONET uses $B=0.714$ and $C=0.600$ (A. Smirnov, personal communication, 2006). The agreement is quite fair given the fact that different codes are involved into the calculations and that the adopted atmospheric, geometric, etc. conditions also differ.

In Fig. 3 the development of the coefficients for Models 1 and 2 is shown. Coefficient $A$ of Model 1 displays the largest variation as a result of increasing OOB transmittance, whereas coefficients $B$ and $C$ also vary but within only a few percents. The same conclusion holds for both coefficients of Model 2, for which the overall variations are less than $\sim 2\%$. The detailed results are listed in Table 2.

The coefficients obtained with Model 2 for the filter used in the continental USA are $B=0.713$ and $C=0.586$. These values are again close to what AERONET actually uses, $B=0.714$ and $C=0.599$ (A. Smirnov, personal communication, 2006). The coefficients determined for the two AERONET filters are very similar since the filter curves are not significantly different either in FWHM or central wavelength. Consequently, the behaviour of the coefficients of Model 1 as a function of the OOB response is also similar to that seen for the filter used at the FORTH site.

3.3 An SPM-2000 filter

Schmid et al. (1996) used sun photometers in the 940-nm band to retrieve the columnar water vapour in parallel with other determinations from co-located radiosonde and...
microwave radiometer equipment. This investigation is of critical importance because the authors were able to determine independently the water vapour transmittance and the water vapour columnar amount. Thus, the corresponding coefficients for Model 2 could be calculated and compared with those determined through line-by-line calculations. (B. Schmid, private communication, 2007) kindly provided us with the spectral response curve of the filter used in their 1996 paper, as shown in their Fig. 1. We were able to determine the coefficients as $B = 0.576$ and $C = 0.625$, while Schmid et al. (1996) had found $B = 0.549$ and $C = 0.629$ with the FASCOD3P code. The agreement is satisfactory considering the different codes and the different molecular absorption data involved in the calculations.

For the site in Bern, Schmid et al. (1996) determined the water vapour content independently and established the filter coefficients experimentally. Note that the latter determinations differ from those of the radiative transfer codes, although the statistical significance is questionable ($< 4\sigma$ in B and $< 2\sigma$ in C). Unfortunately, the OOB response of this filter is not known and we cannot quantitatively estimate its contribution. Nevertheless, we tried several different OOB responses and it can be shown that coefficient C does decrease with increasing OOB level as observed. However, coefficient B also decreases instead of increasing (their Table 1; Schmid et al., 1996). Thus, in the absence of a well-determined OOB response it is not easy to estimate the extent to which the differences in the filter coefficients could be attributed to the OOB effect.

3.4 Coefficient dependence

The filter coefficients reported up to now are based on data from all model atmospheres (e.g. Table 1). We have determined the corresponding coefficients separately for six model atmospheres using the AERONET filter deployed in Crete, Greece assuming an OOB response of zero. It is found that these coefficients are correlated with the total water vapour amount of the atmosphere (Table 3). This fact suggests that the current parametrizations need to be improved in order to describe adequately the water vapour transmittance in all types of atmospheric profiles. The resulting variations in the water...
vapour estimates are of the order of a few percents (less than \(\sim 3\%\)).

The effect of the observing altitude upon the filter coefficients has also been explored. As in the calculations just above, a perfect bandpass filter was adopted and the site altitude was varied from sea level up to 3.5 km, every 0.5 km (Table 4). Altitudes of 0.1 and 0.3 km were also applied since a large number of sites are located at altitudes of this range. Additional calculations were performed for two special cases, namely the Bern (560 m) and Jungfraujoch (3580 m) sites. Ingold et al. (2000) published filter coefficients based on various radiative transfer codes for these two sites and a relative comparison is desirable. Indeed, the relative variations in the coefficients \(A\), \(B\) and \(C\) of Model 1 (1\%, 14\%, 5.1\%) between the low and high altitude sites of Bern and Jungfraujoch are very similar to those seen in the data presented by Ingold et al. (2000). Their Table 1 indicates values of 1.7\%, 13\%, and 6.3\%, respectively, based on LBLRTM 5.10.

4 Discussion

The effect introduced by the finite OOB response of filters used in sun photometers is explored in this work along with different parametrizations of the water vapour transmittance. The OOB response may be small, of the order of \(10^{-4}\) or less, but the wavelength integration extends over a large interval (>700 nm), whereas the far stronger in-band response extends over only a few nanometers. In addition, different radiative transfer models predict slightly different optical depths, which in turn interferes with the relationship between \(T_w\) and \(W\).

A possible way to visualize the differences in the calculated \(T_w\) introduced by the OOB response of a filter is to simulate the atmospheric transmittance for known PW conditions and then attempt to retrieve PW with the parametrized functions of a virtual filter. Note that the transmittances are calculated here by taking into account the OOB contribution, whereas the parametrized function only assumes the coefficients for zero OOB response. Figure 4 shows the percentage difference in the determination of PW.
for USSA and for optical masses of 1, 1.5, 2.0, and 3.0. Under these conditions, PW is underestimated with respect to the exact water vapour content of USSA (1.416 cm). The effect is small but systematic. Under real conditions, the actual differences might be smaller since the coefficients reported in Table 2 are based on data from all six atmospheres listed in Table 1. If we only use USSA to determine the filter coefficients, the agreement is improved but the effect is still present, and becomes even worse when retrieving PW for other atmospheric profiles. This approach assumes that the device signal at the top of the atmosphere can be calculated theoretically, which is not the actual case.

The common practice is the utilization of “modified Langley plots” to determine the “air-mass zero” (AM0) voltage ($V_0$), where the logarithm of the observed voltage ($V$) is plotted against $m_w^C$ (Eq. 5), according to

$$\ln(V) = \ln(V_0) - (A + B(m_w \cdot w)^C). \tag{5}$$

If $A$ is different from zero, then Eq. (5) is valid for Model 1, whereas if $A$ is set to zero, then Model 2 can be adopted. Since coefficient C decreases with increasing OOB response (Table 2), it is clear that the correct X-values will consequently be lowered. Thus, the corresponding AM0 voltage will be higher than the voltage that would be determined assuming a perfect bandpass filter. Given this condition and the fact that the recorded voltage is independent of the filter coefficients, then it can be shown through Eq. (5) that

$$w < \frac{1}{m_w} \left[ \frac{A' - A + B'(m_w w_0)^C'}{B} \right]^{\frac{1}{C'}} \tag{6}$$

where only the coefficients marked with a prime incorporate the out-of-band contribution. It is assumed that the best estimate of the precipitable water, $w_0$, will be given by the parametrized function with these coefficients (prime sign). Equation (6) can be
simplified in the case of Model 2 to
\[
\frac{w}{w_0} < (m_w w_0)^{C'/C-1}
\]  
(7)
since \(A' = A = 0\) and \(B' \approx B\) (Table 2). This equation shows that the water vapour amount is underestimated by 1–3% for OOB responses in the range of \(25 \times 10^{-6}\) to \(100 \times 10^{-6}\).

Note also that if the OOB response increases the goodness of the fits for Model 1 is still acceptable, whereas the fits get worse for Model 2 (Table 2). In the case of an OOB response of \(10 \times 10^{-6}\) or less, this effect is not significant. Thus, it is concluded that high OOB responses should be taken into account in the filter coefficient determination in an attempt to minimize systematic errors.

As noted in Sect. 3.4 the coefficients show a clear dependence on the integrated water vapour amount of the atmospheric profile adopted in the calculations. It is therefore desirable to use a parametrized function which would accurately describe PW amounts from the largest possible number of different atmospheres.

Here, we propose to combine Model 1 and Model 2 into a new function (Model 3) of the form
\[
T_w = e^{-[A \cdot (m_w w)^C + B \cdot (m_w w)^C]} = e^{-(A \cdot w + B) \cdot (m_w w)^C}.
\]  
(8)
As will be discussed in what follows, Model 3 can describe the water vapour transmittance better than Model 1 or Model 2, presumably for any atmospheric profile and for a wide range of water vapour and air mass values (through \(W\)). An advantage of this function over Model 1 is that if \(w \to 0\), then \(T_w \to 1\), whereas Model 1, in this case, predicts a constant offset \((e^{-A})\). In addition, it allows for the calibration of the zero air mass voltage through modified Langley plots without modification. This is stressed because more complicated functions could be developed to better fit the data, but then would not lend themselves to a linear relation between the logarithm of the observed voltage and the power of the water vapour optical mass. Figure 5 shows the difference in water vapour transmittance between the predictions of Models 1, 2 and 3 and the line-by-line calculations, and for a number of atmospheric profiles. Generally, Model 3
performs better than the other models in a variety of different atmospheric environments. The advantage of this model is that a single set of coefficients can be used to represent very different environmental conditions (including site elevation), instead of considering site-specific coefficients.

As a further test, we simulated fixed amounts of PW based on all atmospheric profiles reported in Table 1, using values differing widely from the default one. The selected PW values were 0.5, 1.0, 2.0, 3.0, 4.0, and 5.0 cm. The simulated data points were also limited in air mass (<4) and in transmissivity (>5%), whichever condition was true. This resulted in more than 1300 data points that could be used to retrieve PW with the aid of Models 1, 2 and 3. The solutions of Models 1 and 2 are algebraic, while that of Model 3 is numerical, given its specific functional form. The coefficients used in these models were determined using all atmospheric profiles with their default values as stated in Table 1.

In Fig. 6 we show the percentage difference between the retrieved and the true water vapour as a function of the true PW. It is evident that Model 3 performs satisfactory over the full range of the simulated PW values. Models 1 and 2 show a smaller degree of uniformity in retrieving PW over the same range. This is an important point because determining the filter coefficients for a certain atmospheric profile, e.g. the USSA profile, does not imply that the retrieved PW will be correct over all its full observable range. AERONET Level 2.0 data show that there exist sites that experience yearly variations in PW of an order of magnitude or more (e.g. the GSFC site). In such cases, a model is needed to provide correct estimates of PW from ~0.5 cm to 5.0 cm. Furthermore, Fig. 6 shows that for any given PW, Model 3 provides the smallest scatter as a function of varying air mass or atmospheric profile.

Results displayed in Table 4 imply that altitude can have an impact of about 2% on the estimated PW at low-altitude sites, e.g. for a site located at 300 m that would be using coefficients calculated for zero elevation. It is evident that as altitude increases the retrieval errors increase accordingly, if its effect is not taken into consideration.

Although all the individual effects considered above may be of the order of only a few
percents, it is argued that they should be properly taken care of to avoid systematic errors. Accuracy issues related to the hardware design and implementation constitute a different topic, which is beyond the scope of this work. An experimental validation of the proposed model, using results from field campaigns with sun photometers, microwave radiometers, GPS sensors and radiosonde devices is currently in development.

5 Conclusions

The method of determining the water vapour with sun photometers is well proven, but there are certain issues that may introduce small errors in the estimation of PW under realistic conditions. Our simulations show that the out-of-band contribution may have a non-negligible impact on the retrieved PW. Therefore, filters in the 940-nm band should have an OOB rejection of $10^{-5}$ or better. In addition, the observing site’s altitude is found to affect the coefficients used to model the water vapour transmittance as a function of PW. These coefficients should therefore be calculated for each individual filter (depending on its transmittance and OOB rejection) and exact location of use.

The residuals of the parametrized transmittances show that the current functions (Models 1 and 2) cannot compensate for the different amounts of water vapour existing in various model atmospheres. A new model with three coefficients (Model 3) is therefore proposed. It is found to perform better (with reduced bias) than the existing models when subjected to widely varying atmospheric profiles. It is also characterised by a small scatter, conducive of reduced random errors, even at large slant column water vapour amounts. Model 1 performs better than Model 2 in terms of correctly estimating PW. However, both models tend to overestimate PW, by up to 5%, at high PW values ($\geq 4$ cm). Under dry conditions ($w<1$ cm), Models 1 and 2 underestimate PW by just a few percents. The analysis shows that Model 3 provides more accurate estimates of PW (by 2% on the average) over a wide range of water vapour amounts.

Acknowledgements. The authors would like to thank A. Smirnov and B. Schmid for supplying the digital data of the filters used in the calculations.
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Table 1. Major parameters and their range.

| Parameter       | Value (range)                  |
|-----------------|--------------------------------|
| Atmospheres     | MLS, MLW, USSA TRO, SAS, SAW  |
| Solar Zenith angle | 0° (2°) 82°                 |
| Aerosol turbidity $\beta$ | 0.015–0.405              |
| OOB             | 1, 5, 10, 25,               |
| transmittance ($\times 10^{-6}$) | 50, 75, 100              |
Table 2. Model coefficients for an AERONET filter.

| Out-of-band | Model 1 | $\chi^2$ | Model 2 | $\chi^2$ |
|-------------|---------|----------|---------|----------|
|             | A       | B        | C       | B        | C       |
| 0           | -0.0317 | 0.743    | 0.574   | 0.713    | 0.587   | 0.65    |
| $1 \times 10^{-6}$ | -0.0267 | 0.737    | 0.577   | 0.69–0.69| 0.713    | 0.588   | 0.63–0.65|
| $5 \times 10^{-6}$ | -0.0294 | 0.740    | 0.576   | 0.69–0.71| 0.713    | 0.587   | 0.64–0.67|
| $10 \times 10^{-6}$ | -0.0327 | 0.743    | 0.574   | 0.69–0.74| 0.713    | 0.587   | 0.64–0.69|
| $25 \times 10^{-6}$ | -0.0416 | 0.751    | 0.568   | 0.68–0.80| 0.713    | 0.584   | 0.64–0.72|
| $50 \times 10^{-6}$ | -0.0542 | 0.751    | 0.559   | 0.65–0.85| 0.713    | 0.581   | 0.67–0.97|
| $75 \times 10^{-6}$ | -0.0660 | 0.773    | 0.552   | 0.60–0.90| 0.712    | 0.578   | 0.70–1.13|
| $100 \times 10^{-6}$ | -0.0762 | 0.781    | 0.545   | 0.57–0.92| 0.712    | 0.575   | 0.72–1.29|
Table 3. Dependence of model coefficients on atmospheric profile and total water vapour amount.

| Atmosphere | w   | Model 2 \( B \) | \( C \) |
|------------|-----|-----------------|--------|
| SAW        | 0.416 | 0.704          | 0.586  |
| MLW        | 0.852 | 0.714          | 0.584  |
| USSA       | 1.416 | 0.710          | 0.584  |
| SAS        | 2.081 | 0.715          | 0.581  |
| MLS        | 2.922 | 0.726          | 0.579  |
| TRO        | 4.115 | 0.740          | 0.574  |
Table 4. Dependence of model coefficients on site altitude.

| Altitude (km) | Model 1 |       | Model 2 |       |
|--------------|---------|-------|---------|-------|
|              | A       | B     | C       | B     | C     |
| 0.0          | -0.0317 | 0.743 | 0.574   | 0.713 | 0.587 |
| 0.1          | -0.0338 | 0.742 | 0.572   | 0.711 | 0.585 |
| 0.3          | -0.0252 | 0.727 | 0.575   | 0.704 | 0.585 |
| 0.5          | -0.0142 | 0.712 | 0.576   | 0.697 | 0.584 |
| 0.560        | -0.0179 | 0.715 | 0.575   | 0.696 | 0.585 |
| 1.0          | -0.0087 | 0.690 | 0.577   | 0.681 | 0.582 |
| 1.5          | -0.0119 | 0.678 | 0.574   | 0.666 | 0.581 |
| 2.0          | -0.0183 | 0.672 | 0.569   | 0.652 | 0.581 |
| 2.5          | -0.0218 | 0.660 | 0.562   | 0.636 | 0.581 |
| 3.0          | -0.0195 | 0.638 | 0.558   | 0.616 | 0.579 |
| 3.5          | -0.0261 | 0.629 | 0.548   | 0.601 | 0.583 |
| 3.580        | -0.0273 | 0.628 | 0.547   | 0.599 | 0.583 |
Fig. 1. The filter coefficients $A$, $B$, and $C$ of Model 1 and $B$ and $C$ of Model 2 are plotted as a function of the out-of-band transmittance. The coefficients for an ideal gaussian filter are assigned an out-of-band transmittance of $10^{-7}$ instead of zero in order to use the logarithmic scale in the x-axis.
Fig. 2. Water vapour optical depth as a function of $W$ for OOB transmittances of 1 and $75 \times 10^{-6}$ (plus signs and dots, respectively). The OOB effect shows up mainly at high $W$. 
Fig. 3. Variations in filter coefficients $A$, $B$, and $C$ of Model 1, and $B$ and $C$ of Model 2, as a function of the OOB transmittance. The data is for a filter that has been actually used on an AERONET sun photometer in Crete, Greece. The coefficients in the case of an ideal filter are assigned an OOB transmittance of $10^{-7}$ instead of zero in order to use the logarithmic scale in the x-axis.
Fig. 4. The U.S. standard atmosphere is invoked to simulate a signal assumed to be sensed by filters of different out-of-band transmittances. The water vapour content is estimated through Model 2, whose coefficients are calculated for an ideal filter (OOB transmittance equal to zero). In this case, PW is systematically underestimated. The different aerosol optical depths used in the calculations show up as different positions of the same symbol at any x-value.
Fig. 5. Residual water vapour transmittance ($T_{\text{model}} - T_{\text{simul}}$) as a function of slant water vapour, obtained with three different atmospheric profiles. The simulated data are created under the assumptions appearing in Table 1. The proposed model performs acceptably well under both low and high water vapour conditions.
Fig. 6. Accuracy of the retrieved PW with three possible models. The difference between the retrieved and the actual PW is shown for all three models as a function of the true PW. Model 3 shows a relatively stable behaviour over the whole range of PW values used in this study. In addition, it displays the smallest degree of scatter as a function of air mass, for any given PW.