On the importance of proper noise modelling for long-term precipitable water vapour trend estimations

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ABSTRACT

Time-series of precipitable water vapour (PWV), derived from continuous Global Positioning System (GPS) observations, are analysed for the two South African stations HRAO and SUTH. Since water vapour is a major greenhouse gas, observed changes in atmospheric PWV could be indicative of weather and climate change. Our main contribution is a realistic noise model of the PWV observations which enables one to draw correct conclusions about the significance of the derived PWV increase or decrease for given time spans longer than five years. It is demonstrated that the PWV residuals that are obtained after fitting a trend and yearly signal to the data are, due to the simple model’s exclusion of short-term scatter, much larger than the PWV uncertainties provided by the GPS analysis software. Although a better solution for the associated uncertainties is obtained by using the variance of these PWV residuals for the uncertainty rescaling, it is shown that the ARMA(1,1) noise model better represents the associated statistical uncertainties than the simple white noise model. The ARMA(1,1)-derived PWV trend uncertainties are approximately 2 times greater than those for a rescaled white noise model. Finally, it is argued that the variability of the annual signal prevents any trend estimation using time series shorter than about five years. A quantitative measure is presented to determine the minimum period of continuous GPS observational data required to measure PWV trends to a specified accuracy. As result of our study, we conclude that no statistically significant PWV trends are observed at the two GPS stations between 1998 and 2006.
feedback acting alone approximately doubles the warming from what the warming would be for fixed atmospheric water vapour contents (Cess et al., 1990).

Pielke (2005) points out that the effects of environmental change are experienced by people and ecosystems regionally, which necessitates the study of PWV on a regional level (e.g. at GPS sites) as opposed to only studying temperature and PWV using global or zonal averages. Furthermore, southern Africa is considered to be a “high-risk hydroclimatic environment,” since its rainfall-to-runoff conversion is less than 5% for approximately half of its surface area, compared to the world mean of 35% (Schulze, 2005). Consequently, studies of possible environmental changes are of utmost importance in this region.

In this paper we present results from long-term monitoring of PWV at two South African GPS stations, namely HRAO (located at the Hartebeesthoek Radio Astronomy Observatory, Krugersdorp) and SUTH (collocated at the GeoForschungsZentrum’s superconducting gravimeter at Sutherland). It will be shown that the choice of the noise model to be applied to the PWV time-series will have an impact on the estimated PWV trend uncertainties. The precise quantification of the associated uncertainties is essential when GPS-derived PWV trends are to be used to quantify regional environmental change.

**PWV measurement methodology**

A derivation, from first physical principles, of the delay experienced by an electromagnetic wave traversing the atmosphere, such as a signal travelling from a GPS satellite to a ground-base receiver, can be consulted at Combrink et al. (2004). The dispersive nature of the ionosphere and the non-dispersive nature of the troposphere at radio wavelengths are apparent from this derivation.

Using the two frequencies of signals emitted by GPS satellites, the effect of free electrons in the ionosphere on the propagation of radio signals can, to first order, be cancelled by forming the so-called “ionosphere-free linear combination” so that the ionospheric delay can be modelled and corrected for. The remainder of the atmospheric delay, basically due to the neutral lower atmosphere, can be estimated by GPS processing software, where it is typically mapped to zenith.

The zenith total delay (ZTD) can further be divided into a hydrostatic and a wet component. The hydrostatic component, which can also be modelled and corrected for, is a function of atmospheric pressure at the GPS site, while the wet component further depends on temperature and the amount of atmospheric PWV above the GPS site (cf. Bevis et al., 1992; Combrink et al., 2004). Therefore, water vapour delays the GPS signal and by measuring this delay one can easily

![Figure 1. The time-series of GPS-derived PWV for HRAO. The fitted 4-parameter model and the linear trend are also displayed.](image-url)
calculate the amount of PWV if pressure and temperature measurements are available.

The GPS (observational) data were processed using the GIPSY software package (Webb and Zumberge, 1995). A horizontal tropospheric gradient model has been applied since it improves the precision of the estimates in most cases (Bar-Sever et al., 1998, Miyazaki et al., 2003). The New Mapping Functions (NMF) (Niel, 1996) were used to map delays to zenith and a 15-degree elevation cut-off angle was used. Ocean loading (GOT00.2) was also incorporated in the processing (Scherneck and Bos, 2002).

The pressure and temperature values at the GPS stations required for the estimation of PWV from ZTD, were obtained from the NCEP/NCAR Reanalysis Project (Kalnay et al., 1996, NCEP, 2006). The data were interpolated using techniques presented and verified by Combrink (2006).

At each of the two GPS sites, HRAO and SUTH, one PWV value was estimated for each day from 1998.0 to 2006.0, using daily mean estimates of ZTD, pressure and temperature. Conservative atmospheric pressure uncertainties were used in order to obtain appropriate magnitudes of the PWV uncertainties. The effect of any ZTD outlier in the hourly estimates is significantly reduced because it is averaged out by calculating daily means of ZTD.

**Data analysis and results**

Eight years of daily PWV measurements at HRAO are shown in Figure 1, from which it is evident that the PWV data are dominated by a large annual signal. Our objective is therefore to fit both a linear trend and an annual signal to the data to separate the long-term changes from the seasonal effect. Following Gradinarsky et al. (2002) and Haas et al. (2003) we fitted the following four-parameter model to the PWV data:

\[
\text{PWV}(t) = a_0 + a_1 t + a_2 \cos(2\pi t + \phi_1) + a_3 \cos(2\pi t + \phi_2)
\]  

(1)

with \(t\) in years. We therefore estimate an initial offset parameter, a linear trend and the amplitude and phase of a seasonal signal.

The obtained trends are practically independent of most of the seasonal influences and of absolute constant biases (Gradinarsky et al., 2002) and can therefore be used to sense changes in the mean PWV.

A weighted least-squares method, using the squares of the obtained formal PWV uncertainties provided by GIPSY as the diagonal elements of the covariance matrix, was used for an initial linear regression model fit. The modelled annual signal and its linear trend are also presented in Figure 1.

For both HRAO and SUTH, based only on the weighted least-squares analysis, we find very small formal trend uncertainties for the 8-year period of 0.002 mm/year. Consequently, in order to test whether our obtained uncertainties are reliable, we computed the reduced chi-square statistic which is defined as

\[
\chi^2_{\text{reduced}} = \frac{1}{N - 4} \sum \left( \frac{\text{PWV}_i - a_0 - a_1 t_i - a_2 \cos(2\pi t_i)}{\sigma_i} \right)^2
\]

(2)

where \(N\) is the number of observations and \(\sigma_i\) is the uncertainty of the \(i\)-th observation.

We find values of \(\chi^2_{\text{reduced}} \approx 300\) for HRAO and \(\chi^2_{\text{reduced}} \approx 200\) for SUTH while one expects values around 1 if the noise is uncorrelated and our PWV uncertainties are correct. For the moment we will assume that our model presented in Equation (1) is adequate (cf. Figure 1). The influence of variability in the annual signal will be discussed later in this article.

The large reduced chi-square values imply that the values of \(\sigma\) are too small, *i.e.* that the PWV uncertainties estimated from the GIPSY-derived ZTD measurements are too small.

In order to correct for the fact that GIPSY underestimates the error in the PWV values, the trend uncertainties were scaled by \(\sqrt{\chi^2_{\text{reduced}}}\). The obtained trends and their uncertainties are presented in Table 1, in the columns labelled “White noise”.

Another possible cause for the high \(\chi^2_{\text{reduced}}\) obtained, could be that the noise in the data is not uncorrelated, *i.e.* that it is not white noise which is implicit in our weighted least-squares analysis. To check whether the correct noise model was used, a power spectrum plot was made of the resulting residuals (observations minus model) and is shown in Figure 2.

It is evident that the power spectrum of the residuals better fits an autoregressive moving average (ARMA) model (Brockwell and Davis, 1987), rather than a white-noise model implicit in the initial linear regression. This is attributed to the existence of temporal correlations.

An ARMA(1,1) model is defined by:

\[
X_i = \phi X_{i-1} + \Theta Z_{i-1} + Z_i
\]

(3)

where \(X_i\) is the observation at time \(i\), \(Z_i\) is a Gaussian zero-mean random variable with standard deviation \(\sigma\), \(\phi\) is the autoregressive (AR) parameter and \(\Theta\) is the moving average (MA) parameter. These three parameters can be estimated from the residuals using the GRETl (GNU Regression, Econometrics and Time-series Library, available from http://gretl.sourceforge.net) software, which determines the values producing the maximum likelihood. The parameters for the ARMA(1,1) model depicted in Figure 2 are \(\phi = 0.60 \pm 0.02\), \(\Theta = 0.18 \pm 0.02\) and \(\sigma = 3.42\).

The power density \(P\) of the ARMA(1,1) model described by (3), is given by

\[
P(f) = \frac{2\sigma^2(1 + \phi^2 + 2\Theta \cos(2\pi f))}{\Delta f^2(1 + \phi^2 - 2\Theta \cos(2\pi f))} \text{ for } f = \left[0, \frac{1}{2\Delta f}\right]
\]

(4)

where \(\Delta f = 1\) day. The frequency ranges from zero to the Nyquist frequency, which is one cycle per two days. The three parameters describing the ARMA(1,1) model,
namely $\theta$, $\phi$ and $\sigma$, are then used to compute a new covariance matrix $C$ using the following algorithm:

$$C_i = \sigma^2 \left[ \frac{1}{1 + \phi \theta^i} \frac{1}{1 - \phi^i} \right]$$

where $\gamma = \sigma^2 \left[ \theta + \phi \theta^i \frac{1}{1 - \phi^i} \right]$ for $i = 0$

$$\theta \left[ \frac{1}{1 - \phi^i} \right]$$

for $i > 0$. (5)

A new covariance matrix, obtained from the ARMA model, is consequently used in a weighted least-squares analysis in order to determine the four parameters, and realistic uncertainties associated with them, for the model described in (1).

The reduced chi-squared values were re-computed for each of the considered periods and are shown in Table 1. The used ARMA(1,1) model accounts for all the noise, since the $\chi^2_{\text{reduced}}$ values approach 1 for all the periods analysed.

Gradinarsky et al. (2002) also applied the $\chi^2_{\text{reduced}}$ scaling to the estimated PWV trend values. They also realised that the PWV residuals did not resemble white noise and applied a filter to the residuals to make them white before performing the least-squares fit. However, it is not clear how their prefiltering affected the trend uncertainties. Our trend uncertainties using the ARMA(1,1) noise model seem to produce values that are around 1.2 times larger than theirs.

The estimated PWV trends and their associated uncertainties for different periods and noise models for

<table>
<thead>
<tr>
<th>Period</th>
<th>HRAO White noise</th>
<th>HRAO ARMA(1,1)</th>
<th>HRAO $\chi^2$</th>
<th>SUTH White noise</th>
<th>SUTH ARMA(1,1)</th>
<th>SUTH $\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1998.0 – 1999.0</td>
<td>$-2.30 \pm 1.83$</td>
<td>$-1.22 \pm 0.38$</td>
<td>1.05</td>
<td>$-4.41 \pm 5.91$</td>
<td>$-5.31 \pm 7.77$</td>
<td>0.76</td>
</tr>
<tr>
<td>1999.0 – 2000.0</td>
<td>$-4.60 \pm 1.34$</td>
<td>$-4.42 \pm 2.20$</td>
<td>1.02</td>
<td>$4.94 \pm 1.44$</td>
<td>$4.55 \pm 2.07$</td>
<td>1.37</td>
</tr>
<tr>
<td>2000.0 – 2001.0</td>
<td>$-2.64 \pm 1.47$</td>
<td>$-5.67 \pm 3.44$</td>
<td>1.01</td>
<td>$-3.44 \pm 1.19$</td>
<td>$-5.35 \pm 2.25$</td>
<td>1.10</td>
</tr>
<tr>
<td>2001.0 – 2002.0</td>
<td>$25.51 \pm 2.92$</td>
<td>$26.32 \pm 5.92$</td>
<td>1.02</td>
<td>$19.21 \pm 5.74$</td>
<td>$17.01 \pm 5.98$</td>
<td>1.24</td>
</tr>
<tr>
<td>2002.0 – 2003.0</td>
<td>$-1.37 \pm 1.41$</td>
<td>$-0.52 \pm 3.18$</td>
<td>1.02</td>
<td>$2.27 \pm 1.35$</td>
<td>$2.71 \pm 2.07$</td>
<td>1.17</td>
</tr>
<tr>
<td>2003.0 – 2004.0</td>
<td>$-0.38 \pm 1.43$</td>
<td>$-0.11 \pm 2.45$</td>
<td>1.05</td>
<td>$-1.94 \pm 1.09$</td>
<td>$-1.99 \pm 2.07$</td>
<td>0.91</td>
</tr>
<tr>
<td>2004.0 – 2005.0</td>
<td>$-0.60 \pm 1.44$</td>
<td>$-0.30 \pm 2.89$</td>
<td>1.01</td>
<td>$0.71 \pm 1.18$</td>
<td>$1.10 \pm 2.08$</td>
<td>1.10</td>
</tr>
<tr>
<td>2005.0 – 2006.0</td>
<td>$-1.75 \pm 1.38$</td>
<td>$-6.38 \pm 2.23$</td>
<td>1.07</td>
<td>$-5.48 \pm 1.15$</td>
<td>$-5.50 \pm 2.11$</td>
<td>1.02</td>
</tr>
<tr>
<td>1998.0 – 2000.0</td>
<td>$0.25 \pm 0.32$</td>
<td>$0.22 \pm 0.65$</td>
<td>1.04</td>
<td>$1.52 \pm 0.29$</td>
<td>$1.50 \pm 0.62$</td>
<td>1.14</td>
</tr>
<tr>
<td>1999.0 – 2001.0</td>
<td>$0.88 \pm 0.33$</td>
<td>$0.82 \pm 0.71$</td>
<td>1.01</td>
<td>$-0.78 \pm 0.30$</td>
<td>$-0.86 \pm 0.51$</td>
<td>1.28</td>
</tr>
<tr>
<td>2000.0 – 2002.0</td>
<td>$-0.37 \pm 0.37$</td>
<td>$-0.42 \pm 1.01$</td>
<td>1.01</td>
<td>$0.25 \pm 0.42$</td>
<td>$0.45 \pm 0.62$</td>
<td>1.21</td>
</tr>
</tbody>
</table>
both stations are presented in Table 1. Since the noise parameters were re-estimated independently for each period, we may find different trend uncertainties for each period. Similarly, there is also quite a wide range in the trend values themselves (we attribute the unreliable values for the 2001.0-2002.0 period to a significant number of data gaps in that particular period in both time-series). After a minimum number of years (not less than three to four years, as depicted from Table 1) the different trends observed over different periods are probably not indicative of measurement or modelling errors, but of meteorological changes during the observation period. However, for the short periods of one to two years the observed variations are larger than one should expect by looking at the ARMA(1,1) uncertainty. For example, for a one year period at HRAO the trend varies between -4.38 to 4.42 mm/year while the average ARMA(1,1) trend uncertainty is only 2.5 mm/year. Statistically, a deviation of 8.8 should only occur less than 0.1% of the cases (Student’s t-test with). Thus, it seems that our predicted uncertainty is still too small. This is probably caused by the fact that for short periods the slope and the annual signal cannot be separated adequately in the least-squares fit. This is aggravated by the presence of data gaps. Furthermore, each year is slightly drier or wetter than other years, and the amplitude is also not perfectly symmetric. Since we only estimate a yearly signal with a constant amplitude and phase over the whole period, some mismodelling is certain to occur. This is quite a severe problem since the yearly signal is much larger than the trend value we want to investigate which makes that a small yearly variation can have an impact on the trend estimation. Fortunately, this problem disappears with longer time-series since this will help the separation of the annual term from the trend and will help to average out the annual variability. If one looks at the range of the estimated trend values for a period of six years (cf. Table 1), one can see that both at HRAO and SUTH the variation is within one standard deviation of the estimated ARMA(1,1) uncertainty.

At both HRAO and SUTH we find that the PWV trend values obtained using the reduced chi-squared method and the ARMA noise model are very similar to each other for the longer periods, while the uncertainties of these trends are substantially smaller for the reduced chi-squared method for all considered periods. Again considering the longer periods (i.e. more than five years of observations), no significant increase or decrease in PWV is observed at HRAO, while a small negative PWV trend may exist at SUTH. However, no conclusion could be made with high confidence about significant increases or decreases in mean PWV at these stations.

The PWV trend uncertainty behaviour over time

It is interesting to know how the PWV trend uncertainty diminishes as more and more observations are made over the years. For this purpose we will first assume white noise. If in reality the PWV noise is perfectly described by our ARMA(1,1) model, one can predict what the variance of the residuals will be, namely

$$\sigma(0) = \sigma^2 \frac{1+ \phi^2 + 2\phi}{1- \phi^2}$$

from Equation (6). If no yearly signal existed, the formal estimated trend uncertainty \( \delta \), using a white noise model in the least-squares regression is (Zhang et al., 1997):

$$\delta = \sqrt{\frac{\sigma(0) \cdot \frac{12}{N(N^2-1)}}}$$  (7)

where \( N \) is the number of daily observations. For given values of the ARMA(1,1) parameters, this formula describes the behaviour of the PWV trend uncertainty over time assuming white noise. Note that since we rescaled the uncertainty of the trend by applying the reduced chi-square scaling, we are using the variance of the PWV residuals and not the uncertainties provided by GIPSY. However, we know from the power spectrum plot (cf. Figure 2) that an ARMA(1,1) noise model is closer to reality. If this ARMA(1,1) model is now not only used to predict the variance of the residuals but also to construct the covariance matrix for the weighted least-
squares estimation, one gets uncertainties which are a factor of \(-2.1\) larger than one would get by using Equation (7).

This can be explained by looking at Figure 2: The area underneath the power spectrum represents the variance of the PWV residuals, which is thus \(\gamma(0)\). However, the trend line is mostly affected by the long period noise. This can be made plausible by considering the trend as being a sinusoid with a very long period. Thus for estimating the trend the effective noise is \(P(0)\times\Delta T/2\) (the area underneath the power spectrum if there were no decrease in power at the high frequencies). Since the average noise power, the dotted line in Figure 2, will always be below the power at zero frequency, the ARMA noise will produce a larger trend uncertainty than white noise. One can derive that the ARMA(1,1) increase of the uncertainty in the trend relative to the reduced-\(X^2\)value approximates for large \(N\):

\[
\frac{\sigma_{\text{ARMA}}^2}{\sigma_{\text{white}}^2} = \frac{1+\theta^2 + 2\phi\theta(1-\phi)}{(1-\phi^2 - 2\phi)(1+\theta^2 + 2\theta\phi)} \approx 2.1 \tag{8}
\]

Thus Equation (7) should be scaled by the value from Equation (8) to get the true uncertainty for given value of the ARMA(1,1) parameters and a given number of daily PWV observations.

A comparison of the mean 1-sigma uncertainties from Table 1 are presented per station in Table 2. We find that the formal uncertainties derived from the white noise modelling are typically \(-2.0\) times smaller than those from the ARMA(1,1) noise modelling, which is very close to the value of 2.1 as suggested by Equation (8). Furthermore, tests conducted excluding 5%, 10% and even 20% of the data showed that data gaps hardly have any effect on the amplification of trend uncertainties (Equation (8)).

The different trend uncertainties are presented in Figure 3. The graph shows that after three years the trend uncertainty magnitudes from ARMA(1,1) noise modelling and the scaling of Equation (7) with Equation (8) are almost equal in magnitude. However, due to the variability of the trend estimation (cf. Table 1), due to the presence of conspicuous signals not entirely modelled, we consider that no analysis should be done using a period shorter than five to six years.

Table 2. The mean 1-sigma uncertainties of the estimated PWV trends (in mm/year) at HRAO and SUTH using white noise and ARMA(1,1) noise modelling, as a function of the number of years of data used in the analysis.

<table>
<thead>
<tr>
<th>Years of Data</th>
<th>HRAO</th>
<th>SUTH</th>
</tr>
</thead>
<tbody>
<tr>
<td>White noise</td>
<td>ARMA(1,1)</td>
<td>White noise</td>
</tr>
<tr>
<td>1</td>
<td>1.65</td>
<td>3.21</td>
</tr>
<tr>
<td>2</td>
<td>0.34</td>
<td>0.74</td>
</tr>
<tr>
<td>3</td>
<td>0.17</td>
<td>0.39</td>
</tr>
<tr>
<td>4</td>
<td>0.12</td>
<td>0.25</td>
</tr>
<tr>
<td>5</td>
<td>0.09</td>
<td>0.18</td>
</tr>
<tr>
<td>6</td>
<td>0.07</td>
<td>0.13</td>
</tr>
<tr>
<td>7</td>
<td>0.05</td>
<td>0.10</td>
</tr>
<tr>
<td>8</td>
<td>0.03</td>
<td>0.08</td>
</tr>
</tbody>
</table>

The trend uncertainties presented in Figure 3 are computed using the full covariance matrix \(C\) (using the constant variance of the residuals or the ARMA(1,1) covariance matrix as given by Equation (5)) in the least-squares fit. If \(H\) is the matrix containing the model derivatives with respect to the offset, linear trend and the amplitude and phase of the annual signal, then the least-squares uncertainty of the estimated parameters are given by the diagonal elements of \((H'CH)^{-1}\).

Based on the results depicted in Figure 3, one can avoid the constructing the covariance matrix (Equation (5)), which would be necessary to compute the ARMA(1,1) noise model. In fact, in order to obtain a reliable estimate of the trend uncertainty, it is only necessary to

- Estimate the trend using a weighted least-squares fitting by applying the model presented by Equation (1).
- Compute the ARMA(1,1) parameters \(\sigma, \phi, \Theta\), and derive \(\gamma(0)\).
- Compute the white-noise trend uncertainty \(\hat{\sigma}_T\) (Equation (7)).
- Compute \(\frac{\hat{\sigma}_{\text{ARMA}}}{\hat{\sigma}_{\text{reduced-}\chi^2}}\) (Equation (8)).
- Obtain the final trend uncertainty by multiplying \(\hat{\sigma}_T\) with \(\frac{\hat{\sigma}_{\text{ARMA}}}{\hat{\sigma}_{\text{reduced-}\chi^2}}\).

Conclusions

We have shown that the formal daily PWV uncertainties provided by GIPSY-derived ZTD values are unrealistically small. It is well known that the same applies to the uncertainties of the positions provided by GIPSY (Johnson and Agnew, 1995). To solve for this problem it was standard practice in the analysis of GPS position time-series to rather use the variance of the residuals as a realistic estimate of the error of the measurements. By using the reduced chi-square method to appropriately scale and obtain more realistic trend uncertainties, the PWV trend uncertainty is increased by a factor of \(-15\).

Next we have shown that ARMA(1,1) is a better model for the noise, which again influences the estimated trend uncertainty. By using the right noise model, one not only obtains \(\chi^2_{\text{reduced}} \approx 1\), but also the correct power spectrum for the noise.

Both Equation (8) and Table 2 confirm that the uncertainty of the trend is approximately 2 times larger than for the reduced chi-squared method, while the noise power spectrum is more realistic.
By estimating the trend for different sections of the available data, it was demonstrated that for periods shorter than five years the variability in the annual signal influences the trend estimation. Therefore, the ARMA(1,1) noise model can only be applied for time-series longer than five years to ensure that this effect is negligible.

For the analysed stations, the improvement in the noise modelling allows us to be more confident that no significant PWV trends are observed, which implies that no significant change in the atmospheric water vapour content at these locations can be extracted for the analysed period.

Lastly, we have derived a new procedure to compute reliable trend uncertainties based on white-noise uncertainty (Equations (7)) and ARMA(1,1) model parameters (Equation (8)) without the need of recomputing the large covariance matrix required by this last model. After three years, the simplified formula provides similar uncertainties as the complete ARMA(1,1) model.

The presented noise modelling techniques could also be applied to the PWV data of the ~40 other GPS stations in South Africa, Inkaba yeAfrica’s geographical research focus area; although the other stations have shorter time-series of continuous GPS observations than HRAO and SUTH, it is evident from the preceding discussion that the obtained PWV trend accuracies would improve as more data are collected. This proposed study would be useful to determine whether regional trends of PWV exist over the subcontinent.

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References

Figure 3. The estimated trend uncertainty under different assumptions: using Equation (7), using the PWV uncertainties estimated from the residuals and white noise assumption, scaling Equation (7) with Equation (8) and finally assuming ARMA(1,1) noise in the Least-Squares fit.
Africa.


Editorial handling: M. J. de Wit and Brian Horsfield