Nr 130, 2008

SMHI

Meteorologi

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An empirical model approach

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Cover photo by Mikaell Ottosson Löfvenius shows the Dobson ozone spectrophotometer #30 inside the hut and ready for observation through window in the slant roof.

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Report Summary / Rapportsammanfattning

Issuing Agency/Utgivare	Report number/Publikation
Swedish Meteorological and Hydrological Institute S-601 76 NORRKÖPING Sweden	**130** Report date/Utgivningsdatum

Author (s)/Författare

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Title (and Subtitle/Titel

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Abstract/Sammandrag

At Vindeln monitoring of the total ozone has been done using the Dobson spectrophotometer #30 since 1991. The fundamental observation is done by observing the direct solar radiance. However, when clouds cover the sun an observation of the zenith radiance is collected. This type of measurement is called a zenith observation and by using an empirical relation one can deduce the total ozone. Up to now an old empirical relation based on data from Boulder USA has been applied. In this report we present the development and testing of a site specific empirical relation.

Key words/sök-, nyckelord

Total ozone, zenith sky, Dobson

Supplementary notes/Tillägg	Number of pages/Antal sidor	Language/Språk
This work was supported by the Swedish Environment Protection Agency (Miljöövervakningen) Nr 211 0742	12	English

ISSN and title/ISSN och titel

0283-7730 SMHI Meteorology

Report available from/Rapporten kan köpas från:

SMHI
S-601 76 NORRKÖPING
Sweden

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1. Introduction

Within the Environmental Monitoring of the Swedish Environment Protection Agency measurements of the total ozone has been done by the use of Dobson spectrophotometer #30. The instrument is located at the Svartberget Experimental Forest in Vindeln (latitude 64°14'N, longitude 19°36'E, 225 m.a.s.l.) and it has been in operation since 1991. The fundamental observation is done by observing the direct solar radiance. However, when clouds cover the sun an observation of the zenith radiance is collected. This type of measurement is called a zenith observation and by using an empirical relation one can deduce the total ozone. Up to now an old empirical relation based on data from Boulder USA has been applied. In this project we have used the data from 1991 onwards to develop and test a site specific empirical relation.

2. Instrument and data processing

The instrument used for the total ozone observations is a Dobson spectrophotometer. Its basic operation is described by Dobson (1957a and 1957b) and by Komhyr (1980). The uncertainty and potential error sources are discussed thoroughly by Basher (1982). Therefore, in the following paragraphs only a brief description of the instrument and the method of measurement will be presented.

2.1 Theory of the measurement

If I(λ) is the solar radiance in a small spectral interval centred at λ and at the height *z* in the atmosphere then the relative change in the radiance due to absorption and scattering processes in a finite layer *dz* is given by

$$dI(\lambda) / I(\lambda) = k_1(\lambda)\, \omega \, \sec ZA \, dz + k_2(\lambda)\, \delta_R \sec ZA \, dz + \delta_a \sec ZA \, dz$$

where $k_1(\lambda)$ = ozone absorption coefficient at λ
ω = ozone density at *z*
secZA = secant of the solar zenith angle ZA
$k_2(\lambda)$ = Rayleigh scattering coefficient at λ
δ_R = molecular density at *z*
δ_a = aerosol scattering at *z*

Integration from the surface of the Earth up to the top of the atmosphere gives

$$^{10}\log [I(\lambda) / I_\infty(\lambda)] = - k_1(\lambda) \int_0^\infty \omega \sec ZA \, dz - k_2(\lambda) \int_0^\infty \delta_R \sec ZA \, dz - \int_0^\infty \delta_a \sec ZA \, dz$$

where $I_\infty(\lambda)$ is the radiance at the top of the atmosphere. The integrals are approximated to reduce the equation to

$$^{10}\log [I(\lambda) / I_\infty(\lambda)] = - k_1(\lambda)\, OZ\, \mu - \beta(\lambda)\, m - \delta_a \sec ZA$$

where OZ is the integrated ozone (total ozone) in a vertical column, the slant column is found by the factor μ also called the relative optical airmass for ozone, $\beta(\lambda)$ is the Rayleigh scattering optical thickness in a vertical column and m is the relative optical airmass for a molecular atmosphere and δ_a is the aerosol scattering optical thickness in a vertical column. As a first approximation δ_a is assumed to be independent of the wavelength in the narrow wavelength band that is used.

Applying the equation for two separate wavelengths λ_1 and λ_2, then subtract one from the other and solve it for OZ gives

$$OZ = \left\{ {}^{10}\log \left[I_\infty(\lambda_1) / I_\infty(\lambda_2) \right] - {}^{10}\log \left[I(\lambda_1) / I(\lambda_2) \right] - m \left[\beta(\lambda_1) - \beta(\lambda_2) \right] - \sec ZA \left[\delta_a - \delta_a \right] \right\} / \mu \left[k_1(\lambda_1) - k_1(\lambda_2) \right]$$

where μ, m and secZA can be determined from the position of the site and the time. Thus two of the terms in this equation can be determined based on data measured in the laboratory namely $\mu [k_1(\lambda_1) - k_1(\lambda_2)]$ and $m [\beta(\lambda_1) - \beta(\lambda_2)]$. The term $\sec ZA [\delta_a - \delta_a]$ will be zero based on the assumption that δ_a is a constant. The term ${}^{10}\log [I(\lambda_1) / I(\lambda_2)]$ is the one measured by the spectrophotometer and ${}^{10}\log [I_\infty(\lambda_1) / I_\infty(\lambda_2)]$ can be determined by measuring over a range of μ-values and extrapolating the results to the top of atmosphere.

In practise the measurements are done for two pairs of wavelengths. When the two pairs of wavelengths are selected in a smart way the effect of the assumption that δ_a is constant is not critical and the resulting term will be negligible.

Table 1. Wavelength pairs used by the Dobson and the corresponding Rayleigh scattering and ozone absorption coefficients used up to 31 December 1991.

Wavelength pair	Short (nm)	Long (nm)	Diff ozone abs	Diff Rayleigh
A	305.5	325.4	1.748	0.116
B	308.8	329.1	1.140	0.113
C	311.45	332.4	0.800	0.110
D	317.6	339.8	0.360	0.104

Table 2. Wavelength pairs used by the Dobson and the corresponding Rayleigh scattering and ozone absorption coefficients used from 1 January 1992, Bass-Paur scale.

Wavelength pair	Short (nm)	Long (nm)	Diff ozone abs	Diff Rayleigh
A	305.5	325.4	1.806	0.114
B	308.9	329.1	1.192	0.111
C	311.45	332.4	0.833	0.109
D	317.6	339.8	0.374	0.104

2.2 Direct sun observation

The fundamental observation for the Dobson instruments in general is the so called *direct sun* observation (DS) using the AD-wavelength pair. This is the type of measurement used during intercomparisons (calibrations) when operative instruments are compared with reference instruments. The Dobson #30 was calibrated versus the world standard in 1990 at Boulder, USA, when it was refurbished prior to the start of the monitoring at Vindeln. The next calibration and service was in Arosa, Switzerland, in 1995, versus Dobson #65, which is the world secondary standard. Then, in 2001 and 2007 it was calibrated at Hohenpeissenberg in Germany versus the regional standard Dobson #64. At all these intercomparisons Dobson #30 has proved to be very stable and only small adjustments have been applied.

2.3 Zenith sky observation

The DS-observation can only be done when the sun is not obscured by clouds. It is possible to make relatively good DS-observations when the clouds are relatively thin. However, there is a limit when the clouds become too thick to get a signal strong enough to catch a reliable DS-observation. In these cases the procedure is to measure the zenith sky radiance (ZS, zenith sky observation). The zenith sky radiance can emerge from either cloud free blue sky or from the base of clouds. The first type of observation is denoted ZB (zenith blue) observation and the second one ZC (zenith cloud) observation.

The equation deduced in section 2.1 should not be applied to zenith measurements because the path of the radiation is not as assumed there. This because the radiation measured from the zenith blue sky is scattered once or several times in the atmosphere and thus the path is not known. To overcome this obstacle an empirical approach is applied.

During clear days quasi-simultaneous DS and ZB-observations are done. In the old days the result was plotted giving so called zenith sky charts. From these charts one could find relations between ZB and DS-observations. Today, instead of plotting on a paper an algorithm is fitted to the data set.

3. Model approach

Assume that the total ozone, OZ, can be found from the following approach

$$OZ_{ZB} = \sum\sum c_{ij}\ \mu_i\ N_j$$

where the c_{ij} is a set of coefficients to be determined, μ is the airmass and N is the respective ZB-observed value from the instrument. The indexes i and j loop from 0 to 2 and the coefficients, c, are determined to minimise the difference between OZ_{ZB} and OZ_{DS}.

4. Results and discussion

4.1 Zenith blue sky observations

At Vindeln a set of 741 data pairs has been collected over the years. The pairs consist of observations quasi-simultaneous (close in time) of the zenith blue sky radiance and of the direct sun radiance. These were used to determine the coefficients of the model using Matlab®. This resulted in the following coefficients and algorithm.

$$OZ_{ZB} = 1.3914\mu^2N^2 - 3.8875\mu^2N + 1.5739\mu^2 - 2.4599\mu N^2 + 4.4287\mu N + 18.5771\mu + 2.5077N^2 + 50.4204N$$

where μ is the airmass for the ZB-observation and N is the ZB-reading divided by 10 and by μ.

When applied to the data set itself the following Figure 1 shows the agreement between DS-observations and the modelled ZB-observations. Note, that this is not a validation only a verification that the model works. As expected, the Mean Bias Error (deviation) is zero and the Mean Absolute Error) is close to 2.7 DU and the RMSE 3.7 DU.

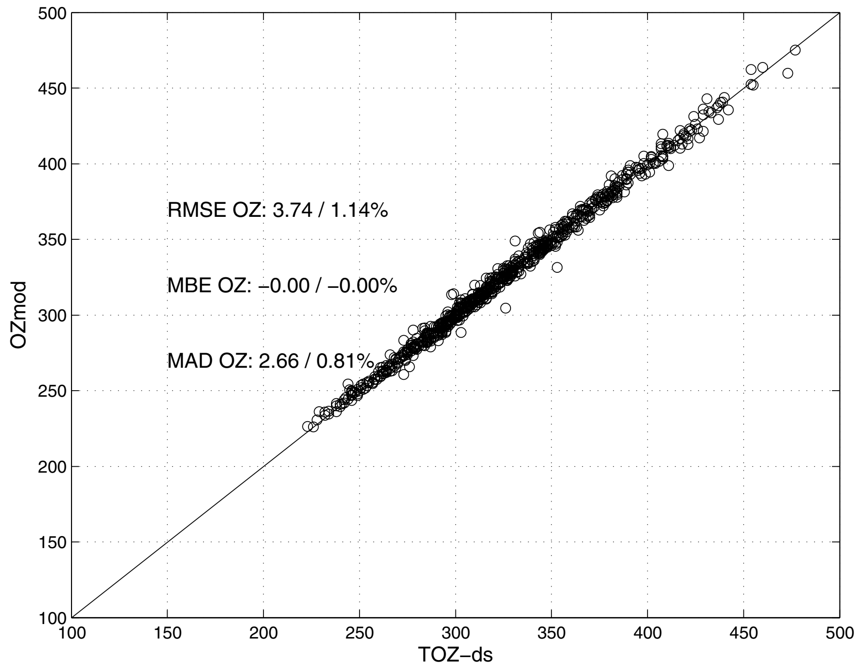

Figure 1. Modelled ZB-total ozone (DU) *is plotted versus measured DS-total ozone* (DU) *at Vindeln for the period 1991-2006. Also indicated are the absolute and relative values* (DU *and* %) *of the Root-Mean-Squared-Error, the Mean Bias Error and the Mean Absolute Error.*

The output expressed as the ratio between modelled ZB and observed DS is plotted versus the relative airmass for the zenith blue observation in Figure 2. It often happens that measurements, where the solar radiation is involved, show a dependence on the solar elevation or as here expressed as the airmass. Fortunately, no such dependence can be seen. The same ratio is also plotted versus time, 1991-2006 in Figure 3. As the date is not included in the model any change over time would reveal eventual drifts in the instruments. From Figure 3 it can be seen that the result is very stable over time with most of the data within ±2%. Less than 6% of the data is outside the range of ±2% from the measured DS-value.

The DS and the ZB observation are only quasi-simultaneous. Therefore, one could expect a less good agreement for observations taken at a larger time interval due to changes in the amount of total ozone. In Figure 4 the ratio between modelled ZB and observed DS total ozone is plotted versus the time difference between the observations. The typical difference is 5 minutes (median and type value). In Figure 4, no dependence on the time difference can be seen.

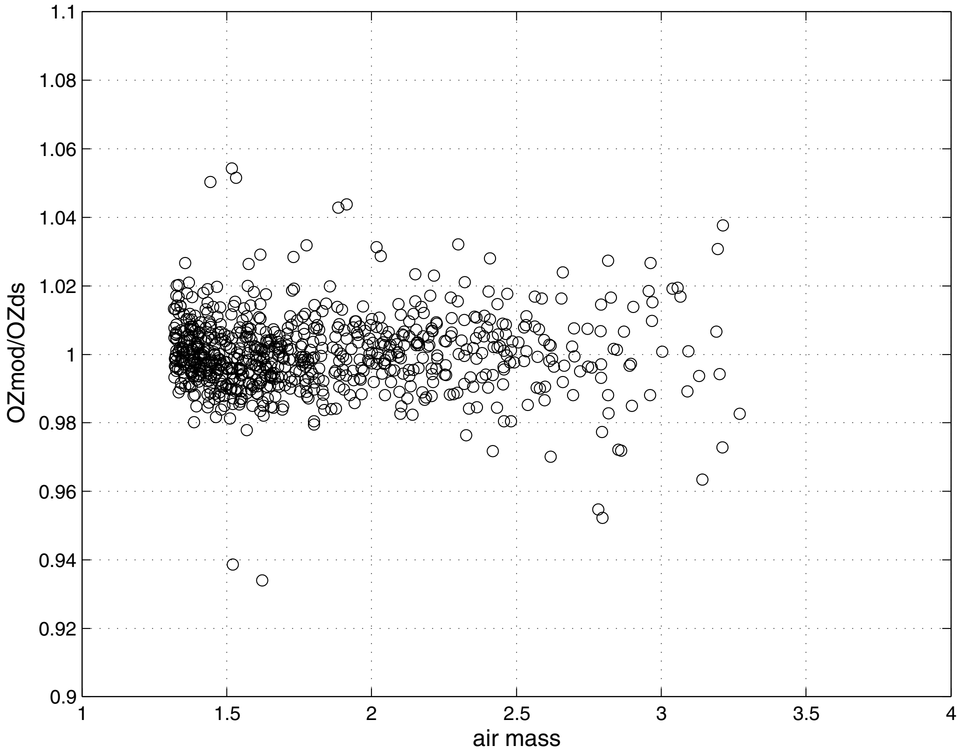

Figure 2. The ratio between modelled ZB and observed DS total ozone versus the relative airmass for the ZB-observation.

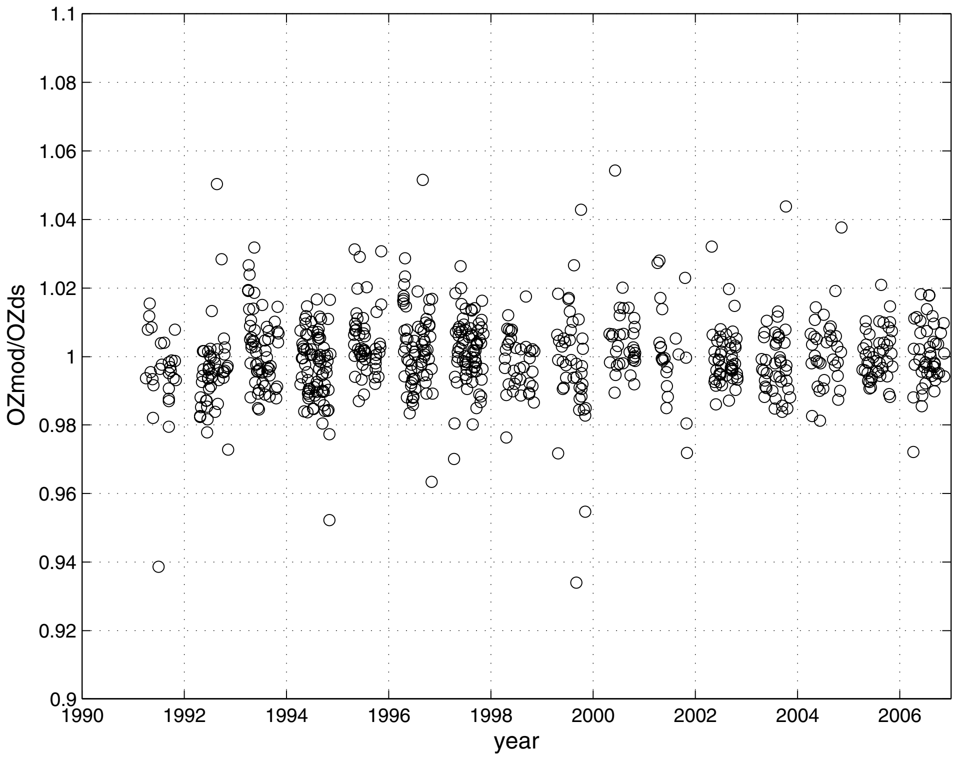

Figure 3. Ratio of ZB-modelled total ozone over observed DS versus time at Vindeln for the period 1991-2006.

Based on the standard direct sun measurement at clear skies of the Brewer ozone spectrophotometer, which is five observations in a sequence recorded within a few minutes, the typical standard deviation will be 1-2 Dobson units or slightly less than 1%. For the Brewer instrument this can be seen as an estimate of the combined natural variation and the precision. Therefore, the observed scatter (mostly within 2%) in the relation between the modelled ZB-total ozone and the observed DS-total ozone can probably be attributed normal measurement precision and to natural variation of the total ozone over the time between the both measurements.

The algorithm should also be independent of the amount of total ozone. Therefore, the ratio was also plotted versus the total ozone as in Figure 5. If any dependence exists it is small. Unfortunately, there is only a few measured values below 250 DU and very few above 450 DU. The algorithm is supposed to be applied even for extreme values, i.e. down to at least 180 DU and up to 575 DU. However, in these extreme conditions one must be very cautious and if possible the algorithm must be validated if such values occur.

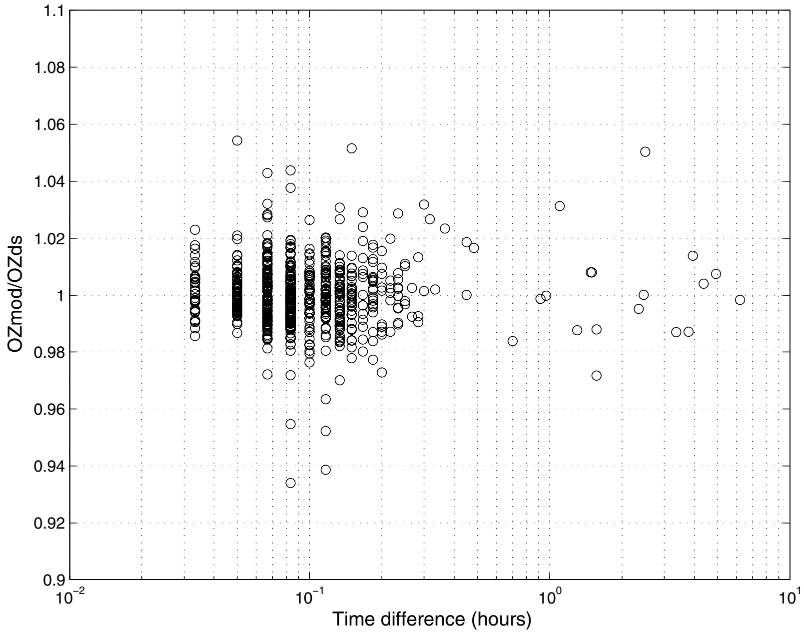

Figure 4. The ratio of ZB-modelled total ozone over observed DS total ozone plotted versus the time difference (hours) between the observations. Time difference is recorded in minutes starting with 2, 3, 4 etc.

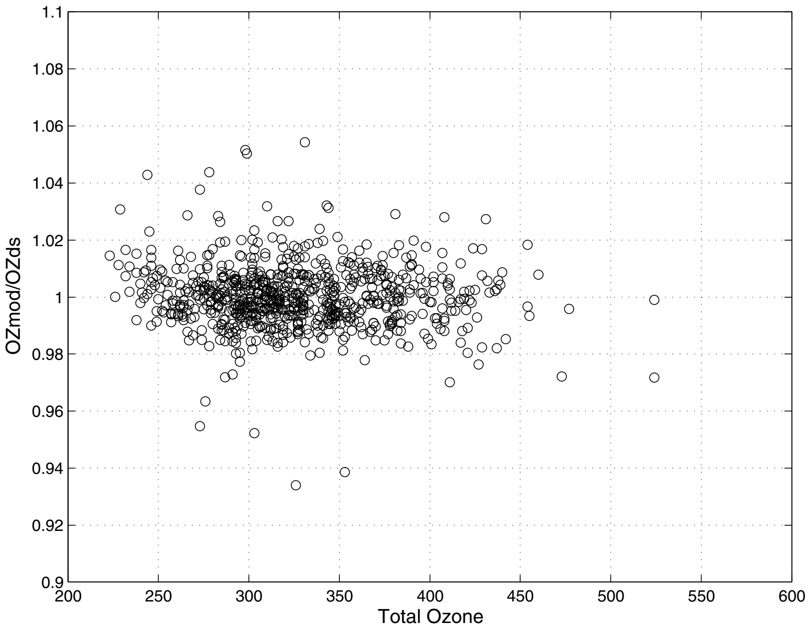

Figure 5. Ratio between ZB-modelled and observed DS total ozone versus the total ozone at Vindeln 1991-2006.

4.2 Validation versus independent data set

For validation the model was applied on independent data from 2007. Independent in the meaning that the data was not used to construct the ZB-model. The result can be seen in Figure 6, where the ratio between modelled and observed total ozone is plotted versus the relative airmass. Two sets of statistics are also presented in the graph. The first numbers relate to all observations. The first one is the absolute value in DU and the second one the relative value in percent compared to the mean. The two last numbers are for the majority of the observations; namely where the airmass is less than 3. Remembering that the ZB-model was based on data with an airmass between 1.3 and 3.3 one cannot expect the model to be correct outside this range. The direct sun observation for the airmass 3.8 is focused sun using the CD-wavelength pair and not the AD-one. This justifies why at least the value at airmass 3.8 can be excluded. The one at airmass 3.0 is excluded as an outlier. The remaining observations and their statistics are then in good agreement with the results presented in Figure 1.

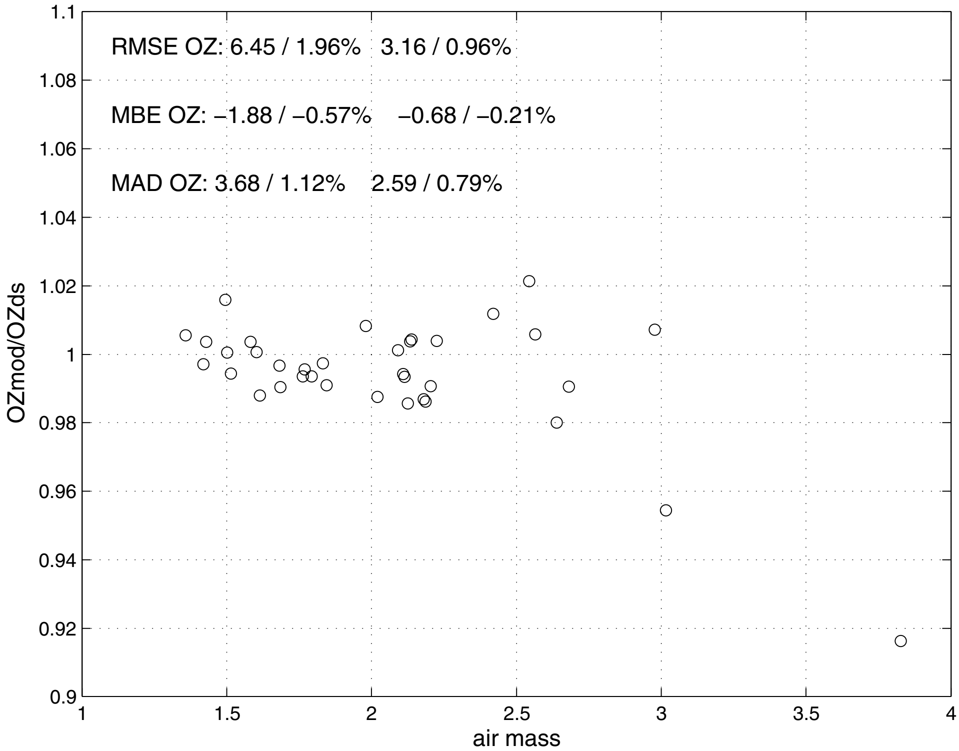

Figure 6. Validation versus independent data for the year 2007.

4.3 Comparison with the zenith blue chart applied on 1951-1966 data

The ZB-model found in this project has also been compared with the graphical ZB-charts that were produced by Rindert (1973) based on the observations in Uppsala 1951-1966. Here we must take into account that Uppsala is situated some 500 km south of Vindeln. The surrounding grounds around the two sites are different. The ground reflects UV-radiation, which in turn may be re-reflected back and some part will contribute to the measured radiance. In particular when snow covers the ground the influence is expected to be substantial. Therefore, the charts valid for Uppsala were not expected to be valid for Vindeln. However, looking at the old Uppsala ZB-charts valid for AD-wavelength pair and correcting for the use of the different ozone absorption coefficients (see Table 1 and 2) it appeared that the result showed an astonishing agreement, Figure 7. Roughly, the difference was as most about ±3% within the most frequent range of observations considering total ozone (200-500 DU) and solar zenith angle (μ-range 1.3 – 2.0)

This remarkable result also shows that we can be quite confident on the quality of the data observed in Uppsala that has been used as reference values for Sweden since the start of the current monitoring.

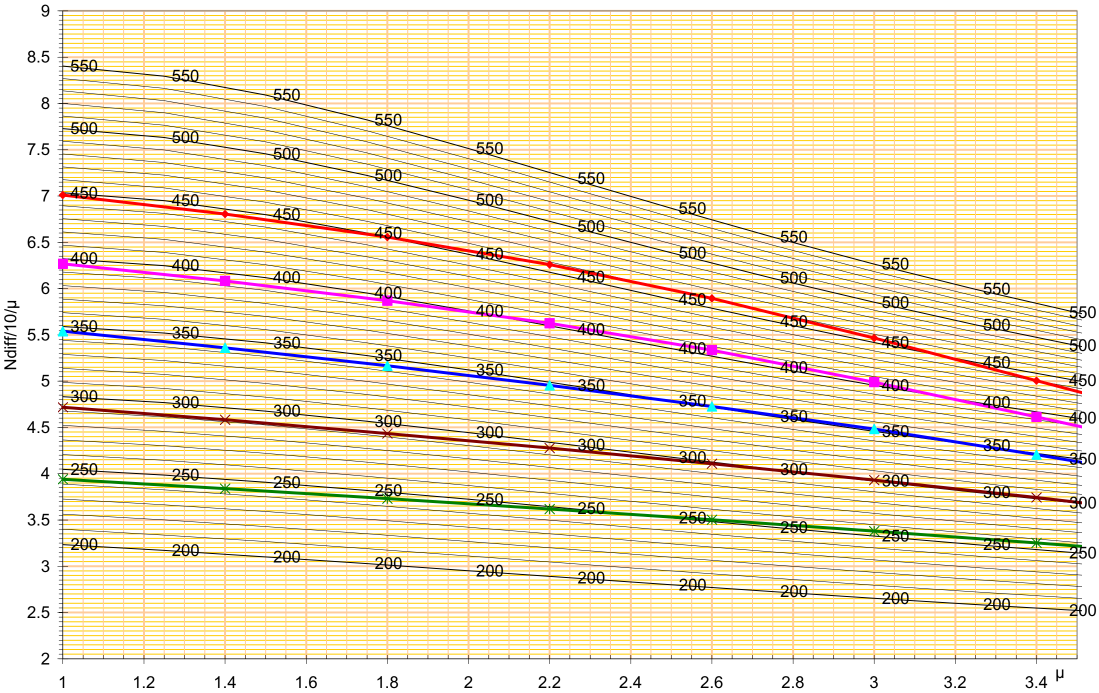

Figure 7. The found algorithm presented as a traditional zenith blue chart for the AD-DS and for Dobson #30. Also included in color is the corresponding lines for total ozone (250, 300, 350, 400 *and* 450 DU) *derived by Rindert* (1975) *converted to the present Bass-Paur scale*.

4.4 Zenith cloud observations

In the same way as for the zenith blue (ZB) observations a set of zenith cloud (ZC) have been compiled. Over the years 269 pairs of observations have been collected. A specific model of the same type as for the ZB-observations was developed, Figure 8. However, the difference between the ZB and the ZC models is minor as can be seen comparing with the upper panel of Figure 9. This encourages the use of the ZB model also for the ZC-observations. There are two factors supporting this. Mostly, the ZC observations inherit a larger uncertainty due to weaker signal and to variations in the cloudiness. The time difference between the ZC and the corresponding DS-observation is by nature larger, which also introduces a larger uncertainty. Looking at the statistics the mean bias error is about +1.5 DU when using the ZB-model to estimate the ZC-total ozone. The RMSE is about 6-7 DU and the MAD about 4-5 DU for both approaches and only slightly less for the specific ZC-model. As can be seen in the lower panels of Figure 9, where the ratio of the ZC modelled value using the ZB-model over the DS-observation versus the relative airmass for the ZC-observation and versus the DS total ozone, there is no significant dependence on these two variables when the ZB-model is applied on the ZC-observations.

In general, there is an indication that one should apply a cloud correction by subtracting a few DU from the value computed by the ZB-algorithm. However, the data set is too small to find out how the correction varies by airmass, total ozone and cloud thickness. The limited number of available values does not contradict the decision to use the corrections, Table 3, suggested by Komhyr (1980).

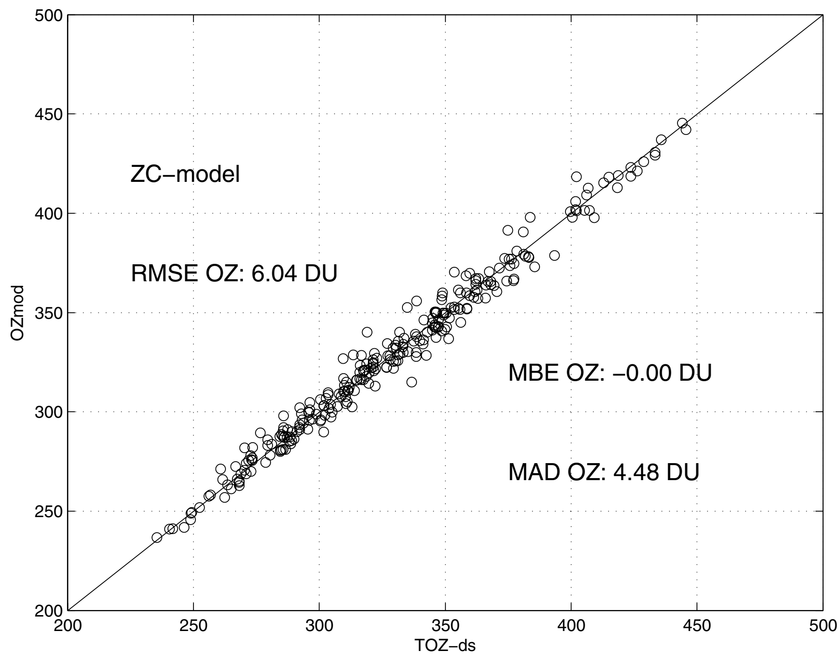

Figure 8. The result of fitting a model to the zenith cloud observations. Modelled versus observed total ozone (DU) *is plotted.*

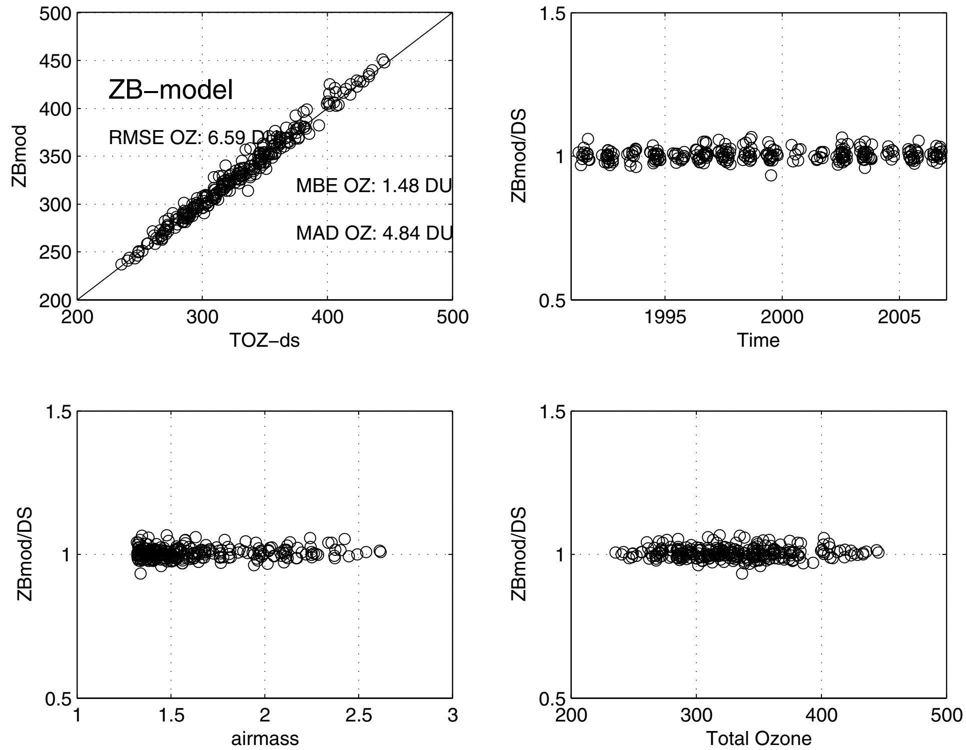

Figure 9. Results of applying the ZB-model to the ZC (zenith cloud) observations are given. Upper left panel shows the ZC-observation modelled by applying the ZB-model. Upper right panel shows the result over time1991-2006. Lower panels show the ratio between the ZC modelled value using the ZB-model and the DS-observation plotted versus the relative airmass for the ZC-observation and versus the DS total ozone.

Table 3.Cloud correction (DU) *for ZC-observations as recommended by Kohmyr* (1980).

Total oz	**Airmass (µ)**							
(DU)	**1**	**1.2**	**1.4**	**1.6**	**1.8**	**2.0**	**2.2**	**2.4**
250	0	0	0	1	1	1	1	1
275	0	0	1	1	2	2	3	3
300	0	1	1	2	3	3	4	4
325	1	1	2	3	4	4	5	6
350	1	2	2	4	5	6	7	8
375	1	2	3	5	6	8	9	11
400	2	3	4	6	7	9	11	13
425	2	3	5	7	9	11	13	15
450	2	4	6	8	10	13	16	18
475	3	4	7	9	12	15	18	21
500	3	5	8	11	14	17	21	24
525	3	6	9	12	16	19	23	27

5. Conclusion

The found zenith sky algorithm for retrieving total ozone using the Dobson #30 seems to be robust over a long period of time. The scatter is small and it can probably also be used slightly outside the range for which it was established.

It has also been shown that the algorithm can be applied on the zenith cloud observations and that the deduced total ozone only needs a small correction.

Data for the period 1991-2007 has been reprocessed and it has also resubmitted to the World Ozone and Ultraviolet Data Centre.

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Acknowledgement. The authors are grateful to Christer Degermark, Pernilla Löfvenius and Annika Degermark who have operated the Dobson with great care over the years. We also thank the Swedish Environment Agency without their support the excellent results would not be available.

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ISSN 0283-7730