
EMPIRICAL BACKGROUND MODEL OF TOTAL OZONE DENSITY OVER BULGARIA

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Abstract: A detailed analysis of the variations of the stratospheric and mesospheric ozone over Bulgaria, in the period 1996-2012, is presented in the article on the basis of ground and satellite measurements of the Total Ozone Column (TOC). The dynamics of the most important components has been studied. Their mean values for the period and the existing long-term trends have been found. The time evolution of the most basic components of the seasonal course has been studied, the existing long-term trends in it and their relations to the stratospheric temperature and quasi-biennial oscillation. Based on these studies and analyses, an empirical model for a daily forecast of TOC over Bulgaria has been created. The main aim of the model is monitoring of the ozone layer and, respectively, the biologically harmful ultraviolet radiation of the Sun related to it which has an effect on human health and life.

Keywords: ozone, modelling TOC, UV radiation, TOC over Bulgaria.

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Introduction

In Bulgaria, there is no institution making stratospheric ozone forecasts and monitoring its level. The National Institute of Geophysics, Geodesy and Geography has been assigned by the government (Ministry of Environment and Water) the task to study ozone: "Conducting research on the ozone layer (stratospheric ozone) over the territory of Bulgaria." The next logical step is creating a model based on the information obtained from this research. The aim of developing the model apart, from its scientific contributions, is also to gain information about the available ozone at a regional level.

The purpose of the present work is to create an empirical functional model describing the average monthly variations of TOC over Bulgaria depending on the season while taking into account possible long-term variations. In this case, a suitable method is presenting of seasonal variations through a decomposition of the daily values in Fourier series with a sliding segment of one year (the decomposition is made up to the fourth harmonic).

One of the first attempts for TOC forecasts based on regressions between satellite data and meteorological variables was made in Canada (Burrows et al., 1994). Most methods to predict TOC depend on statistical relations between ozone and meteorological prediction parameters such as temperature, geopotential height and potential velocity at some pressure levels (Rood and Douglas, 1985; Schubert and Munteanu, 1988; Vaughan and Price, 1991; Allaart, et al., 1993). Models for prediction of the total ozone content on that basis was developed by Poulin and Evans, 1994; Spänkuch and Schulz, 1997; Hood, 1997; McCormack and Hood, 1997; Plets and Vynckier, 2000; Monreal et al., 2002. Modeling total ozone usually serves as an input parameter for the UV index forecast (Lemus-Deschamps et al., 1999, Schmalwieser, et al, 2003; Allaart et al., 2004).

The same as the proposed approach was used by Antón et al. (2010) in the article "Temporal and spatial variabilities of total ozone column over Portugal"; however, the decomposition of Fourier series took part in the model only up to the first harmonic. Bekoryukov V. et al., 1987, used an analogous model based on spherical functions, since it was applied to the whole Earth. The statistical model of McCormick et al. (1992)

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contained quasi-biennial, seasonal, and semi-annual oscillations, a linear component and a first-order autoregressive noise process.

Data analysis

The data row in this study is from ground and satellite measurements. The ground measurements of TOC were made with the sun photometer Microtops II in the National Institute of Geophysics, Geodesy and Geography at the Bulgarian Academy of Sciences, which had been produced by Solar Light Company, USA, <http://www.solarlight.com>. The results from the measurements were received fully automatically from the built-in microcomputer; the only manual operation was targeting the sensors of the device to the sun. The precision of the device given by the factory is 1-2%. The error might reach up to 6 DU by a mean amount of the total content about 300 DU.

The ground measurements with Microtops II were supplemented with satellite data from Ozone Monitoring Instrument (OMI) working on AURA Satellite. The data is available for free on the web of NASA: <http://toms.gsfc.nasa.gov/>. Data are given in a 1°x1° grid resolution. To cover the territory of Bulgaria, data was used from 42 to 44° N and from 23 to 28° E. The relationship between the data of Microtops II and OMI was studied for the period September 2009 to June 2009. Systematic bias between the two types of measurements of about 11 DU was obtained, which permitted to recalculate the data of OMI and calibrate them to the data of Microtops II.

The data row can be expanded to 1996 with data from the Total Ozone Mapping Spectrometer (TOMS) aboard the Nimbus 7 polar-orbiting satellite. Both satellites worked simultaneously for the period from October 2004 to December 2005, and that allowed calibrating the data of TOMS to OMI. Finally, satellite data were calibrated to the ground measurements of Microtops II. Since the resulting continuous data row has been obtained from various devices, it should be considered free of systematic bias.

The time series of the mean monthly values of TOC over Bulgaria, collected through satellite and ground measurements, are displayed in Fig. 1. The well-known seasonal cycle of the total ozone with a spring maximum and an autumn minimum is readily seen. The running average of the mean annual value of the total ozone, presented in Fig. 2, shows three clearly expressed maximums in 1998, 2003-2007 and 2009-2010 and the respective minimums in 2000, 2007 and 2011. The mean value of the running average TOC, displayed with a dotted line, is 308.4 DU. A polynomial best fit of second order is displayed as the most common characteristic of the trend change of the mean annual value which shows an upward trend in the first half of the period and changes into a downward trend in the second half.

It is suitable to make a detailed study of the behaviour of the total ozone over the studied period on the basis of the components of the seasonal cycle. A decomposition of the daily values was made with a sliding time segment of a year with a step of one day, and the components of the seasonal cycle from the first to the fourth harmonic were included in the decomposition (that is mean annual value, yearly oscillation, semi-yearly oscillation, 4- and 3-month oscillation). This corresponds to a decomposition of Fourier series but the amplitudes and phases were defined by the least squares best fit (Bowman et Krueger, 1985) because of data gaps. The results are presented for the period 1997-2012 because 1996 is not complete, and we have the opportunity to use the data from 2013 until now for the second half of 2012.

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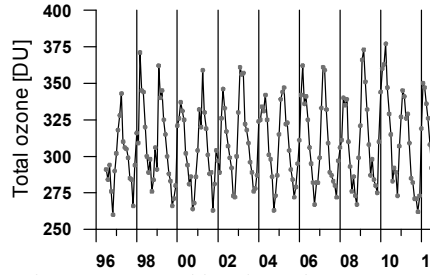


Fig. 1. Mean monthly values of TOC over Bulgaria in the period 1996-2012

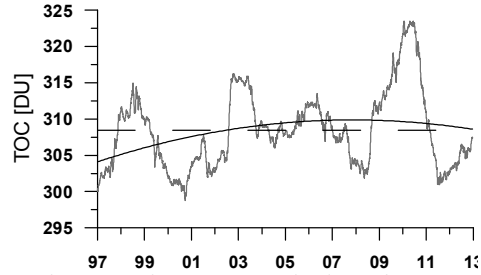


Fig. 2. Running mean annual values of TOC over Bulgaria in the period 1996-2012

The time series of a 12-month amplitude and phase are shown in Fig. 3 and 4. This is the strongest variation of the total ozone related to the seasonal cycle. The amplitude of the annual wave, in the observed period, shows a stable upward trend of about 30 to 40 DU. This signifies an increase of the maximal and a decrease of the minimal value over the year in case there is no significant upward or downward trend. The phase of the annual variability shows a visible downward trend. The phase (that is, the maximum moment of the annual amplitude) is about the 98th day of the year (the beginning of April) as an average for the period. The negative linear trend is 0.9 days/year.

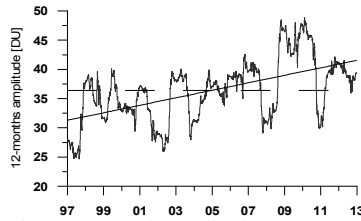


Fig. 3. 12-month amplitude

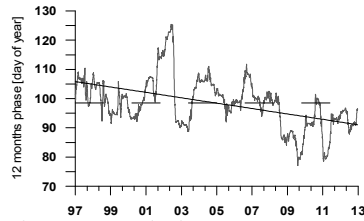


Fig. 4. 12-month phase

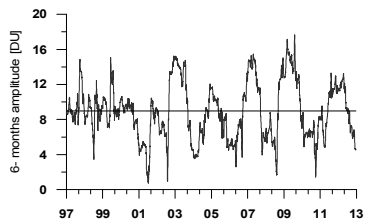


Fig. 5. 6-month amplitude

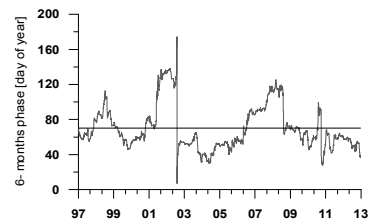


Fig. 6. 6-month phase

The amplitude and the phase of the semi-annual wave of the seasonal cycle of TOC do not show significant trends over the studied period (Fig. 5, 6). The amplitude varies over a wide range: from almost zero to about 16 DU while its average value is 9 DU. The mean value of the phase is the 70th day of the year. A quasi-biennial oscillation is readily seen in the period from 2001 to 2012. The values of the amplitudes of the other two components of the seasonal cycle, with periods of 3 and 4 months (the results are not shown), are close to the measurement error. Their variations are, most probably, of a

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random character. Bowman et Krueger, 1985, received values of the annual amplitudes of about 40 DU and of the semi-annual of about 5 DU (on the same coordinates shown on Fig. 5 and 6), for 1978-1982, which were almost identical to the values received in the present work.

Interrelation between TOC, stratospheric temperature and QBO

Data about the stratospheric temperature over Bulgaria from UK Met Office were used at isobaric level 68 hPa (18 km altitude). This dataset is a result of assimilation in situ and of remotely collected data through a numerical model for analysis of the stratosphere and troposphere. The daily values of the stratospheric temperature over Bulgaria were decomposed in the same way as TOC. The choice of level 68 hPa was made on the basis of experimental determining of the correlation between TOC and temperature at different levels. The best correlation was obtained with a temperature at 68 hPa, which level coincided with the maximum concentration of stratospheric ozone expressed in an amount of ozone of a certain volume.

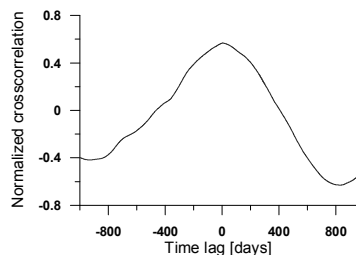


Fig.7. Cross-correlation between temperature at 68hPa and running mean annual value of TOC

The normalized cross-correlation function between the mean annual temperature and the mean annual TOC is displayed in Fig. 7. The maximal value of the correlation – 0.58 is observed with a five-day delay of ozone response. The ozone plays a significant role in the temperature regime of the stratosphere because it absorbs solar radiation but the observed delay shows that a reverse influence of the temperature over the concentration of ozone is also possible (Petzoldt et al., 1994).

Although the quasi-biennial oscillation QBO is a tropical phenomenon, it affects the stratospheric flow from pole to pole through an alteration of the vertical propagation of tropical waves. The quasi-biennial oscillation (QBO) prevails the variability of the equatorial stratosphere (16–50 km) and is easily seen as downward propagating easterly and westerly wind regimes, with an inconstant period averaging roughly 28 months. From a fluid dynamical perspective, the QBO is an enchanting example of a coherent, oscillating mean flow that is driven by propagating waves with periods unrelated to that of the resulting oscillation. Although the QBO is a tropical phenomenon, it affects the stratospheric flow from pole to pole by modulating the effects of extra-tropical waves. The effects of the QBO are not closed to atmospheric dynamics. Chemical constituents, such as ozone, water vapour, and methane, are affected by circulation changes induced by QBO (Baldwin et al., 2001). In this work, value of QBO at level 30 hPa is used.

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The influence of the quasi-biennial oscillation (Tung et al., 1994) can be observed on the amplitudes and phases of the annual and semi-annual component of the seasonal cycle of TOC. The cross-correlations displayed in Fig. 8 and Fig. 9. demonstrate correlation values of up to 50% more significant in the amplitude than in the phase. A positive correlation with a delay of about 200 days and nights can be observed with the amplitude and a negative one with the same delay with the phase.

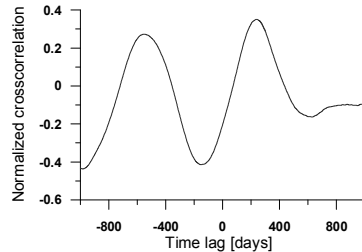


Fig. 8. Cross-correlation between QBO and a 12-month amplitude

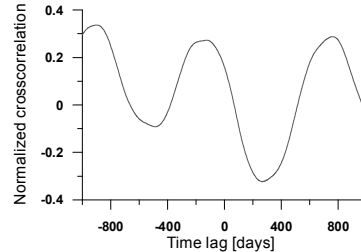


Fig. 9. Cross-correlation between QBO and a 12-month phase

Concept of the model and constants estimation

The concept of the proposed model is based on determining the functional dependence of the smoothed 31-day moving segment of regional TOC values of the season, taking into account the possible long-term trends and depending on the stratospheric temperature at level 68 hPa. Using values adjusted with the sliding time segment allows obtaining daily values but their significance is the monthly average value of a nominal month lasting 31 days and centred on the respective day of the year. The model cannot predict variations of TOC on a temporary scale for less than a month, which is subject to short-term forecasting.

The functional dependency (1) which is taken as the basis of the proposed model represents a functional dependency of four of the seasonal cycle components: the running mean annual value, the amplitudes and phases of the four harmonics for the basic period (one year) of the weather and a dependency of the temperature at 68 hPa and the values of the index QBO. A long-term trend of all the components, represented by a polynomial of a second degree, is additionally introduced. For convenience, the amplitudes and phases of the sinusoidal components of the seasonal cycle are represented by a sine and a cosine component with a zero initial phase by which the functional dependency becomes a multi-linear regression.

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$$\begin{aligned}
 TOC(day) = & a_{00} + a_{01}day + a_{02}T_{68}(day - t_i) + a_{03}QBO(day - t_q) + a_{04}day^2 + a_{05}T_{68}^2(day - t_i) + a_{06}QBO^2(day - t_q) + \\
 & \sum_{n=1}^4 a_{n0} \cos\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 a_{n1} day \cos\left(n \frac{2\pi}{365.25} day\right) + \\
 & \sum_{n=1}^4 a_{n2} T_{68}(day - t_i) \cos\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 a_{n3} QBO(day - t_q) \cos\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 a_{n4} day^2 \cos\left(n \frac{2\pi}{365.25} day\right) + \\
 & \sum_{n=1}^4 a_{n5} T_{68}^2(day - t_i) \cos\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 a_{n6} QBO^2(day - t_q) \cos\left(n \frac{2\pi}{365.25} day\right) + \\
 & \sum_{n=1}^4 b_{n0} \sin\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 b_{n1} day \sin\left(n \frac{2\pi}{365.25} day\right) + \\
 & \sum_{n=1}^4 b_{n2} T_{68}(day - t_i) \sin\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 b_{n3} QBO(day - t_q) \sin\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 b_{n4} day^2 \sin\left(n \frac{2\pi}{365.25} day\right) + \\
 & \sum_{n=1}^4 b_{n5} T_{68}^2(day - t_i) \sin\left(n \frac{2\pi}{365.25} day\right) + \sum_{n=1}^4 b_{n6} QBO^2(day - t_q) \sin\left(n \frac{2\pi}{365.25} day\right)
 \end{aligned} \tag{1}$$

The model is described by $9.6 = 54$ constants plus the two time delays which make a total of 56 constants. An attempt was made for the long-term trend to be represented by a linear function (whereby the numerical constants decreased), but the results proved to be worse than those by a parabolic approximation. On the other hand, the increase in degree, as well as the increase in the number of harmonics of the seasonal move did not noticeably improve the forecast. In this sense, it can be assumed that the numerical constants of the model are optimal. The constants of the model are determined according to the criterion of data best fit: the minimum of the variations squares' sum (the least squares best fit). All the constants take part linearly and can be determined by solving a system of linear equations except for the time delays to temperature and QBO.

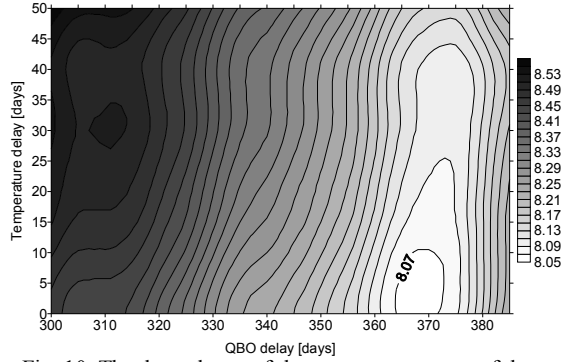


Fig. 10. The dependency of the mean square error of the model from the introduced delays within the respective range

Table. 1. Empirically obtained delays, mean square deviation and mean square error of the model.

Delay Temp	3
Delay QBO	368
RMS	8.058
Mean error	0.000

A procedure based on trials and errors was used to determine the time delays (under the criterion of the least squares best fit). The linear constants of the model were determined for all the possible combinations of the unknown time delay. The mean square deviation was calculated. The procedure of choosing such delays is illustrated in Fig. 10. It can be readily seen that the mean square error shows a minimum at certain values of both time delays which gives ground to choose namely those two values as the most suitable for the model.

Results

The data for TOC (light blue) with which we dispose are presented in Figure 11 compared to the results received from the model (dark blue). As it can be seen, the oscillation of TOC over the years is satisfactorily represented. It can be noted that the model renders account of the alterations by sharp rises of the concentration even though with far more smoothed values (for example the middle of 1998 and the beginning of 2010).

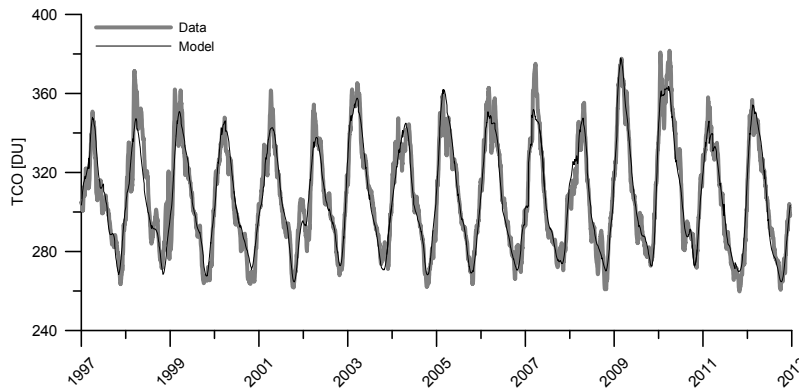


Fig. 11. A comparison of the data with the model values

A statistical analysis of the deviations (the errors) of the model.

The daily values of the error are represented in Figure 12. Those are, in fact, the differences between the values predicted by the model and the real data. As it can be seen, the error varies mainly in the interval ± 20 DU, with few little exceptions. The mean error has, practically, zero value which is a result of the least squares best-fit method. The distribution is close to the Gaussian one as it can be seen in Fig. 13. Autocorrelation coefficient of the errors is less than 0.2 by a time lag of 31 days (data is not shown here).

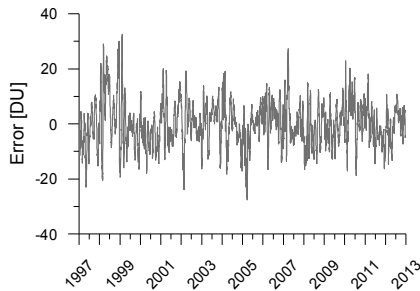


Fig. 12. Daily values of the error of the quadratic model.

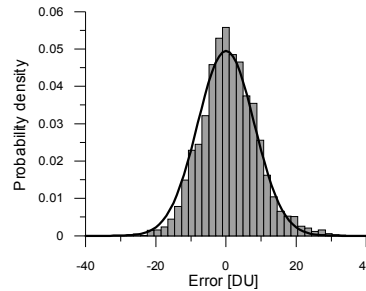


Fig. 13. The probability distribution of the error of the quadratic model.

Comparing the model of Pribullová, et al., 2006, shows a relative error of 6%, Burrows et al., 1994 obtained RMSE 16 DU and 23 DU for two different years (1992 and

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1993). According to Vogel et al., 1995 the RMS error is 20 DU corresponding to an absolute relative error of 7%. Aksoy et al., 2009 calculated RMS error for individual months, and obtained values varied between 7.28 DU and 23.26 DU. Spänkuch and Schulz, 1995 reached 25.2 DU for a winter-spring season, 13 DU for a summer and 18.4 DU for an autumn-winter season for the 10-year period 1978-1988. A comparison of the results of the proposed method with the quoted methods indicates that all methods offer approximately equal error values.

Verification of the model

The data trend and the trend of the model values of TOC for 2013, a year which had not been used for determining of the model's coefficients, are displayed in Fig. 14. The purpose is to make an evaluation of the model through the comparison of model and measured values of TOC. More significant deviations of the model from the data can be observed for the period May – August.

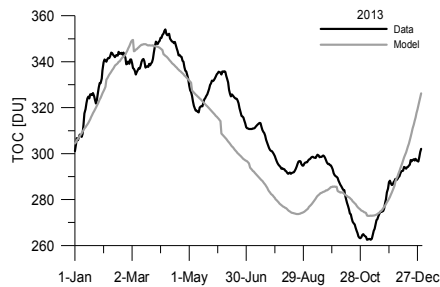


Fig. 14. Data and model for 2013

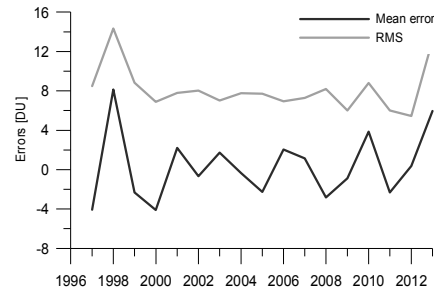


Fig. 15. Mean error and RMS of the model by years

The mean error and RMS for 2013, displayed in Fig. 15, are bigger than the respective values for the whole period 1997-2012 but they do not surpass the biggest error for the separate years (in 1998). One of the possible reasons is the violation of the trend of the seasonal cycle of TOC's components which were put in the model for 2013 purely empirically. Another possible reason is a deviation of the TOC trend from the general regularities introduced in the model in 2013 in particular, like the situation in 1998.

Conclusion

The presented empirical model of the daily values of TOC over Bulgaria describes satisfactorily the general regularities of the TOC trend related to the seasonal changes in the atmosphere as well as the influence of the temperature and the dynamics in the stratosphere in particular while the resulting errors are in the range of the data measurement error. The long-term trends of the components of the seasonal cycle received by the analysis and included in the model are described through parabolic dependencies which pose a certain risk of increases in the error by using of the model beyond the time range for which it has been synthesized. An attempt is made to describe the trends not with a polynomial of second degree but with linear functions (the results

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are not presented). The errors for the period of time 1997-2012 are a little bit bigger than the presented results of the parabolic approximation but are smaller for 2013. The parabolic approximation is nevertheless preferred since it better describes the trend of TOC over the studied period. Further improvement of the model is possible by the accumulation of a longer data row.

The presented model can be used to estimate the state of the ozone layer over Bulgaria and to assess whether there is any hazard of dangerous increases of the ultraviolet radiation of the Sun for people's health.

Acknowledgement

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