Sensitivity of surface UV radiation and ozone column retrieval to ozone and temperature profiles

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Abstract. This paper discusses the influence of ozone and temperature profiles on surface UV radiation, and on total ozone column derived from global irradiance measurements. Measured ozone and temperature profiles from Legionowo, Poland, are used together with typical surface and cloudless atmosphere conditions. The effects of assuming a U.S. standard profile with scaled ozone column instead of actual profiles are analyzed. Variable temperature/ozone vertical distributions and different sets of ozone absorption cross section data may change erythemally weighted radiation by as much as 14% with respect to reference conditions. The mean and standard deviations of errors were generally below 2% but increased another 2-3% for large solar zenith angles. Uncertainties of up to 10% may be caused by using an inappropriate profile in total ozone column retrieval. We analyzed the underlying processes causing the uncertainties by selecting three ozone and temperature profile pairs characterized by the same unscaled total ozone amount but with different vertical distributions. Results obtained for cases with ozone redistribution from the stratosphere to the troposphere are consistent with earlier work. However, if the temperature profiles differ significantly in the stratosphere, an ozone redistribution may lead to a strong decrease in UV doses for high solar zenith angles. It is also shown that differences in ozone maximum height as well as in ozone concentration in the upper troposphere have a significant influence on surface UV radiation.

1. Introduction

Solar UV-B radiation is strongly attenuated by ozone absorption in the Earth's atmosphere. The effectiveness of ozone absorption is a function of the temperature and the path of propagation through atmospheric layers that contain ozone. Hence the absorption of solar UV radiation by ozone does not only depend on the total ozone content but also on the solar zenith angle, atmospheric scattering, and the vertical distribution of ozone and temperature. In radiative transfer models, standard ozone and temperature profiles are usually used since in situ measurements of ozone and temperature profiles are generally not available.

Brühl and Crutzen [1989] showed that a redistribution of stratospheric ozone to the troposphere gives a decrease in the biological UV dose. In a similar study, Tsay and Stamnes [1992] analyzed the effects of shifting ozone from the stratosphere to the troposphere on erythemal UV radiation. They found that such a redistribution tends to decrease the erythemal UV dose for a solar zenith angle of 55° and to increase the dose, by 1-3%, for larger solar zenith angles. In the latter study, synthetic ozone profiles were used and ozone artificially redistributed from the stratosphere to the troposphere. Schwaner et al. [1997] estimated the uncertainties in modeled UV irradiances caused by the limited accuracy of model input data. They found that replacing a standard ozone profile by seasonal profiles may lead to a significant, around +11%, increase in UV irradiance at 290 nm and a solar zenith angle of 60° for winter conditions. For other wavelengths and solar zenith angles the differences were smaller. For summer profiles the opposite results were obtained.

This paper discusses the influence of variable ozone and temperature profiles on surface UV radiation. Furthermore, the implications for ozone column retrieval from global UV irradiance measurements are discussed. Measured ozone and temperature profiles from Legionowo, Poland, are used together with an accurate radiative transfer model to quantify the error made by using standard ozone and temperature profiles compared with actual profiles. The underlying processes causing the deviations are explained using selected cases.

The paper is organized as follows: in section 2 the radiative transfer model is briefly described. This is followed by a presentation of the ozone and temperature profiles used in the study. The sensitivity results are presented and discussed next, followed by the conclusion.

2. Radiative Transfer Model

The radiative transfer model is an upgraded version of the model described by Mayer et al. [1997]. The model is based on the multistream discrete ordinates radiative transfer equation solver DISORT by Stamnes et al. [1988] with pseudospherical corrections as described by Dohalbuck and Stamnes [1991]. The calculations were performed for the 280-400 nm spectral range with a resolution of 0.05 nm. The ozone cross section was taken from Molina and Molina [1986], where not otherwise noted. We
used a tropospheric urban aerosol model with a spring/summer profile and a Heney-Greenstein phase function [Shettle, 1989]. The aerosol optical depth was scaled using the Angstrom turbidity formula with alpha and beta set to 0.11 and 1.3, respectively. The Rayleigh scattering cross sections were calculated according to the parameterization given by Nicolet [1984]. The extraterrestrial irradiances were taken from measurement made by the Solar Ultraviolet Spectral Irradiance Monitor (SUSIM) onboard the space shuttle during the ATLAS-3 mission in November 1994.

Ozone and temperature profiles were either standard profiles or measured profiles described below. To estimate the sensitivity of surface UV radiation to ozone and temperature profiles, the UV erythemal [McKinlay and Diffee, 1987] and DNA damage [Setlow, 1974] doses were calculated together with the UV index (UVI). The latter is defined as the daily maximum effective erythemal weighted irradiance (W/m²) averaged over a duration of 30 min and multiplied by 40 [WMO, 1997]. These radiation quantities were calculated for various solar zenith angles and ground albedo values. In addition, irradiances at 305 and 340 nm were calculated for use in the ozone column sensitivity study.

3. Atmospheric Profiles

The conservation of realism when performing a sensitivity study on the influence of ozone profiles on surface UV radiation is not a trivial task. UV radiation is influenced by molecular, aerosol and cloud scattering, and absorption and surface reflection. Furthermore, the ozone cross section depends on temperature, and hence the ozone absorption is temperature dependent. In a strict sense, a fully realistic sensitivity study should only compare results when all atmospheric and surface variables are identical, except for the variables of interest. Obtaining an adequately sized data set from surface radiation measurements using this criterion is generally impossible. In our radiative transfer modeling, all surface and atmospheric parameters except for the ozone and temperature profiles were fixed to typical surface and atmospheric conditions. In order to perform comparative studies where only the effect of vertical distributions of ozone and temperature is observed, we were obliged to manipulate the atmospheric scenarios. Firstly, the full ozone profiles were multiplied by a scaling factor to have the same total column value. Secondly, the air molecule number density profile of the U.S. Standard Atmosphere [Anderson et al., 1986] was artificially applied throughout the study. There is a risk that those manipulations may produce somewhat unrealistic ozone and Rayleigh extinction profiles. The latter manipulation ignores the effect of temperature on the air molecule number density [Schwander et al., 1997]. We also ignore the influence of temperature on relative humidity which may have an impact on aerosol optical properties. The number of atmospheric homogeneous layers and thus the vertical resolution of the radiative transfer model was 50. Two separate sets of profiles measured in Legionowo, Poland, from measurement made in the period 1979-1997, were prepared for the sensitivity study.

3.1. Data Set 1

Data set 1 consists of a pool of profiles from which extreme influences on surface UV radiation and ozone column retrievals are explored. In total, 50 temperature and ozone profile pairs were analyzed for their influence on the surface erythemal dose rate and total ozone column retrieval. In addition, six standard atmospheric profiles obtained from Anderson et al. [1986] were used. They correspond to midlatitude summer/winter, subarctic summer/winter, tropical, and U.S. standard conditions. All profiles in this data set were scaled to a total ozone column of 350 Dobson units (DU). The actual total columns of the ozone profiles considered here were in the range 274-402 DU.

3.2. Data Set 2

To study the underlying processes of the influence of realistic ozone profiles on UV radiation, pairs of ozone profiles with different vertical distribution but similar total ozone, within the range of ±33%, were selected from the data series. The basis for the selection was the difference in tropospheric ozone amount and in the heights of the tropopause [WMO, 1957] and the ozonopause [Chrgian, 1967]. The tropopause height is often used for studying the changes of total ozone in midlatitudes [Schubert and Munteanu, 1988; Hoinka et al., 1996]. The reason for this was formulated by Steinbrecht et al. [1998] as follows: "The tropopause forms a boundary between the well-mixed, ozone-poor troposphere and the stratified ozone-rich lower stratosphere." When studying the temperature and ozone profiles, one can observe easily the differences in the heights of tropopause and ozonopause. It is really the ozonopause that separates the ozone-poor troposphere from the ozone-rich stratosphere; Chrgian [1967] formulated the ozonopause as "the height above which the ozone partial pressure is growing rapidly." After Ivanova [1972] the heights of tropopause and ozonopause differ in 85% by ± 1 km, but in several cases, the difference can be 4-9 km. Performed selection of ozone profile pairs aimed at separating such cases. For detailed studies, three pairs of ozone profiles were chosen:

3.2.1. Case 1, August 3, 1994 and July 7, 1993, Figures la and lb. The two profiles have major differences in the tropospheric and stratospheric ozone amounts with the first profile having 34 DU more of ozone below the tropopause and 35 DU less above, hence providing a good example of ozone redistribution from the stratosphere to the troposphere. The difference of ozone amount below and above the ozonopause is even larger (Table 1). The second feature is the difference in the tropopause and the ozonopause heights.

3.2.2. Case 2, February 2, 1997 and March 6, 1996, Figures 1c and 1d. The profiles differ only in the heights of the tropopause and the ozonopause.

3.2.3. Case 3, March 15 and 1, 1996, Figures 1e and 1f. There are large differences in the tropospheric and stratospheric ozone amounts. In this case however, ozone is redistributed more evenly in the troposphere then for case 1. In addition, large differences in the tropopause and ozonopause heights are observed. More details about the ozone profiles are provided in Table 1. Ozone profiles for each pair were scaled to the mean total ozone amount of the pair. The ozone soundings are reliable only below 30 km, so above this altitude, constant mixing ratios were used in both data sets. The second profile in each pair is the reference one, so in all calculations the difference is obtained by subtracting the value calculated for the second profile from the one calculated for the first profile. In Figure 1 the reference profiles are plotted with a solid line.

4. Results and Discussion

4.1. Surface UV Radiation

For convenience and/or due to lack of measurements, modelers often use standard ozone and temperature profiles for their radiative transfer calculations. Using the 55 profiles from data set 1, we computed surface erythemal doses for various solar zenith angles and compared the results to corresponding results obtained by using the U.S. Standard Atmosphere.
Figure 1. Ozone and temperature profiles for (a, b) case 1, (c, d) case 2, and (e, f) case 3.
Table 1. Ozone Content (DU) in Atmospheric Layers Against Tropopause and Ozonopause Heights (km) for Chosen Profiles

<table>
<thead>
<tr>
<th></th>
<th>0-5 km Below Tropopause</th>
<th>Above Tropopause</th>
<th>Total Tropopause Height</th>
<th>0-5 km Below Ozonopause</th>
<th>Above Ozonopause</th>
<th>Ozonopause Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>94.08.03</td>
<td>31.1</td>
<td>59.5</td>
<td>280.5</td>
<td>340.0</td>
<td>11.7</td>
<td>64.7</td>
</tr>
<tr>
<td>93.07.07</td>
<td>6.8</td>
<td>25.5</td>
<td>315.5</td>
<td>341.1</td>
<td>9.4</td>
<td>18.6</td>
</tr>
<tr>
<td>Difference</td>
<td>24.3</td>
<td>34.0</td>
<td>-35.0</td>
<td>-1.0</td>
<td>2.3</td>
<td>46.1</td>
</tr>
<tr>
<td>97.02.07</td>
<td>16.0</td>
<td>29.6</td>
<td>263.4</td>
<td>293.0</td>
<td>12.3</td>
<td>33.7</td>
</tr>
<tr>
<td>96.03.06</td>
<td>16.1</td>
<td>30.2</td>
<td>256.8</td>
<td>287.0</td>
<td>10.7</td>
<td>27.4</td>
</tr>
<tr>
<td>Difference</td>
<td>-0.1</td>
<td>-0.6</td>
<td>6.6</td>
<td>6.0</td>
<td>1.7</td>
<td>6.3</td>
</tr>
<tr>
<td>96.03.15</td>
<td>33.4</td>
<td>61.1</td>
<td>280.5</td>
<td>368.0</td>
<td>10.7</td>
<td>55.6</td>
</tr>
<tr>
<td>96.03.01</td>
<td>16.9</td>
<td>25.4</td>
<td>315.5</td>
<td>374.0</td>
<td>7.2</td>
<td>26.7</td>
</tr>
<tr>
<td>Difference</td>
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<td>35.7</td>
<td>-35.0</td>
<td>-6.0</td>
<td>3.5</td>
<td>28.9</td>
</tr>
</tbody>
</table>

The differences were largest for large solar zenith angles with the sounding profiles giving minimum and maximum differences in the doses of -9.4% to 12.3% compared to the U.S. Standard Atmosphere for a solar zenith angle of 85°. The minimum-maximum differences in the doses decrease rapidly with decreasing solar zenith angle. For a solar zenith angle of 70° the largest positive (negative) difference is 2% (-1.8%). For still smaller solar zenith angles, the corresponding numbers are 1.8% and -4%. The standard deviation of the difference for all the various profiles compared with the U.S. standard profile is 1.4%, 1.3%, and 5% at solar zenith angles of 0°, 45°, and 85°, respectively. The corresponding mean differences are -1.2%, -1.0%, and 2.7%. The latter indicates that systematic errors are introduced by applying the U.S. standard profile. This indicates that there are better single atmospheric profiles than the U.S. Standard Atmosphere for the location of these particular ozone soundings.

Various measurements have been performed of the ozone cross section. If instead of the Molina and Molina [1986] measurements we use the ozone cross sections presented by Bass and Paur [1985], the surface erythemal dose rate increases with 3% at 0° solar zenith angle and 1.7% at 85°. The corresponding increases were 2.7% and 1.5%, respectively, when using the ozone cross section due to Daumont et al. [1992]. The differences between doses calculated with different ozone cross sections decrease with increasing solar zenith angles.

To investigate the underlying processes causing the dose rate differences for different ozone and temperature profiles and solar zenith angles, we discuss in some detail the results obtained using data set 2. For case 1, which is a good example of ozone redistribution from the stratosphere to the troposphere, a decrease in UV doses is observed for small and medium solar zenith angles. The largest differences are in the range of 4-8% for an albedo of 0.03 (Figure 2a) and 8-13% for an albedo of 0.5, depending on the spectral response function that is used. For larger solar zenith angles, a small increase in UV doses (up to 3%) for an albedo of 0.03 is observed (Figure 2a). This effect is caused by an increased contribution of diffuse radiation relative to the total radiation [Tsay and Stamnes, 1992]. When scattered above the tropospheric ozone, diffuse radiation has a shorter effective path of propagation through this absorbing layer than the direct beam. However, when we move to very large solar zenith angles, above 80° the differences disappear. This is due to the large air mass and domination of diffuse radiation at these low Sun elevations. For a higher albedo (0.5) the shape of the curve is similar to that for an albedo of 0.03, but positive values of differences in UV doses for larger solar zenith angles are not observed. The higher albedo causes more multiple scattering between the surface and the lower troposphere. This in turn enhances absorption due to tropospheric ozone. For solar zenith angles above 80° the difference is again negative and drops to 4%. The differences in the
UV index (UVI) for the two albedo values are not very large, the maximum differences being 0.4 UVI for an albedo of 0.03 and 1 UVI for an albedo of 0.5 for small zenith angles.

In case 2, practically no difference in the tropospheric and stratospheric ozone exists, and the ozone profiles differ only in the tropopause and ozonopause heights and hence in the ozone maximum heights. An increase in UV doses of around 2% is observed for all spectral response functions and small to medium solar zenith angles and an albedo of 0.03 (Figure 2b). By increasing albedo values up to 0.5, we obtained an increase of 2.3% for all spectral response functions. A vertical distribution of direct and diffused radiation calculated for this case and a solar zenith angle of 15° show that these results are caused by an increased contribution of diffuse radiation in total UV irradiance at the 10 km altitude. The upward shift of the ozone maximum together with the temperature increase in the stratosphere leads to a decrease in direct radiation entering the troposphere. Nevertheless, a decrease in ozone concentration in the layer between 10 and 15 km, which is connected with the difference in the ozonopause heights, causes an enhancement of the diffused component of total radiation and results in increased UV irradiance at the ground level.

For low Sun however, decreases of 8% for the erythemal weighting function, 16% for DNA, and 22% for UVB doses were obtained independently of an albedo. These results can be explained by an increase in ozone concentration at the altitude above 20 km. For high solar zenith angles the radiation reaching the ground is dominated by a diffuse component. Higher ozone concentration in the layer at 25 km leads to a decrease in the amount of "detour photons" that may pass through the stratosphere and reach the ground level [Schwander et al., 1997]. This effect is additionally enhanced by the stronger ozone absorption caused by the temperature increase in the layer between 15 and 25 km (Figure 1d). Hence the weakening of source of diffuse radiation, in the light of longer optical path in the troposphere, for low Sun results in the decrease in UV doses at ground level.

Again, the differences in absolute values of UVI are very small, the maximum values are 0.19UVI and 0.28UVI for an albedo of 0.03 and 0.5, respectively.

Case 3 is characterized by ozone redistribution from the stratosphere to the troposphere and rather large differences in the tropopause and ozonopause heights. Here the UV doses decrease for all solar zenith angles and all spectral response functions. For small and medium solar zenith angles the percentage decrease varies from 2% to 4%, depending on spectral response function, for an albedo of 0.03 (Figure 2c), and from 4% to 6% for an albedo of 0.5. It is striking that no positive differences for high solar zenith angles are observed. Instead, a sudden fall of the differences, even to 16-19% for UVB, depending on albedo, takes place. The largest differences in UVI are of 0.2 to 0.4, depending on albedo.

Although ozone redistribution from the stratosphere to the troposphere takes place in both cases 1 and 3, the results for these two situations are different. Instead of the increase in UV doses obtained for case 1 at higher solar zenith angles, a large decrease is observed for case 3. One of the features that distinguish ozone profiles for cases 1 and 3 is the way in which ozone is redistributed in the troposphere. For the first situation, ozone increase is especially high in the lower troposphere (0-5 km), while in case 3, ozone is evenly distributed throughout the troposphere.

To explain if this feature leads to obtained results, we constructed a "modified" case 1 in the following way: the first ozone profile was replaced by a modified second profile (the reference profile). The modification consisted of redistributing ozone from the stratosphere evenly to the troposphere in the second profile, so the same tropospheric ozone difference of the profiles as in case 1 was obtained. The large ozone difference in the layer 0-5 km, which was characteristic for the first profile of case 1, was reduced. In this way both profiles of "modified" case 1 have the same tropopause and ozonopause heights, and the temperature profiles are the same. All calculations were made in the same way as in case 1, and the results for an albedo of 0.03 are presented in Figure 3. The shapes of the curves for UV spectra for case 1 (Figure 2a) and "modified" case 1 (Figure 3) are very similar, but the results vary in absolute values of the UV differences. However, for the "modified" case 1 we do not observe the drop of the curves for very high solar zenith angles, on the contrary, the positive values of the difference in UV are continuously growing to large values. This indicates that the results obtained for the case 3 can be explained by difference in temperature profiles in the stratosphere, which is much bigger for case 3 than for the case 1 (Figures 1b and 1f). Although the increase in ozone concentration at an altitude of 18 km for case 3 is rather small, the temperature increase above 15 km leads to a strong decrease in direct UV radiation entering the troposphere. At the same moment for case 1, an increase in direct and diffused UV radiation is observed for the same altitude. The difference in the optical properties of the upper stratosphere leads to various results obtained for high solar zenith angles.

4.2. Total Ozone Column Retrieval

The total ozone column may be estimated from global irradiance measurements by forming the irradiance ratio of a wavelength that is strongly absorbed by ozone and one which is weakly absorbed by ozone [Stamnes et al., 1991]. We used the wavelengths 305 and 340 nm and calculated the irradiances at these wavelengths using a triangular slit function with a full width at half maximum of 0.6 nm. For convenience a look-up table (LUT) of the ratios as a function of solar zenith angle and total ozone content was generated. The LUT entries were computed for conditions corresponding to the U.S. Standard Atmosphere. Next, we simulated UV spectra using measured ozone/temperature profiles. From these simulated UV irradiances the ozone column was retrieved. Since all measured ozone profiles were scaled to 350 DU, the deviation of the retrieved ozone column from this total ozone content illustrates the impact of variable ozone and temperature profiles.
The influence of ozone and temperature profiles on UV radiation has been studied. It was found that erythemal UV doses calculated using measured temperature and ozone profiles differed by up to 12% with respect to the U.S. standard profile. Detailed studies of a few selected cases show a significant influence of changes in ozone concentration at different atmospheric altitudes on UV radiation at the ground. The widely discussed effect of ozone redistribution from the stratosphere to the troposphere has been analyzed on the basis of two realistic cases. Obtained results are consistent with other publications as far as temperature differences in the stratosphere are very small, otherwise expected increase in UV doses for high solar zenith angles may be replaced by a strong decrease. For the studied case this decrease was of 4% for erythemal weighting function and an albedo of 0.03.

For the situation when the changes in ozone concentration in the stratosphere take place, we found that the changes in ozone concentration in the upper troposphere which are usually connected with the difference in the ozonopause heights, may overrun the changes caused by the ozone maximum shift for small solar zenith angles. For high solar zenith angles however, this effect is not seen, and the influence of ozone maximum height becomes dominant. The above results show that for research purposes, especially in the Arctic, at low Sun, the real ozone as well as temperature profiles should be utilized. For all cases, the differences obtained for the UV index are rather small and are within the range of recommended UVI forecast quality. This indicates that for UV index forecasting purposes, the long-term, seasonal average ozone, and temperature profiles for a given area may be used.

Discrepancies observed by using different sets of ozone cross section measurements for the reference case (U.S. Standard Atmosphere) was of the order of 3%.

The shape of the ozone profile is of importance when deriving the total ozone column from global irradiance measurements. Uncertainties of up to 9% may be caused by using an inappropriate profile in the retrieval. This maximum difference in our case was observed for a solar zenith angle of 75°, which was the largest angle considered. The average errors are quite low, less than 1.5%. The choice of different ozone absorption cross-section data may cause differences in the retrieved total ozone column of 3%. The overall maximum uncertainty of total ozone retrieval, due to both the ozone/temperature profiles and the ozone cross section uncertainties, is 10%.

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References


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