# Influence of spectroscopic data quality on the modeling of downward solar UV radiation fluxes

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The downward solar fluxes have been modeled in the 280–370 nm spectral range on basis of different experimental data on $NO_2$ and ozone absorption cross sections. This spectral interval is of interest for the problem of total ozone retrieval from spectral measurements of the solar radiation incident on the Earth surface. Absorption by atmospheric gases; molecular and aerosol scattering and absorption; and cloudiness have been taken into account in the calculations. It is shown that the spectral fluxes, calculated with a spectral resolution of 1 nm on the basis of three most popular ozone cross section data sets, differ by 8% and more; the total ozone, retrieved from the solar photometer measurements, can differ by 2%. The difference between fluxes calculated from different data on $NO_2$ absorption cross section is 0.3%.

## Introduction

Measurements of spectral fluxes of solar radiation of the 300–370 nm spectral range, incoming to the Earth's surface, are used to calculate the total ozone in the atmosphere, aerosol optical depth, and other optically active components influencing the Earth climate. To solve the inverse problem of total gas content retrieval, an accurate accounting for molecular absorption parameters is required. At present, a great amount of experimental data on ozone absorption cross sections is available, obtained by different investigators in a sufficiently wide temperature range at different spectral resolution.

According to Ref. 1, the use of ozone absorption cross sections, determined in the GOME experiment[2] and obtained by Bass and Paur,[3] as well as Daumont, Malicet, and Brion[4–6] can significantly influence the ozone retrieval due to data discrepancy. The ozone values, retrieved from satellite radiation measurements with the use of these cross sections, differ by almost 12 DU for the total ozone and almost by 100% for ozone in individual atmospheric layers. Differences in the transmission functions, calculated with the Bass,[3] Daumont,[4] and Molina[8] ozone absorption cross sections, were estimated in Ref. 7 and equaled almost to 10%.

A net of solar photometers measure the incoming solar radiation at IAO SB RAS. The photometers' UV spectral filters allow determination of total ozone in the atmosphere. In this work, we consider the influence of discrepancy in spectral data arrays of ozone and $NO_2$ absorption cross sections on the modeling of downward solar fluxes and the accuracy of total atmospheric ozone retrieval from measurements of solar radiation with the SP6 photometer.

## Modeling of solar UV fluxes

At present, the stationary equation of solar radiation transfer in the scattering and absorbing atmosphere is solved by the method of discrete ordinates DISORT [Ref. 10] allowing correct accounting for multiple radiation scattering at a high calculation rate. Input data for the calculation are the height profiles of optical depth of the gas and aerosol absorption, the albedo of single aerosol scattering, coefficients of molecular (Rayleigh) scattering and absorption, scattering and absorption by clouds, the aerosol and cloudiness scattering phase functions, and the underlying surface albedo.

The optical depth of the atmospheric gas absorption in the UV range is determined from experimental data on absorption cross sections, obtained at varying temperatures and pressures in laboratory conditions. To obtain the absorption value under arbitrary atmospheric conditions, interpolation polynomials are used, describing temperature dependence of absorption cross sections.[11] The main absorbing gases in the 280–370 nm spectral range are $O_3$ and $NO_2$, while atmospheric $SO_2$, BrO, $HNO_2$, OClO, and formaldehydes contribute less.

The values of ozone absorption cross sections, determined experimentally,[3,4–6,8,12,13] are often used in atmospheric calculations. In Ref. 14, it has been recommended to use data from Refs. 3–6.

To model radiation fluxes, we used three data sets from Refs. 3, 4, and 8, because they were obtained with a high spectral resolution and for a wide temperature range. The absolute and relative difference in ozone absorption cross sections at a temperature of 298 K is shown in Fig. 1.

The relative difference in ozone absorption cross sections has been determined with respect to the Bass data,[3] since they are included in the HITRAN-2004 database[15] and quite often used in calculations of atmospheric transfer of solar radiation.

The absolute and relative differences in $NO_2$ absorption cross sections in Refs. 16–18 are shown in Fig. 2. The difference in the 300–350 nm range attains 20%.

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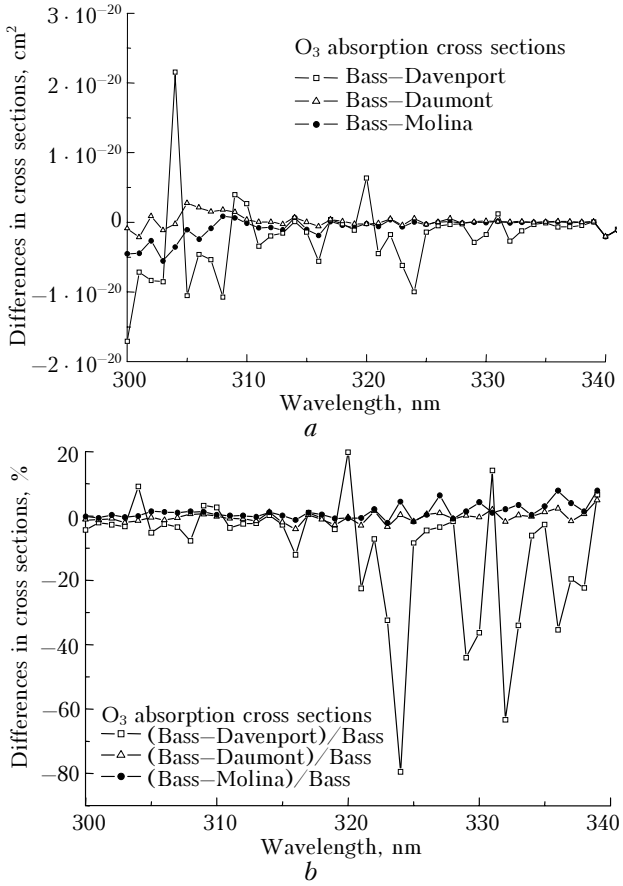


**Fig. 1.** Absolute (*a*) and relative (*b*) differences in ozone absorption cross sections at a temperature of 298 K.

The flux modeling was carried out by AFGL [Ref. 19] for midlatitude summer conditions. The aerosol optical depth was defined by the Angström equation at $\alpha = 1.1$ and $\beta = 0.2$; it varied from 1.4 to 1.32 for 300–400 nm wavelengths. The aerosol scattering phase function was calculated by the Henyey–Greenstein equation[20] with a mean absorption cosine of 0.7. The total ozone was 300 DU. Concentrations of other atmospheric gases were taken according to the AFGL [Ref. 19] meteorological model. In the calculations, ozone[3,4,8] and $NO_2$ [Refs. 16–18] absorption cross sections, as well as Rayleigh and aerosol scattering and absorption were taken into account. The calculations were performed with a spectral resolution of 1 nm and the solar zenith angle (SZA) equal to 30°. The results of comparison of downward solar fluxes at the Earth level, calculated with different ozone absorption cross sections, are shown in Fig. 3.

When comparing the fluxes with Molina[8]–Bass[3] and Daumont[4]–Bass[3] cross sections, the relative difference was determined with respect to the fluxes, calculated with Bass[3] cross sections, while the comparison for the fluxes with Daumont[4] and Molina[8] cross sections was determined with respect to the fluxes calculated with Daumont[4] ones. The relative difference in the calculated with Molina[8] and Bass[3] data is 8% and higher; and for Daumont[4] and Bass[3] data it is not higher than 2%.

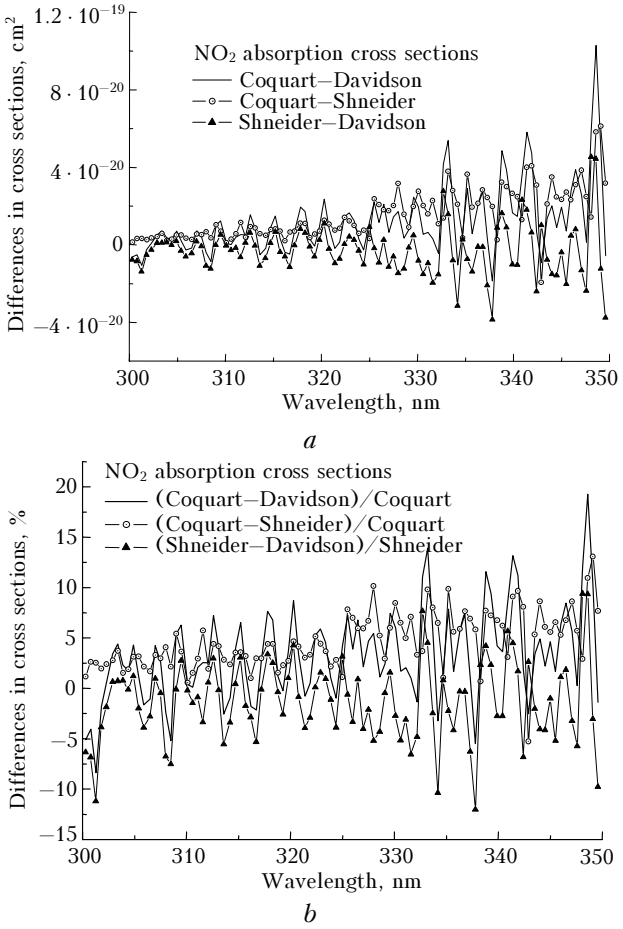


**Fig. 2.** Absolute (*a*) and relative (*b*) differences in $NO_2$ absorption cross sections at a temperature of 298 K.

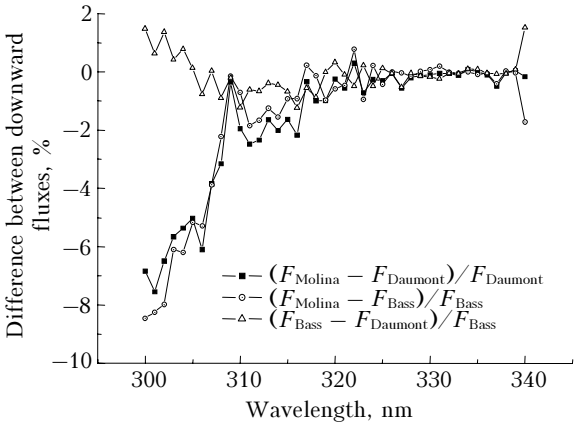


**Fig. 3.** Relative difference between downward solar fluxes at the Earth level, calculated with the Molina,[8] Bass,[3] and Daumont[4] ozone absorption cross sections. SZA = 30°.

The comparison of downward fluxes calculated with $NO_2$ absorption cross sections according to Coquart,[16] Davidson,[17] and Shneider[18] data is shown in Fig. 4. The relative difference between fluxes in the 280–370 nm range does not exceed 0.3%. The difference in data on $NO_2$ absorption cross sections less influences calculations of fluxes as compared with those in ozone data, since the concentration of

$NO_2$ in the atmosphere is by an order of magnitude less then of $O_3$. Differences in $NO_2$ absorption cross sections do not noticeably influence the results of ozone retrieval, while they play an essential part in problems of $NO_2$ determination.

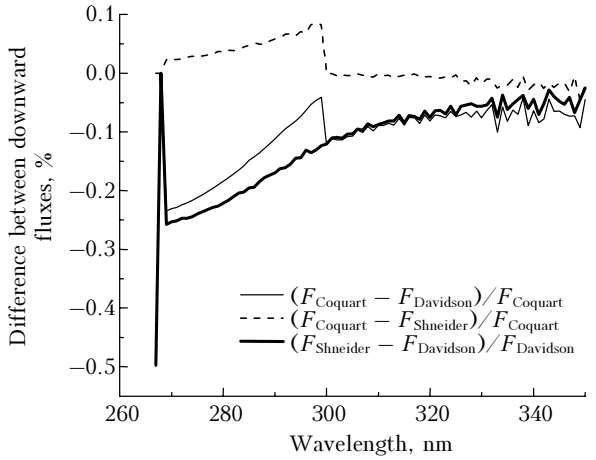


**Fig. 4.** Relative difference between downward fluxes at the Earth level calculated with $NO_2$ absorption cross sections according to Coquart,[16] Davidson,[17] and Shneider[18] data. SZA = 30°.

The comparison results are shown in Figs. 3 and 4 for SZA = 30°. Absolute values of solar radiation downward fluxes at SZA = 30 and 75° under cloudy and cloudless conditions are shown in Fig. 5.

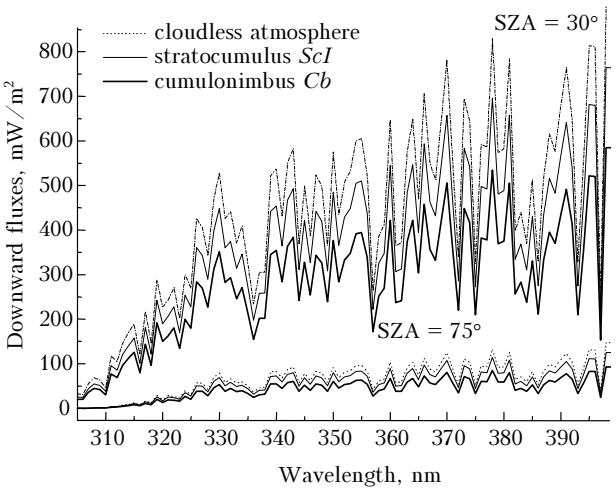


**Fig. 5.** Downward solar fluxes at the Earth level at different SZA values for cloudless atmosphere and in the presence of cumulonimbus *Cb* and stratocumulus *ScI* clouds.[21,22] Absorption by $O_3$ [Ref. 3] and $NO_2$ [Ref. 16], Rayleigh absorption and scattering and multiple scattering by aerosol and clouds are taken into account.

We considered two types of clouds,[21] i.e., *Cb* with relatively high optical depth ($\tau = 10$), located at a low air layer of 1.8–2 km, and *ScI* with low optical depth ($\tau = 2.81$), located in the upper troposphere at an altitude of 12.4–13 km. Optical properties of liquid droplet clouds (attenuation factor, albedo of single scattering $\omega$, and mean scattering cosine) were defined according to the model from Ref. 22. The scattering phase function was calculated by the Henyey–Greenstein equation.[20] Clouds significantly attenuate the UV radiation coming to the Earth's surface. The considered types of clouds *ScI* and *Cb* attenuated the downward fluxes by 16 and 34%, respectively, as compared with cloudless atmosphere.

An increase in the atmosphere optical depth due to clouds (or an increase in SZA) results in radiation attenuation; in this case, relative influence of differences in cross sections on calculations of downward fluxes increases. To solve the problem of total ozone content (TOC) retrieval in the atmosphere from the incoming UV radiation measurements, the measurement data for fluxes in cloudless atmosphere at large SZA are the most suitable.

## Influence of ozone absorption cross section data on retrieval of total ozone content in the atmosphere

The total ozone content (TOC) can be retrieved based on measurements of AEROSIBNET SP6 and SP8 photometers[9] at different SZA. The TOC is the function of the ratio of signals $F_{308\,nm}$ and $F_{324\,nm}$, measured by the SP6 photometer in two UV channels with filter centers at wavelengths of 308 and 324 nm with accounting for the calibration constant $C$:

$$\mathrm{TOC} \sim Cf\left(\frac{F_{324\,nm}}{F_{308\,nm}}\right).$$

One of the effective ways to solve the inverse problem of the TOC retrieval is tabulation of ratios of downward fluxes at two wavelengths, calculated for a large set of zenith angles and TOC values.[23] The use of close wavelengths allows neglecting the influence of incorrect definition of aerosol parameters and Rayleigh absorption in the modeling. The ratio of photometer signals measured with accounting for the calibration constant $C$ is compared with the modeled ratio and the TOC is determined. Errors in definition of input modeling parameters can result in noticeable errors in the TOC retrieval.[24]

We performed the modeling for to show how differences in data on ozone absorption cross sections influence the accuracy of the TOC retrieval. The fluxes were calculated by the method of discrete ordinates with spherical correction of the atmosphere SDISORT.[25] The aerosol optical depth was defined by the Angström equation at $\alpha = 1.3$ and $\beta = 0.2$. We used the annual average temperature and pressure profiles. An initial TOC value was set equal to 350 DU, which is close to the average annual value at the measurement site. TOC values, obtained in solving the inverse problem with ozone absorption cross sections, measured by Molina,[8] Bass,[3] and Daumont,[4] at different SZA values, are compared in the Table below.

**Table. TOC, retrieved with the use of Molina,[8] Bass,[3] and Daumont[4] ozone cross sections**

| SZA, deg | TOC(1/cos(SZA)) | | | Relative difference in TOC, % | |
|---|---|---|---|---|---|
| | Bass | Molina | Daumont | Bass–Molina | Bass–Daumont |
| 75 | 1.3523 | 1.2556 | 1.3327 | 7.1538 | 1.4485 |
| 70 | 1.0233 | 1.0045 | 1.0297 | 1.8374 | –0.62161 |
| 60 | 0.7 | 0.68774 | 0.70337 | 1.7516 | –0.4818 |
| 50 | 0.5445 | 0.53497 | 0.54633 | 1.75 | –0.33566 |
| 40 | 0.45689 | 0.44884 | 0.45825 | 1.7631 | –0.29648 |
| 30 | 0.40415 | 0.39695 | 0.40524 | 1.7792 | –0.26992 |
| 20 | 0.37246 | 0.36584 | 0.37342 | 1.7784 | –0.25698 |

It is evident that the relative difference in TOC increases with the rise of SZA, attaining 7 and 14% when comparing Bass and Molina, as well as Bass and Daumont data.

## Conclusion

Popular Molina,[8] Bass,[3] and Daumont[4] ozone absorption cross sections differ more than by 4% within the 300–370 nm spectral range. This results in almost 8% difference in calculated downward solar fluxes near the Earth's surface at SZA = 30° with a spectral resolution of 1 nm. The relative difference between the fluxes increases as the zenith angle increases.

The use of Coquart,[16] Davidson,[17] and Shneider[18] data on $NO_2$ absorption cross sections in the 300–370 nm spectral range does not essentially influence the calculations of the incoming solar radiation; differences in fluxes do not exceed 0.3%.

TOC values, retrieved with the ozone absorption cross sections by Molina[8] and Daumont,[4] differ from those with Bass[3] cross sections by 1.8 and 0.62%, respectively, at SZA < 70°.

The performed modeling has shown that Daumont[4] and Bass[3] data on ozone absorption cross sections are most suitable for calculating the solar radiation transfer in the 280–370 nm range. This agrees with the results of Refs. 1 and 14.

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