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PHOTODETACHMENT RATES FOR O^- AND O_2^- IN THE D LAYER OF THE IONOSPHERE AS FUNCTION OF SOLAR ZENITH ANGLE AND SOLAR ACTIVITY

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Abstract. We present the results of calculation of photodetachment rates for negative ions in the D layer of the ionosphere, using recent photodetachment cross-section measurements. The calculations have been made for the standard atmosphere by means of the TUV (Terrestrial UltraViolet) code. We have obtained dependences of the photodetachment rates on altitude and solar zenith angle. The nonlinear nature of these dependences causes similar variations in the role of the photodetachement processes with altitude and solar zenith angle as compared to other processes in the middle atmosphere and the lower ionosphere, especially under terminator conditions. Calculations with solar spectrum for 2011–2020 for the summer/winter solstice and the spring/autumn equinox have shown no quantitative difference between the photodetachement rates for ions in the D layer of the ionosphere.

Keywords: ionosphere, D layer, photodetachment.

INTRODUCTION

Geophysicists worldwide agree that the D layer of the ionosphere is underexplored to date despite being studied for decades. There is a plenty of reasons for this situation. They are analyzed and discussed in detail, for example, in [Danilov and Vlasov, 1973; Mitra, 1977; Whitten and Poppoff, 1977; McEwan 1975; Brassier and Solomon, 1987; Kozlov, 2021; Kozlov, 2022; Bekker, 2022].

One of the main reasons is the lack of knowledge about reaction rate constants for many photochemical reactions, including the rate of photodetachment $\rho\left(x^-\right)$ of electrons from negative ions. Available articles use the same quantities of $\rho\left(x^-\right)$ [s^{-1}] [Mitra, 1977]:

$$\rho\left(O_2^-\right)\approx 0.33,\ \rho\left(O^-\right)\approx 1.4,\ \rho\left(O_3^-\right)\approx 0.04,$$

$$\rho\left(NO_2^-\right)\approx 10^{-2\pm1},\ \rho\left(CO_3^-\right)\approx 1.5\cdot 10^{-3}.$$

The literature pays almost no attention to determining (theoretical or experimental) the photodetachment rate. No references are made to the well-known works [Hasted, 1965; Massey, 1979; Smirnov, 1978; Smirnov, 1983], where the photodetachment from negative ions is considered as a physical process, though using obsolete data. There is usually no information about the dependence of $\rho\left(x^-\right)$ on the solar zenith angle, altitude H, and solar activity, hence the need for knowing these dependencies is evident. This can lead to inaccuracies in simulating the D-region since negative ions at H<90 km play a fairly prominent role.

In this paper, we attempt to eliminate the above shortcomings for the primary negative ions O^- and O_2^-. Unfortunately, we cannot make such calculations for complex cluster negative ions CO_2^-, NO_2^-, O_2^- because of the absence of information on these ions, in particular reliable photodetachment cross-sections.

INITIAL DATA

The usual formula for calculating $\rho\left(x^-\right)$ is:

$$\rho\left(X^-\right)=\int_{\lambda_n}^{\lambda}\varepsilon(\lambda, H)\sigma(\lambda)d\lambda,$$

where λ_n is the threshold solar emission wavelength at which the photodetachment from O_2^- and O^- occurs; $\sigma(\lambda)$ is the photodetachment cross-section; $\varepsilon(\lambda, H)$ is the solar flux at a given altitude H at a wavelength λ. The value $\lambda_n\left(O^-\right)$ is well-known and is equal to 855 nm (1.45 eV). There is a spread in values for O_2^-; however, according to [Hasted, 1965] we can take $\lambda\left(O_2^-\right)\approx 2480$ nm (0.5 eV).

Figure 1 shows the $\sigma(\lambda)$ values we use [Janalizadeh, Pasco, 2020]. Estimating $\varepsilon(\lambda, H)$ requires specifying the solar spectrum for $\lambda\leq 800$ nm and the model of the atmosphere through which emission propagates.

We use two solar spectra (Figure 2). The first spectrum was taken from World Meteorological Organization [WMO, 1985]. It is climatic (mean). The second spectrum is available in [SSI, 2020] with solar activity variation in 11-year cycle (the curve in Figure 2 corresponds to 2018). We calculate radiation transfer for the standard atmosphere by the pseudo-spherical four-flux

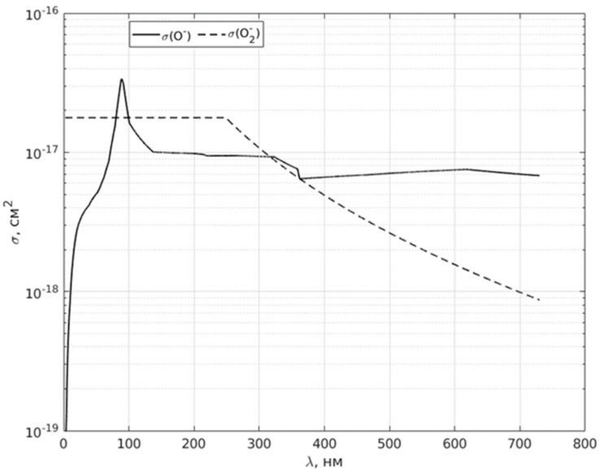

Figure 1. Photodetachment cross-sections for O_2^- and O^- according to Janalizadeh and Pasko [2023].

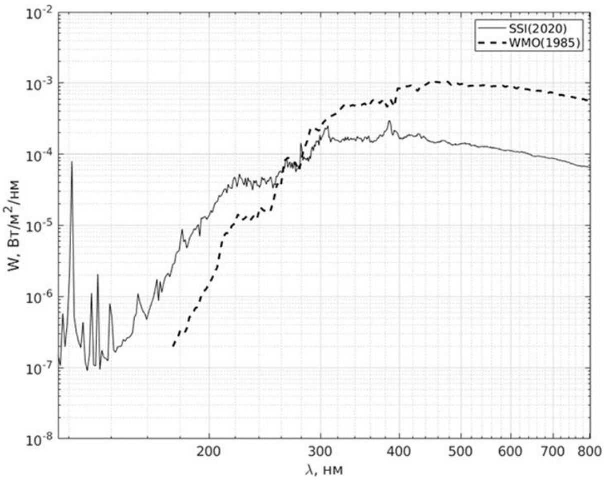

Figure 2. Solar spectra used in photodetachment calculation

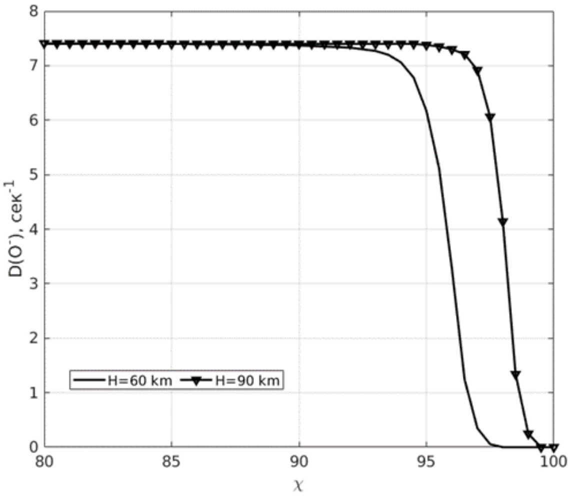

Figure 3. Photodetachment rate for negative ion O– at altitudes of 60 and 80 km for the spectrum (NOAA, 2020).

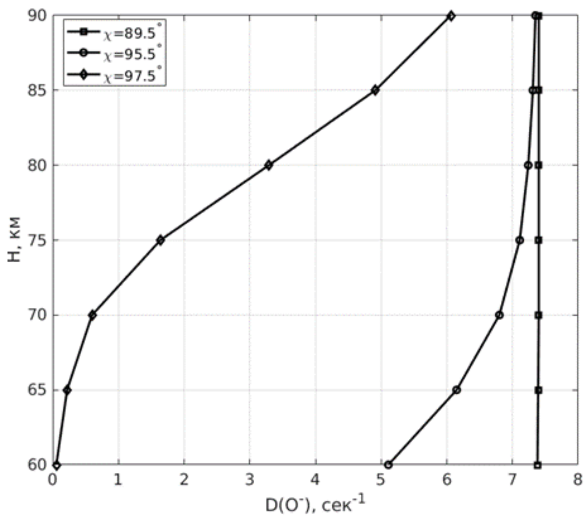

Figure 4. Altitude dependence of O^- photodetachment rate at 89.5°, 95.5°, and 97.5° zenith angles for the spectrum [NOAA, 2020]

method of discrete ordinates [Stamnes et al, 1988]. Albedo is 0.1 and aerosol fraction is 0.25 according to [Elterman, 1968].

Final fluxes $\varepsilon(\lambda, H)$ are evaluated by the TUV code (v. 5.3.2) [Madronich, 1993, 1998] for H=60–90 km with a 5 km step. The solar zenith angle χ varies within 60–100°. This yields maximally unified results suitable for numerical simulation in any set of coordinates, season, and UT.

RESULTS AND DISCUSSION

The photodetachment rates $\rho(O^-)$ and $\rho(O_2^-)$ depending on H and χ for the modern spectrum [NOAA, 2020] are listed in Tables 1 and 2. Figures 3 and 4 plot rates of photodetachment from O^- for the spectrum [NOAA, 2020] as function of the solar zenith angle for two altitudes bounding the D layer and as function of altitude (see Figure 4) for three zenith angles. The dependences for $\rho(O_2^-)$ and for the spectrum [WMO, 1985] are qualitatively the same, differing only in magnitude. Analysis of the results allows the following conclusions:

a) At $\chi \le 80$, photodetachment rates are constant at any H under any level of solar activity (Figure 3). The values $\rho(O^-) = 1.29\ s^{-1}$, $\rho(O_2^-) = 0.477\ s^{-1}$ calculated for the spectrum [WMO, 1985] are quite close to the commonly used values (see Introduction). However, for the current spectrum [NOAA, 2020], which we consider to be more reliable, $\rho(O^-) = 7.41\ s^{-1}$, $\rho(O_2^-) = 2.44\ s^{-1}$, which far exceed the previous values.

b) The χ values at which it is necessary to take into account the decrease in $\rho(X^{-1})$ depends only on H. This effect starts at H=60 km and gradually propagates to higher altitudes as χ increases.

c) Additional calculations to check the dependence $\rho(X^-)$ on solar activity in the 11-year cycle and on season, made using the database of spectra [NOAA, 2020] for 2010–2020, have shown that year- to-year and seasonal variabilities of $\rho(O^-)$ and $\rho(O_2^-)$ under

Table 1

Photodetachment rate for O^- [s^{-1}]

χ, degrees	60 km	65 km	70 km	75 km	80 km	85 km	90 km
<80	2.44	2.44	2,44	2.44	2.44	2.44	2.44
88.5	2.41	2.43	2.44	2.44	2.44	2.44	2.44
89.5	2.41	2.43	2.44	2.44	2.44	2.44	2.44
90.5	2.39	2.42	2.43	2.44	2.44	2.44	2.44
91.5	2.37	2.40	2.43	2.43	2.44	2.44	2.44
92.5	2.34	2.37	2.40	2.43	2.44	2.44	2.44
93.5	2.28	2.33	2.36	2.40	2.42	2.43	2.44
94.5	2.12	2.24	2.30	2.34	2.38	2.41	2.43
95.5	1.55	1.91	2.13	2.24	2.30	2.34	2.38
96.5	0.28	0.80	1.38	1.80	2.06	2.21	2.28
97.5	0.009	0.036	0.12	0.40	0.94	1.48	1.88
98.5	0.00	0.00	0.00	0.005	0.03	0.095	0.31
99.5	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 2

Photodetachment rate for O_2^- [s^{-1}]

χ, degrees	60 km	65 km	70 km	75 km	80 km	85 km	90 km
<80	7.4	7.4	7.4	7.4	7.4	7.4	7.4
88.5	7.38	7.4	7.4	7.4	7.4	7.4	7.4
89.5	7.38	7.39	7.4	7.4	7.4	7.4	7.4
90.5	7.36	7.39	7.4	7.4	7.4	7.4	7.4
91.5	7.34	7.37	7.39	7.4	7.4	7.4	7.4
92.5	7.3	7.34	7.37	7.39	7.4	7.4	7.4
93.5	7.2	7.29	7.33	7.37	7.39	7.4	7.4
94.5	6.78	7.11	7.24	7.31	7.35	7.38	7.4
95.5	5.11	6.15	6.80	7.11	7.24	7.31	7.35
96.5	1.24	2.89	4.62	5.82	6.60	7.03	7.21
97.5	0.06	0.22	0.60	1.64	3.29	4.91	6.06
98.5	0.00	0.00	0.00	0.03	0.20	0.52	1.34
99.5	0.00	0.00	0.00	0.00	0.00	0.00	0.00

sunlit conditions do not exceed 1 %.

d) At sunrise and sunset, considering the dependences $\rho\left(O^-\right)$ and $\rho\left(O_2^-\right)$ on χ becomes essential for studying the quiet and disturbed D layer.

CONCLUSIONS

The negative ions O_2^- and O^- are primary in the complex chemical chain of their transformation into cluster negative ions. The use of the $\rho\left(O^-\right)$ and $\rho\left(O_2^-\right)$ coefficients, calculated in this work for current solar spectra [NOAA, 2020] when simulating the D layer, will lead to a decrease in the negative ion density and to an increase in the rate of the electron density n_e variation, which will primarily have an effect on propagation of LF and VLF waves. This should be taken into account when interpreting radio monitoring data. Thus, the new coefficients of photodetachment of electrons from O_2^- and O^- will improve the accuracy of D-layer models.

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