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An Exact Method for Determination of the 6300 Å Oxygen Line Intensity by the Use of $N(h)$ Ionospheric Profiles

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1. Introduction

It has been established that, at undisturbed geomagnetic conditions during the night, the general mechanism leading to the red oxygen line emission is the dissociative recombination of O_2^+ ions and, to a significantly lower degree, that of NO^+ ions [1-4]. In 1959 a semi-empirical formula had been deduced [5], relating the 6300 Å intensity to some measured ionospheric parameters — f_0F, $h'F$. This formula reflects in general the behaviour of the intensity of the red emission during the night, but we do not have sufficient coincidence between the values observed and those theoretically calculated. A theoretically established relation on the basis of a new theory of F-region was given in 1972 [6], which reflects far better the relationship between the red emission and the radio-measured parameters of the F-region. In addition to the parameters used by Barbier, we include the thickness of the layer Z, the density scale H and the parameter of the exponent p, at an exponential decrease of the electron density in the overmaximal part of the F-region. An attempt at simultaneous measurement of the 6300 Å emission and of the parameters of the F-region was made [7], in which we obtained very good agreement between the theoretical and experimental data.

The following formula has been used for the theoretical calculation of the intensity of the 6300 Å emission by dissociative recombination:

$$I_{6300}=0.076\int_{150}^{500}\frac{\varepsilon . K_1[O_2] . R . N_e . dh}{1+\frac{K_2[N_2]}{A}} \tag{1}$$

where ε is the effective number of the atoms $O(^1D)$ produced at each action of recombination. If we take into account the cascade transition $^1S-^1D$, we could assume that $\varepsilon\approx 1$. K_1 is the rate constant of the exchange reaction:

$$\text{(2)} \qquad O^+ + O_2 \rightarrow O_2^+ + O \; K_1$$

A is Einstein's coefficient; $A=0.0091\ s^{-1}$, K_2 is the quenching rate constant of the de-excitative reaction:

$$\text{(3)} \qquad O(^1D) + N_2 \rightarrow N_2 + O(^3P) \; K_2$$

R is the ratio O^+/N_e, which changes with the height.

The concentrations of O_2 and N_2 are taken from a model, and $N_e(h)$ is measured directly by ionograms or by rocket measurements.

This formula has, however, an essential defect; it requires the knowledge of the ratio R at every height and this can be obtained by rocket experiments only. Consequently, it can hardly be used for practical calculations.

In the present paper a new method of calculating I_{6300} is given, in which only data from ionosonds and atmospheric models are used.

2. Method

Let us present formula (1) in the following form:

$$\text{(4)} \qquad I_{6300} = 0.076 \int_{150}^{500} \frac{\varepsilon \cdot K_1[O^+] \cdot [O_2] \cdot dh}{1 + \frac{K_2[N_2]}{A}}.$$

In the above formula the concentration of $O^+(h)$ can be obtained in the following way:

For the range of 150 – 500 km, in which the red line is emitted, we can write the following equation:

$$\text{(5)} \qquad [O^+] + [NO^+] + [O_2^+] = N_e,$$

expressing the quasi-neutrality of the plasma in this region.

At these night conditions the equilibrium concentration of O_2^+ is given by:

$$\text{(6)} \qquad [O_2^+] \approx \frac{K_1[O^+][O_2] + K_6[N_2^+][O_2]}{\alpha_D(O_2^+) \cdot N_e}$$

where $\alpha_D(O_2^+)$ is the rate constant of the dissociative recombination for O_2^+ ions, and K_6 is the rate constant of the exchange reaction between N_2^+ and O_2. It was shown [8] that $K_1 \approx 4 \times 10^{-11}\ cm^3\ s^{-1}$ and $K_6 \approx 2 \times 10^{-18}\ cm^3 s^{-1}$. Taking also into account that $[O^+] \gg [N_2^+]$, we could neglect the second term in the numerator of (6), and therefore equation (6) takes the form:

$$\text{(7)} \qquad [O_2^+] \approx \frac{K_1 \cdot [O^+] \cdot [O_2]}{\alpha_D(O_2^+) N_e}.$$

The equilibrium concentration of NO^+ is

$$\text{(8)} \qquad [NO^+] \approx \frac{K_3[O^+][N_2] + K_4[N_2^+][O] + K_5[N^+][O_2]}{\alpha_D(NO^+) N_e}$$

where K_3, K_4 and K_5 are the rate constants of the corresponding exchange reactions, and $\alpha_D(NO^+)$ is the velocity of the dissociative recombination of NO^+ ions.

In the range of 180—300 km, where about 90 per cent of the integral value of 6300 Å line is emitted [9], we have:

$$[N_2] > [O_2] \approx [O], \tag{9}$$

$$[O^+] \gg [N_2^+] > [N^+]. \tag{10}$$

We assume that $K_3 \approx 10^{-10} \div 10^{-12}\ \mathrm{cm^3\,s^{-1}}$; K_4 $2.5 \times 10^{-10}\ \mathrm{cm^3 s^{-1}}$ and $K_5 \approx 2$ $2 \times 10^{-10}\ \mathrm{cm^3 s^{-1}}$ [10]. At these values of the rate constants and according to (9) and (10) we make the following evaluations:

$$K_4[O][N_2^+] \quad K_5[N^+][O_2] \ll K_3[N_2][O^+] \tag{11}$$

and the expression (8) is reduced to

$$[NO^+] \approx \frac{K_3[N_2][O^+]}{\alpha_D(NO^+) . N_e}. \tag{12}$$

The substitution of (7) and (12) in (5) leads to

$$[O^+] = \frac{\alpha_D(NO^+) . \alpha_D(O_2^+) . N_e^2}{\alpha_D(NO^+) . \alpha_D(O_2^+) . N_e + \alpha_D(O_2^+) K_3[N_2] + \alpha_D(NO^+) K_1[O_2]}. \tag{13}$$

In this manner formula (13) expresses the behaviour of $[O^+]$ by the behaviour of the concentration of the most frequently and most easily measured ionospheric parameter — the electron density N_e. We know that the variations in the concentration of the neutral compounds and the rate constants depend mainly on the temperature and consequently, under undisturbed geomagnetic and solar conditions, they can be determined from the known models.

The substitution of the expression (13) in (4) leads to the following formula for λ 6300 Å intensity:

$$I_{6300} = 0{,}076 . A . \varepsilon \int_{150}^{500} \frac{K_1 \alpha_D(NO^+) . \alpha_D(O_2^+)[O_2] N_e^2 . dh}{(\alpha_D(NO^+) . \alpha_D(O_2^+) N_e + \alpha_D(O_2^+) . K_3[N_2] + \alpha_D(NO^+) K_1[O_2])(A + K_2[N_2])} \tag{14}$$

The expression (14) reflects the behaviour of the λ 6300 Å line intensity as a function only of the electron density at a given atmospheric model. This formula can easily be reduced to a convenient form for numerical integration.

3. Experimental Verification of the Method

As an example of the application of the method to the experimental observations, the initial data are shown in Fig. 1. The intensity of the line 6300 Å is determined in the Observatory at Stara Zagora, Bulgaria ($\varphi = 42°27$ N, $\Lambda = 23°41$ E), by a zenith tilting-filter photometer. The accuracy of the registration of λ 6300 is about 5 per cent. Two moments were selected on October 29, 1973, at 21^{h}00^m and 22^{h}00^m LT. The observations of the ionosphere were performed at the ionospheric station near Sofia

($\varphi = 42°41$ N, $\Lambda = 23°21$ E). The distance between the two points of observation is about 200 km. The calculation of the $N_e(h)$ profiles is done by a laminar method [11]. Fig. 1 shows also the three atmospheric models used at exospheric temperatures of 500°K, 800°K and 1000°K, according to Jacchia's revised model [12].

Since from the $N_e(h)$ profiles the distribution of electron density is obtained up to the maximum of the F-layer, in the over-maximal part of the same layer the parabolic distribution to Z_m-level is used, the exponential distribution being used above it. Here Z_m is the semi-thickness of the F-layer.

The following rate constants were used for the calculations: $\alpha_D(O_2^+) = 2.2 \times 10^{-7}$ cm^3 s^{-1}, $\alpha_D(NO^+) = 4.5 \times 10^{-7}$ cm^3 s^{-1}, $A = 0.0091$ s^{-1}, $K_3 = 21 \times 0^{-12}$ cm^3 s^{-1} and two different values for K_1:

$$K_1' = 4 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1} \text{ [13] and}$$

$$K_1'' = 2 \times 10^{-1} \text{ cm}^3 \text{ s}^{-1} \text{ [14].}$$

With these constants and according to the data from Fig. 1, the following results were obtained, as presented in Table 1 and in Fig. 1:

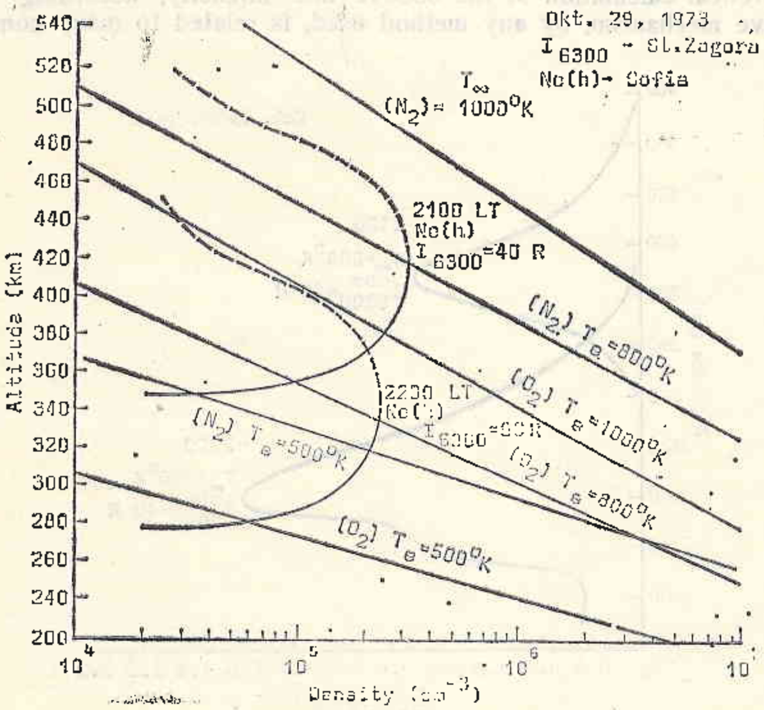

Fig. 1

It is obvious from the Table that at $T_\infty = 500°$K the model gives extremely low values and is, in general, unfit in this case for the very low values of the atmospheric density. In the two other cases, however, the coincidence is very good. One of them is at $T_\infty = 800°$ K and $K_1 = 4 \times 10^{-11}$ cm^{3}s^{-1},

Table 1

T	21h00m LT 6300=40 R		22h00m LT 6300=90 R	
°K	$K_1'=4\times10^{-11}$	$K_1''=2\times10^{-11}$	$K_1'=4\times10^{-11}$	$K_1''=2\times10^{-11}$
500°K	0.5 R	0.2 R	1.1 R	0.6 R
800°K	$\boxed{38\ \mathrm{R}}$	21 R	$\boxed{89\ \mathrm{R}}$	44 R
1000°K	79 R	$\boxed{43\ \mathrm{R}}$	181 R	$\boxed{96\ \mathrm{R}}$

and the other one at $T_\infty = 1000°K$ and $K_1 = 2\times10^{-11} cm^3s^{-1}$. Besides, it has been found that the most essential contribution in the intensity of the 6300 Å emission is that of the terms $\alpha_D(NO^+) . \alpha_D(O_2^+)N_e$ and, at lower heights, the term $(A+K_1N_2)$.

4. Estimation of the Precision of the Method

The theoretical calculation of the 6300 Å line intensity, according to the dissociative mechanism, by any method used, is related to many conditions.

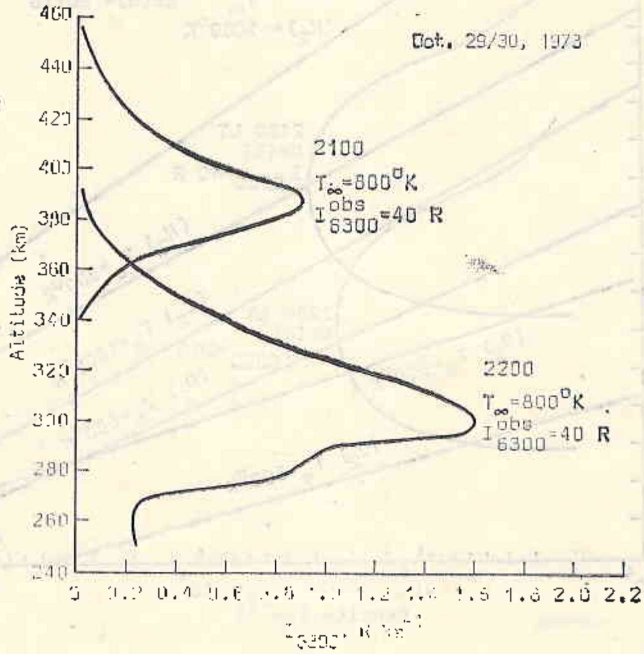

Fig. 2

In the first place this refers to the choice of the rate constants of the reactions. It follows from the calculations in the example given above that a change by a factor of 2 only in the value of the very important constant K_1 of reaction (2) leads to an equal change in the red line intensity. The analysis of formula (14) and the example given in Fig. 1, Table 1 and Fig. 2 show that the choice of this constant is of essential importance. Besides that it is accepted that the values of $\alpha_D(O_2^+)$ and $\alpha_D(NO^+)$ are known with greater confidence, while on the other hand the inaccuracy in their measurement plays a small part in the calculation of the 6300 Å line intensity.

Another source of errors is the unknown exact temperature dependences of the rate constants of the dissociative and exchange reactions which, in combination with the lack of sufficient knowledge on the temperature distribution at the given moment, could also lead to uncertain results.

Notice should also be taken of the fact that the problem of exact calculation of the products from the dissociative recombination is reduced to the choice of the most reliable atmospheric model at a given case. On the other hand, as in the case of rate constants of the temperature dependence reactions, this is connected with the knowledge of the value T_∞.

In the case presented in Fig. 1, Table 1 and Fig. 2, the calculations are in best agreement with the experimental data at $T_\infty=800°K$ and $K_1=4\times10^{-11}$ cm^{3}s^{-1}, and also at $T_\infty=1000°K$ and $K_1=2\times10^{-11}$ cm^{3}s^{-1}. Of course, it is hardly possible to overcome this difficulty only by the use of photometric and ground-based ionospheric data.

It may be recommended that the choice of the atmospheric model for the calculation of the 6300 Å line intensity, at a given night, be done according to some of the lowest values of the red oxygen line, for which we must be sure that there exist no other generative mechanisms besides the dissociative recombination. By the model thus chosen, in which we have the best coincidence, we make the calculations for all other points during the night.

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Точный метод определения интенсивности красной кислородной линии 6300 Å посредством использования ионосферных профилей

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(Резюме)

Описан точный метод определения интенсивности красной кислородной линии 6300 Å. Этот метод позволяет определить λ_{6300} как функцию только электронной концентрации, которая легко получается по данным ионосферной станции. Полученные теоретические результаты с достаточной точностью совпадают с экспериментальными данными, полученными в Обсерватории по изучению свечения ночного неба в г. Стара-Загора. Рассмотрены возможные источники ошибок и сделаны предложения для будущих измерений.