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COMPONENTS EXCITED STATE IN THE UPPER ATMOSPHERE

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Abstract. The role of metastable ionospheric components of oxygen and nitrogen atoms and molecules is considered for F2-region ionospheric processes. The main attention was paid to investigation of the processes with oscillatory excited state of the nitrogen molecules N_2 (Nu). The density calculation of this component was made for the ten oscillating levels (Nu=1…10), using the time-depended diffuse equation. Bolzman distribution was not taken into account. The role of diffusive and photochemical processes in N_2 (Nu) dynamics was discussed. The calculations were made on the basis of ionosphere-plasmasphere model along a magnetic field tube with possibility of calculating time-altitude distributions of main ionospheric ions, including ions excited states.

It is well known that the excited species play a very important role in determining the structure and properties of the upper atmosphere. Models of the metastable species have been developed in a number of papers [1], [7], [8]. Using these models helps solve in details the problems of the ion and neutral composition, the thermal balance and the results of this model can be compared with observations of optical emissions as well as measurements of the minor constituents. The purpose of the paper is to analyze the connection between metastable and ionic constituents.

In this paper we shall describe our calculations results of the following metastable species: $O(^1D)$, $O(^1S)$, $O^+(^2D)$,, $O^+(^2P)$, $N(^2D)$, $N(^2P)$ and vibrationally excited states of $N_2(N_2^{(v)})$.

The model of ionosphere-plasmosphere system is reported in [2]. The vibrational relaxation equation was included in the total system of model equations for altitudes of 120-400 km.

The continuity equation for each level of vibrationally excited molecular nitrogen $N_2^{(v)}$ is

$$\frac{\partial n_v}{\partial t} = -\frac{\partial (n_v \cdot V_{zv})}{\partial z} - \alpha_v \cdot n_v + Q_v , \tag{1}$$

where n_v – the number density of molecular nitrogen in level v(1-10); Q_v, L_v - production and loss rate of n_v [Table 1], z is the vertical coordinate and will be assumed that the magnetic field line is vertical.

V_{zv} diffusion velocity is

$$V_{zv} = -D\left(\frac{1}{n_v}\cdot\frac{\partial n_v}{\partial z} + \frac{1}{T_n}\cdot\frac{\partial T_n}{\partial z} + \frac{1}{H}\right), \tag{2}$$

$$D = \frac{5\cdot 10^{18}}{M}\left(\frac{T_n}{300}\right)^{3/4}, cm^2 \cdot c^{-1}, \tag{3}$$

$[M] = [O] + [O_2] + [N_2]$.

Using (1), (2), (3)

$$\frac{\partial n_v}{\partial t} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial n_v}{\partial z} + \beta \cdot n_v\right) - \alpha_v \cdot n_v + Q_v , \tag{4}$$

where $\lambda = D$, $\beta = D\left(\frac{1}{T_n}\frac{\partial T_n}{\partial z} + \frac{1}{H}\right)$.

Table 1

№	Reaction	
1.	$O(^1D)+N_2 \xrightarrow{k_1} N_2^{(\nu)}+O(^3P)$	$k_1 = 5*10^{-11}$
2.	$N+NO \xrightarrow{k_2} N_2^{(\nu)}+O(^3P)$	$k_2 = 2.2*10^{-11}$
3.	$N_2^{(\nu)}+O(^3P) \xrightarrow{k_3} O(^3P)+N_2^{(\nu_1)}$	$k_3 = 1.2*10^{-13}\exp(-23/T^{1/3})$
4.	$N_2^{(\nu_1)}+N_2^{(\nu_2)} \xleftrightarrow{k_4} N_2^{(\nu_1-1)}+N_2^{(\nu_2+1)}$	$k_4 = 3*10^{-12}$
5.	$N_2^{(\nu_1)}+e \xleftrightarrow{k_5} N_2^{(\nu_2)}+e$	$k_5 = \exp(P_1+P_2+P_3/T_e+P_4/T_e)$
6.	$O^+ +N_2^{(\nu)} \xrightarrow{k_6} NO^+ +N$	$\log k_6 = a_\nu+b_\nu T_n+c_\nu T_n^2+d_\nu-16$

Where $P_1, P_2, P_3, P_4, a_\nu, b_\nu, c_\nu, d_\nu$ - coefficients [2].
The source and loss terms for (1) are given by [7].

$$Q_1^{(\nu)} = \nu \cdot k_1 \cdot \left[O\left(^1D\right)\right]\cdot\left[n_{\nu-1}\right],$$

$$\alpha_1^{(\nu)} = (\nu+1)\cdot k_1\left[O\left(^1D\right)\right],$$

$$Q_2^{(\nu)} = k_2 \cdot [N]\cdot[NO]\cdot W_N,$$

$$\alpha_2^{(\nu)} = 0,$$

$$Q_3^{(\nu)} = k_3 \cdot \left[O(^3P)\right]\cdot\left(\nu\cdot n_{\nu-1} + (\nu+1)\cdot n_{\nu+1} e^{\frac{\theta}{T_n}}\right),$$

$$\alpha_3^{(\nu)} = k_3 \cdot \left[O(^3P)\right]\cdot\left(\nu\cdot e^{\frac{\theta}{T}} + (\nu+1)\right)$$

$$Q_4^{(\nu)} = k4\left(\sum_{\nu_2=0}\nu_1(\nu_2+1)n_{\nu_1-1}n_{\nu_2+1} + \sum_{\nu_2}\nu_2\cdot(\nu_1+1)\cdot n_{\nu_1+1}\cdot n_{\nu_2-1}\right), \qquad (5)$$

$$\alpha_4^{(\nu)} = k_4\cdot\left(\sum_{\nu_2=0}^{8}\nu_1\cdot(\nu_2+1) + \sum_{\nu_2=1}^{8}\nu_2\cdot(\nu_1+1)\right)\cdot\left[n_{\nu_2}\right],$$

$$Q_5^{(\nu)} = \sum_{\nu_1\neq\nu_2} A_{\nu_1\nu_2}\cdot\left[n_{\nu_2}\right]\cdot\left[N_e\right],$$

$$\alpha_5^{(\nu)} = \sum_{\nu_1\neq\nu_2} A_{\nu_2\nu_1}\cdot\left[N_e\right],$$

$$A_{\nu_1\nu_2} = \exp\left(P_1 + \frac{P_2}{T_e} + \frac{P_3}{T_e^2} + \frac{P_4}{T_e^3}\right),\quad A_{\nu_2\nu_1} = A_{\nu_1\nu_2}\cdot l^{\frac{\theta}{T_e}},$$

$$Q_6^{(\nu)} = 0,$$

$$\alpha_6 = k_6\cdot(\nu+1)\cdot\left[O^+\right],$$

$$\log k_6 = a_\nu + b_\nu\cdot T_n + c_\nu\cdot T_n^2 + d_\nu\cdot T_n^3 - 16,$$

$$n_\nu = n_0\exp\left(-\frac{\nu E_{10}}{T_n}\right)$$

where n_i – number density nitrogen in vibrational level ν, $W_n = 0{,}25$.

D binary diffusion coefficients for molecular nitrogen assumed to be independent of vibrational excitation; y acceleration of gravity; Q_i - production rate of n_i; L_i - logs rate of n_i. Production and loss terms are contained in Table 1 for the i-th level. We will assume that molecular nitrogen can be represented with a harmonic oscillator. In this paper we do not assume a Boltzmann distributions vibrationally excited Nitrogen $\left(N_2^{(\nu)}\right)$.

Equation (1) was solved numerically with the lower boundary at 120 km and the upper boundary at 400 km. Time and height integration step lengths were 300 sec and 4 km respectively. The lower boundary condition is $n_\nu = \frac{Q_\nu}{\alpha_\nu}$.

For the boundary condition at 400 km we can set the diffusion flux term in equation (1) to zero. The initial condition

$$n(z) = n(z_0)\exp\left(-\int_{z_0}^{z}\frac{dz}{H}\right) \tag{6}$$

and to integrate Equation (1) over several days the solution was independent of the initial conditions.

The $O(^1D)$ is electronically excited in metastable state oxygen atom that decays primarily by emission of 630.0 nm radiation. The $O(^1D)$ atoms produced in reactions

$O_2 + h\nu_{(1350-1750)} \rightarrow O(^3P) + O(^1D)$

$$O_2^+ + e \rightarrow O(^1D) + O \text{ and } OH^+ + e \rightarrow \begin{matrix} O+H \\ O(^1D)+H \end{matrix} \tag{7}$$

undergo radiative decay with a life time 147s and the resulting red-line emission can be observed from the ground.

The so-called green line produced by the atomic oxygen transition $O(^1D{-}^1S)$ and resulting in photon emission at $557{,}7^0 A$. The based for the sources of $O(^1S)$ to be electron impact of O, dissociative recombination of O_2^+ and photodissociation of O_2

$$\begin{aligned} e + O &\rightarrow O(^1S) + e \\ O_2^+ + e &\rightarrow O(^1S) + O(^3P) \\ O_2 + h\nu &\rightarrow O(^1S) + O \end{aligned} \tag{8}$$

The $O(^1D)$ atom is very effectively quenched by molecular nitrogen and may be realized in two ways:

$$O(^1D) + N_2 \rightarrow \begin{matrix} N_2^* + O \\ N + NO \end{matrix} \tag{9}$$

Additional energy is necessary for the dissociation of N_2 via reaction (9). This energy 1.29 ev may be in photodissociation of molecular oxygen for the $\lambda \le 121.8nm$. The reaction (9) plays a very important role in the D-region [3]. Fig. presents the altitude profiles $\left[O(^1D)\right]$ and $\left[O(^1S)\right]$ obtained in our calculation. This results in a satisfactory agreement with the experiments data (Fig. 1).

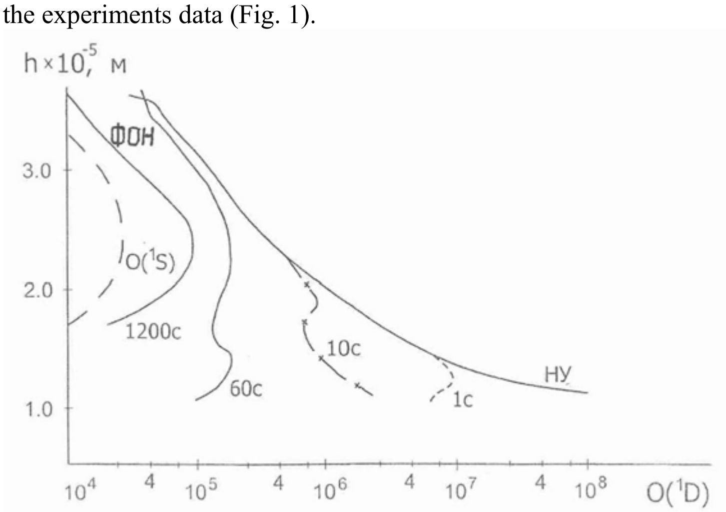

Fig.1. Height-time behavior of electronically excited oxygen $O(^1D), O(^1S)$.

The $N(^2D)$ atom reacts very effectively with molecular oxygen . The reaction

$$O_2 + N(^2D) \rightarrow NO + O \tag{10}$$

is the main process of NO production in the lower E-region and the upper part D-region [5], [6]. It is important to note that atomic nitrogen excited in ^2D metastable state for which the radiative lifetime is $\approx 10^5 s$ has very weak intensities of the emission at $5200^0 A$.

The photodissociation

$$N_2 + h\nu \rightarrow N(^4S) + N(^2D) \quad (11)$$

is an important source in the 800-to 1000 ^0A spectral range [4], [5], [8]. Fig. presents the altitude profiles concentrations of $N(^2D)$ (Fig. 2).

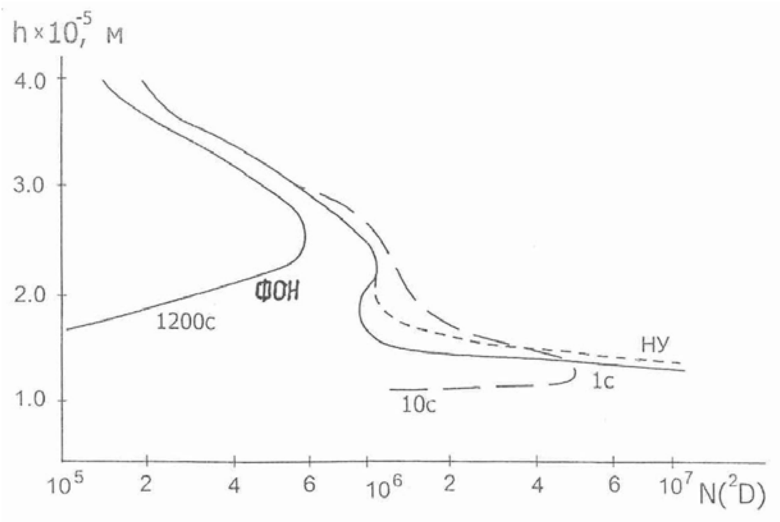

Fig.2. Height-time behavior of electronically excited atomic nitrogen $N(^2D)$.

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