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MATHEMATICAL MODELING OF METASTABLE COMPONENTS IN THE IONOSPHERE OF THE EARTH

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A formulation (different from those adopted earlier) of the problem of numerical modeling of the altitude-time behavior of vibrationally excited molecular nitrogen has been presented. A conservative and absolutely stable difference scheme for the continuity equation with allowance for convective transfer has been proposed. The results of numerical calculations of the altitude-time behavior of different ionospheric parameters obtained on a mathematical model of ionospheric-plasmaspheric interactions have been given. The important role of vibrationally excited molecular nitrogen for such conditions has been noted. The times of establishment of the disturbed to background values of the concentrations of the excited components and the electrons and their temperatures have been determined.

Introduction. The role of metastable components in both gas lasers [1, 2] and ionospheric processes [3] is known fairly well at present. Their energy may decrease due to de-excitation, producing visible emission lines from whose measurements one determines the concentration of particles. It may also become the kinetic or vibrational energy of their molecules and may pass into the environment in endothermic reactions. The processes of deactivation of such components in chemical reactions occur with much higher rates than those for neutral components. Mathematical modeling is currently one basic method of investigation of different processes natural experiments for which are very laborious. Numerical experiment based on a physicomathematical model has a significant advantage, which lies in the possibility of calculating situations repeatedly and obtaining numerical results.

In this work, we present a physicomathematical model for calculation of ionospheric parameters along the geomagnetic tube of force for disturbed conditions such as the temperatures of the O^+ and $H^+(T_i)$ ions and electrons (T_e), the components of the neutral-wind velocities (v_{nx} and v_{ny}), the concentrations of the excited components $O(^1D)$, $O(^1S)$, $N(^4S)$, $N(^2D)$, $N(^2P)$, NO, $N_2^{(v)}$, N_2, $O_2(^1\Delta_g)$, and O_2, the positive ions $O^+(^4S)$, $O^+(^2D)$, $O^+(^2P)$, H^+, O_2^+, N_2^+, and $NO^+(n_i)$, and electrons (n_e).

It is well known that, at the present time, there is no evidence for the existence of the uniqueness and stability of a numerical solution for a coupled and nonlinear system of differential equations describing these parameters. The computational experiment conducted will make it possible to consider the problem on the stability of a numerical solution in input parameters. In the previous investigation [4], the problem of stability has been considered as the influence of a change in the input parameters from the background values toward decreasing values on the solution reaching these values. In this work, we investigate the case of a change in the input parameters toward their increase relative to the background values and the solution reaching subsequently the background values. By doing so, we may judge the stability of the model constructed from the input data.

Description of the Model (Basic Equations). The altitude-time distribution of the ith sort of charged components along the line of force is described by the equation

$$\frac{\partial n_i}{\partial t} + B\frac{\partial (n_i v_i)}{\partial s} = F_i - \alpha_i n_i\,, \tag{1}$$

where n_i is the concentration, v_i is the velocity along the line of force whose length varies within $-s_0 < s < s_0$, s_0 is the lower boundary of the line of force at an altitude of 125 km, and F_i and α_i are the terms of formation and loss of ions in photochemical reactions (see Tables 1 and 2). For the velocity of ions we write the following expression:

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TABLE 1. Reaction of Neutral Components

Reaction	Rate constant	Reaction	Rate constant
$O(^3P) + O(^3P) + N_2 \to \begin{array}{l} O_2(^1\Delta_g) + N_2, p_1 = 0.9 \\ O_2(b^1\Sigma^1_g) + N_2, p_2 = 0.1 \end{array}$	$9.9 \cdot 10^{-34} \exp(470/T)$	$O_2 + e^* \to O_2(^3\Sigma^+_u) + e$	$\langle \sigma_5 v_5 \rangle$
		$O_2(A^3\Sigma^+_u) + N_2 \to O_2 + N_2$	$4 \cdot 10^{-11}$
		$O_2(^1\Delta_g) + O(^3P) \to O_2 + O$	$13 \cdot 10^{-14}$
$O(^1D) + N_2 \to O(^3P) + N_2$	$5.0 \cdot 10^{-11}$	$O_2(a^1\Delta_g) \to O_2 + \hbar\nu$	$3.3 \cdot 10^{-3}$ sec^{-1}
$O(^1D) + O_2 \to O(^3P) + O_2$	$5.0 \cdot 10^{-11}$	$O_2(b^1\Sigma^+_g) \to O_2 + \hbar\nu$	0.1 sec^{-1}
$O(^1D) \to O(^3P) + \hbar\nu$	0.0068 sec^{-1}	$N_2 + e^* \to N(^4S) + N(^2D) + e$	$\langle \sigma_6 v_6 \rangle$
$O + e^* \to O(^1D) + e$	$\langle \sigma_1 v_1 \rangle$	$N_2 + h\nu \to N(^2D) + N(^4S)$	J, sec^{-1}
$N(^2D) + O_2 \to \begin{array}{l} O(^3P) + NO, p_1 = 0.2 \\ O(^1D) + NO, p_2 = 0.8 \end{array}$	$6 \cdot 10^{-12}$	$N(^2D) + O \to N + O$	$7 \cdot 10^{-13}$
		$N(^2D) + O_2 \to NO + O$	$6 \cdot 10^{-12}$
		$N(^2D) + e \to N + e$	$(3.6—6.5) \cdot 10^{-10} (T_e/300)^{1/2}$
$O_2 + \hbar\nu \to O(^1D) + O(^3P)$	J, sec^{-1}	$N(^2P) + O \to N(^2D) + O$	$1 \cdot 10^{-11}$
$O(^1S) + N_2 \to O(^3P) + N_2$	$<5.0 \cdot 10^{-17}$	$N(^2P) + O_2 \to NO + O$	$2 \cdot 10^{-12}$
$O(^1S) + O_2 \to O(^3P) + O_2$	$5.0 \cdot 10^{-17}$	$N(^2P) \to N(^2D) + \hbar\nu$	$3 \cdot 10^{-2}$
$O(^1S) \to O(^1D) + \hbar\nu$	1.06 ± 0.32	$N_2(A^3\Sigma^+_u) + O(^3P) \to N_2 + O(^1S)$	$4 \cdot 10^{-11}$
$O(^1S) \to O(^3P) + \hbar\nu$	0.045 ± 0.014	$N_2(A^3\Sigma^+_u) + O_2 \to N_2(x^1\Sigma^+_g) + O_2$	10^{-13}
$O + e^* \to O(^1S) + e$	$\langle \sigma_2 v_2 \rangle$	$N_2(A^3\Sigma^+_u) + NO \to N_2 + NO(^2\Sigma^+)$	$7 \cdot 10^{-11}$
$O_2(^1\Delta_g) + O_2 \to 2O_2$	$2 \cdot 10^{-18}$	$N_2(A^3\Sigma^+_u) + N \to N(^2D) + N_2$	$5 \cdot 10^{-11}$
$O_2(^1\Delta_g) + O_2(^1\Delta_g) \to O_2(b^1\Sigma_u) + O_2$	$3 \cdot 10^{-14}$	$N_2(A^3\Sigma^+_u) \to N_2 + \hbar\nu$	0.5 sec^{-1}
$O_2 + e^* \to O_2(^1\Delta_g) + e$	$\langle \sigma_3 v_3 \rangle$	$N_2 + e^* \to N_2(^3\Sigma^+_u) + e$	$\langle \sigma v \rangle$
$O_2 + e^* \to O_2(b^1\Sigma^+_g) + e$	$\langle \sigma_4 v_4 \rangle$	$N(^4S) + NO \to N_2 + O$	$2.5 \cdot 10^{-11} \exp(—167/T)$
$O_2(b^1\Sigma^1_g) + N_2 \to O_2 + N_2$	$15 \cdot 10^{-15}$	$N(^4S) + O_2 \to NO + O$	$2.4 \cdot 10^{-11} \exp(—3970/T)$
$O_2(b^1\Sigma^1_g) + O(^3P) \to O_2 + O$	$1 \cdot 10^{-15}$		

$$v_i = \frac{1}{R_i + S_{ij}} \left[m_i g \sin I + S_{ij} v_j + R_i v_{nx} \cos I - \frac{k}{n_e} \frac{\partial (n_e T_e)}{\partial s} - \frac{k}{n_j} \frac{\partial (n_j T_j)}{\partial s} \right]. \qquad (2)$$

Here v_{nx} is the meridian component of the neutral-wind velocity.

The altitude-time distribution for the electronic and ionic (O^+ and H^+) temperatures along the line of force is written as

$$\frac{3}{2} k N_e \frac{\partial T_e}{\partial t} = B \frac{\partial}{\partial s} \left(\frac{\lambda_e}{B} \frac{\partial T_e}{\partial s} \right) + \sum_i \frac{3 m_e N_e}{m_i} \nu_{ei} k (T_i - T_e) + Q_e - L_{e,n}\,, \qquad (3)$$

$$\frac{3}{2} k n_i \frac{\partial T_i}{\partial t} = B \frac{\partial}{\partial s} \left(\frac{\lambda_i}{B} \frac{\partial T_i}{\partial s} \right) + 3 n_i \nu_{ie} k (T_e - T_i) + \sum_n \frac{3 m_i n_i}{m_i + m_n} \nu_{in} k (T_n - T_i) + Q_i - L_i\,, \qquad (4)$$

where Q_e, Q_i, $L_{e,n}$, and L_i are the rates of heating and cooling of thermal electrons and ions due to the ion-molecular reactions. The meridian component of the neutral-wind velocity v_{nx}, which appears in Eq. (2), is found by solution of the system

TABLE 2. Reaction of Positive Ions

Reaction	Rate constant	Reaction	Rate constant
$O^+(^4S) + H \rightarrow O + H^+$	$4 \cdot 10^{-10}(T_{ef}/300)^{0.5}$	$O_2^+ + e \rightarrow \begin{matrix} O(^1D) + O, p_1 = 0.9 \\ O(^1S) + O, p_2 = 0.1 \end{matrix}$	$2 \cdot 10^{-17}(300/T_e)^{1/2}$
$O^+(^4S) + O_2 \rightarrow O_2^+ + O$	$2.8 \cdot 10^{-11}$		
$O^+(^4S) + N_2 \rightarrow NO^+ + N$	$2 \cdot 10^{-12}$		
$H^+ + O \rightarrow O^+(^4S) + H$	$3.5 \cdot 10^{-10}(T_{ef}/300)^{0.5}$	$O_2^+N(^4S) \rightarrow NO^+ + O$	$1.8 \cdot 10^{-10}$
$O^+(^2D) + O \rightarrow O^+(^4S) + O$	$<0.3 \cdot 10^{-11}$	$O_2^+ + NO \rightarrow NO^+ + O_2$	$4.4 \cdot 10^{-10}$
$O^+(^2D) + N_2 \rightarrow O^+(^4S) + N_2$	$(7 \pm 3) \cdot 10^{-11}$	$O_2^+(a^4\pi_u) + N_2 \rightarrow N_2^+ + O_2$	$4 \cdot 10^{-10}$
$O^+(^2P) + O \rightarrow O^+(^4S) + O$	$(5.2 \pm 2.5) \cdot 10^{-11}$	$O_2^+(a^4\pi_u) + O_2 \rightarrow O_2^+(x^2\pi_g) + O_2$	$5.1 \cdot 10^{-10}$
$O^+(^2P) \rightarrow O^+(^4S) + \hbar\nu$	0.047 sec^{-1}	$N_2^+ + O_2 \rightarrow O_2^+ + N_2$	$5 \cdot 10^{-11}$
$N_2^+ + O \rightarrow O^+(^4S) + N_2$	$1 \pm 0.3 \cdot 10^{-12}(300/T)^{0.23}$	$N_2^+ + O \rightarrow NO^+ + N(^2D)$	$(1.4 \pm 0.3) \cdot 10^{-10}(300/T)^{0.44}$
$O^+(^2P) \rightarrow O^+(^2D) + \hbar\nu$	0.05 sec^{-1}	$N_2^+ + e \rightarrow N(^2D) + N$	$2.5 \cdot 10^{-7}(300/T_e)^{1/2}$
$O^+(^2D) + N_2 \rightarrow N_2^+ + O$	$(7 \pm 3) \cdot 10^{-11}$	$NO^+ + e \rightarrow \begin{matrix} N(^2D) + O, p_1 = 0.8 \\ N(^4S) + O, p_2 = 0.2 \end{matrix}$	$4.3 \cdot 10^{-7}(300/T_e)$
$O^+(^2D) + O_2 \rightarrow O_2^+ + O$	$7 \cdot 10^{-10}$		
$O^+(^2P) + N_2 \rightarrow N_2^+ + O$	$(4.8 \pm 1.4) \cdot 10^{-10}$		
$O^+(^2P) + O_2 \rightarrow O_2^+ + O$	$4.8 \cdot 10^{-10}$		

$$\frac{\partial v_{ny}}{\partial t} = \frac{\xi}{\sin^2 I} \frac{\partial^2 v_{ny}}{\partial s^2} - \frac{1}{\rho_n} \sum_{j=1}^{5} n_j R_j v_{ny} - 2\Omega \sin \varphi v_{ny} - \frac{1}{\rho_n} \frac{\partial P_n}{\partial y}, \tag{5}$$

$$\frac{\partial v_{nx}}{\partial t} = \frac{\xi}{\sin^2 I} \frac{\partial^2 v_{nx}}{\partial s^2} - \frac{1}{\rho_n} \sum_{j=1}^{5} n_j R_j (v_{nx} - v_j \cos I) + 2\Omega \sin \varphi v_{ny} - \frac{1}{\rho_n} \frac{\partial P_n}{\partial x}. \tag{6}$$

Here v_{ny} is the zonal component of the neutral-wind velocity, $\xi = 3.34 \cdot 10^{-6} T_n 0.17/\rho_n$ is the kinematic viscosity of the neutral gas, and $\partial P_n/\partial x$ and $\partial P_n/\partial y$ are the meridian and zonal components of the pressure gradient of the neutral gas (they are calculated according to [5]).

The altitude-time distribution of small components under the assumption that, in the region of altitudes and middle latitudes in question, the line of force coincides with a local vertical may be represented as

$$\frac{\partial n_k}{\partial t} + \frac{\partial (n_k v_k)}{\partial s} = F_k - \alpha_k n_k. \tag{7}$$

Here F_k and α_k are the terms of formation and loss of particles in photochemical reactions (see Tables 1 and 2) and v_k is the molecular velocity of motion of the kth component, which is determined from an equation of the form

$$g + \frac{1}{\rho_k} \frac{\partial P_k}{\partial s} + \frac{1}{\rho_k} \sum_{j \neq k} n_j R_{jk} (v_k - v_j) = 0, \tag{8}$$

where $\rho_k = m_k n_k$ is the partial density of the gas, $P_k = k n_k T_n$ is the partial pressure of the gas, and $R_{jk} = S_{jk} \rho_k$. Then the expression for the molecular velocity of motion of the kth component is written as

$$v_k = \frac{\sum\limits_{j\neq k} S_{jk} n_j v_j}{\sum\limits_{j\neq k} S_{jk} n_j} - D_k \left(\frac{1}{n_k} \frac{\partial n_k}{\partial s} + \frac{1}{H_k} + \frac{1}{T_\text{n}} \frac{\partial T_\text{n}}{\partial s} \right), \tag{9}$$

where $D_k = \dfrac{kT_\text{n}}{m_k \sum\limits_{j\neq k} s_{jk} n_j}$ is the coefficient of molecular diffusion and $H_k = \dfrac{kT_\text{n}}{m_k g}$ is the altitude scale of the kth component.

For molecules obeying the Maxwell distribution we have

$$S_{jk} = \frac{16}{3} \frac{\mu_{jk}}{m_k} \sigma_{jk}^2 \left(\frac{\pi T_\text{n}}{2\mu_{jk}} \right)^{1/2},$$

where $\sigma_{jk} = \dfrac{\sigma_k \sigma_j}{\sigma_k + \sigma_j}$, $\mu_{jk} = \dfrac{m_k m_j}{m_k + m_j}$, and σ_k and σ_j are the average diameters of colliding molecules.

Substituting the expression for v_k from (9) into (7), we obtain a parabolic-type partial differential equation

$$\frac{\partial n_k}{\partial t} = \frac{\partial}{\partial s} \left(D_k \frac{\partial n_k}{\partial s} + \beta_k n_k \right) - \alpha_k n_k + F_k, \tag{10}$$

where

$$\beta_k = D_k \left(\frac{1}{H_k} + \frac{1}{T_\text{n}} \frac{\partial T_\text{n}}{\partial s} \right) - \frac{\sum\limits_{j\neq k} s_{jk} n_j v_j}{\sum\limits_{j\neq k} s_{jk} n_j}.$$

In the continuity equation for heavy ions

$$\frac{\partial n_i}{\partial t} = F_i - \alpha_i n_i \tag{11}$$

we disregard transfer.

Continuity Equation for Vibrationally Excited Molecular Nitrogen. An equation describing the altitude-time distribution of vibrationally excited nitrogen $N_2^{(v)}$ for each vibrational level (v) will be represented in the form

$$\frac{\partial n_v}{\partial t} = -\frac{\partial}{\partial z} (n_v v_{\text{n}z}) - \alpha_v n_v + F_v, \tag{12}$$

where n_v is the concentration of $N_2^{(v)}$ at the levels $v = 1, ..., 9$, $v_{\text{n}z}$ is the vertical component of the molecular-diffusion rate, and F_v and α_v are the terms allowing for the formation and loss of $N_2^{(v)}$ in photochemical reactions (Table 3). The molecular-diffusion rate is determined as

$$v_{\text{n}z} = -D \left(\frac{1}{n_v} \frac{\partial n_v}{\partial z} + \frac{1}{T_\text{n}} \frac{\partial T_\text{n}}{\partial z} + \frac{1}{H} \right), \tag{13}$$

where $H = \dfrac{kT_\text{n}}{mg}$ is the altitude scale of $N_2^{(v)}$, m is the mass of an N_2 molecule, and T_n is the temperature of the neutral gas;

TABLE 3. Table of Chemical Reactions of Vibrationally Excited N_2

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

Note. P_1, P_2, P_3, and P_4 are the coefficients and a_ν, b_ν, c_ν, and d_ν are the coefficients of [5].

$$D = \frac{5\cdot 10^{18}}{N}\left(\frac{T_n}{300}\right)^{3/4} \tag{14}$$

without allowance for the vibrational level of $N_2^{(\nu)}$.

After the substitution of (13) into (12), we obtain

$$\frac{\partial n_\nu}{\partial t} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial n_\nu}{\partial z} + \beta n_\nu\right) - \alpha_\nu n_\nu + F_\nu\,. \tag{15}$$

Here we have $\lambda = D$ and $\beta = D\left(\frac{1}{T_n}\frac{\partial T_n}{\partial z} + \frac{1}{H}\right)$.

The system of equations (15) is supplemented with the lower and upper boundary conditions. The lower boundary conditions are determined from the assumption of photochemical equilibrium, whereas the upper ones are determined from the condition of equality of the particle flux to zero.

The vibrational temperature of $N_2^{(\nu)}$ is calculated from the formula

$$T_\nu = \frac{\theta}{\ln\left(1 + \frac{\sum_{\nu=0}^{8} N_2^{(\nu)}}{\sum_{\nu=1}^{8} N_2^{(\nu)}}\right)}, \tag{16}$$

where $\theta = 3390$ K.

According to Table 3, the rates of formation and loss for $N_2^{(\nu)}$ will be written in the form

$$Q_1^{(\nu)} = \nu k_1\,[O\,(^1D)]\,n_{\nu-1}\,, \quad \alpha_1^{(\nu)} = (\nu + 1)\,k_1\,[O\,(^1D)]\,,$$

$$Q_2^{(\nu)} = k_2\,[N]\,[NO]\,W_{N_2}^{(\nu)}\,, \quad \alpha_2^{(\nu)} = 0\,,$$

$$Q_3^{(\nu)} = k_3\,[O\,(^3P)]\,(\nu n_{\nu-1} + (\nu + 1)\,n_{\nu+1}\exp(\theta/T_n))\,, \quad \alpha_3^{(\nu)} = k_3\,[O\,(^3P)]\,(\nu\exp(\theta/T_n) + (\nu + 1))\,,$$

$$Q_4^{(\nu)} = k_4\left(\sum_{\zeta=0}\nu\,(\zeta + 1)\,n_{\nu-1}n_{\zeta+1} + \sum_{\zeta=1}\zeta\,(\nu + 1)\,n_{\nu+1}n_{\zeta+1}\right), \quad \alpha_4^{(\nu)} = k_4\left[\sum_{\zeta=0}\nu\,(\zeta + 1) + \sum_{\zeta=1}\zeta\,(\nu + 1)\right]n_\zeta\,,$$

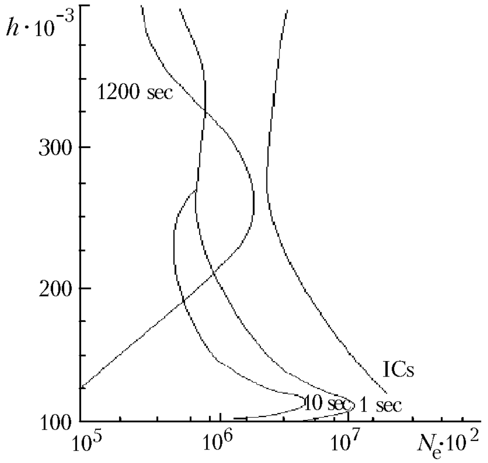

Fig. 1. Altitude-time behavior of N_e beginning from the initial disturbed conditions (ICs) to background values (t = 1200 sec).

$$Q_5^{(\nu)} = \sum_{\nu \neq \zeta} A_{\nu\zeta} n_\zeta N_e \,, \quad \alpha_5^{(\nu)} = \sum_{\nu = \zeta} A_{\nu\zeta} N_e \,,$$

where $A_{\nu\zeta} = \exp\,(P_1 + P_2/T_e + P_3/T_e^2 + P_4/T_e^3)$, $A_{\zeta\nu} = A_{\nu\zeta}\exp\,(\theta/T_e)$, and $W_{N_2}^{(\nu)}$ is the probability of formation of a vibrational level (in the work, we have i = 1–4 and $W_{N_2}^{(\nu)} = 0.25$), ($Q_6^{(\nu)} = 0$ and $\alpha_6^1 = k_6(\nu + 1)\ [O^+]$).

Method of Numerical Solution. The system of differential equations of second order (1–6), (10), and (15), which describes the altitude-time behavior of ionospheric-thermospheric parameters, is nonlinear and coupled. The only method of its solution is a numerical one. We have solved Eqs. (3) and (4) by the method of ordinary running, (5) and (6) by that of matrix running, and (10) and (15) by the flux variant of the running method [10, 11].

Input Data. In the work, we have presented the results of calculations along a tube of force with a base at the altitude h_0 = 125 km. The calculations were carried out for the high geomagnetic (k_p = 3) and solar ($F_{10.7}$ = 234) activity on January 22, 1979. The exospheric flux of UV solar radiation, the values of the absorption, photoionization, and elastic- and inelastic-collision cross sections, and the coefficients of thermal conductivity and friction were taken from [3]. The basic neutral components $[O(^3P)]$, $[N_2(x_1\Sigma_g^+)]$, $[O_2(x^3\Sigma_g^-)]$, [H], and [He] and their temperature T_n were calculated from the model of [5]. The reactions (see Table 1) involving "fast" electrons with an energy higher than 1 eV were allowed for; the rate coefficient of this reaction under the assumption of the Maxwell distribution of particles was calculated from the formula

$$k = \frac{1}{T_e^{3/2}} \sqrt{\frac{8}{m\pi}} \int_0^\infty \varepsilon\sigma\,(\varepsilon)\, \exp\,(-\,\varepsilon/T_e)\, d\varepsilon \,.$$

The excitation cross sections $\sigma(\varepsilon)$ were approximated according to [8].

Results of Numerical Calculations. In the work, we have presented the results of numerical calculations obtained with a time step of integration of τ = 0.01 sec for the time $0 < t \leq 1$ sec without allowance for transfer processes. Subsequently the calculations were carried out for τ = 0.1 sec with allowance for transfer in a diffusion approximation. In this connection, the decrease in $[N_e]$ at the initial time $t \leq 1$ sec (Fig. 1) is attributable only to photochemical processes, since the diffusion lifetime of particles is much longer than this time. The numerical experiment has shown that the ionospheric parameters, such as $N_2^{(\nu)}$, T_e, and N_e, are restored from the disturbed conditions to background values over a period of 20 min, on the average. The decrease in the concentration N_e below the background one is attributable to the influence of $[N_2^{(\nu)}]$ (the last reaction in Table 3). It is well known that, for the average solar activity F = 140, middle latitudes $\varphi = 45^o$, and equinox conditions, we have $[N_m F2] \approx (1\text{–}2) \cdot 10^6\ cm^{-3}$ at the altitude $h_m F \approx 250$ km. In Fig. 1, it is seen that $[N_e]$ at the altitude $h_m F2$ changes from an initial value of $2 \cdot 10^7$

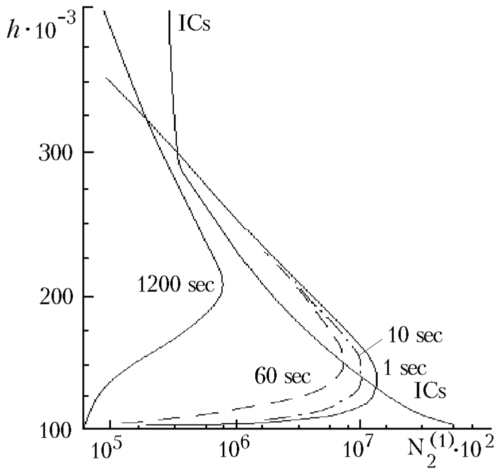

Fig. 2. Calculated altitude-time behavior of vibrationally excited $N_2^{(1)}$ for the first vibrational level.

cm^{-3} to $7 \cdot 10^5$ cm^{-3} in 50 sec, thus decreasing to $[N_e]$ values lower than the background N_mF2, passing over the background value; then it is restored to a background value of $2 \cdot 10^6$ cm^{-3} over the course of 20 min. We may write min $[N_e] \approx 0.5 N_m$F2 for the case considered. Further restoration of $[N_e]$ to $[N_m$F2$]$ takes several tens of minutes ($\approx$30 min). The reason is that the basic processes at the initial instant of time and with the selected initial conditions are chemical processes with a short lifetime of $\tau < 10$ sec (this determines the selection of the step of integration). At times longer than 1 min, the concentrations of different components substantially increase and diffusion processes begin to take effect.

In Fig. 2, it is seen that fairly high concentrations of $[N_2^{(1)}]$ relative to the background values (the excess is one to two orders of magnitude) are presented at the initial instants of time and to 20 min; at the same time, high values of T_e ($\cong 2 \cdot 10^3$ K) are preserved to times of the order of 1 min. It is precisely the factors noted above that cause N_e to decrease lower than the background value and lead to its further establishment.

The time in which $[O(^1D)]$ from the initial conditions reaches its background values is about 20 min. The basic sources are the excitation of $O(^3P)$ by superthermal electrons (above 130 km), the photodiscussion of molecular oxygen in the Schumann–Runge continuum (to 180 km), the dissociative recombination of O_2^+, and the reaction of interaction of $N(^2D)$ with O_2. The transition of atomic oxygen from the electron-excited state ^1D to the ground state ^3P yields a red line with wavelengths of 630 and 636.4 nm. The radioactive lifetime of $O(^1D)$ is 110 sec.

An analogous distribution is presented in Fig. 3 for $[O(^1S)]$; it is seen that the concentration decreases by two orders of magnitude over a period of the order of several seconds. The $O(^1S)$ atoms are formed mainly in collision of $O(^3P)$ with photoelectrons. The transition from the electron-excited state ^1S to the ^1D state is accompanied by the glow of a green line with a wavelength of 557.7 nm, whereas the transition from ^1S to the ground state ^3P is accompanied by the glow at a wavelength of 297.2 nm.

The transition from the ^2D state to ^4S is accompanied by radiation with a wavelength of 520.0 nm. In this connection, obtaining the altitude-time distribution of such an emission involves the construction of a photochemical scheme making it possible to correctly describe the altitude-time distribution of $[N(^2D)]$. We may assume at present that such a scheme has been developed in sufficient detail. It is noteworthy that the reaction of cooling of $N(^2D)$ on $O(^3P)$ may proceed by two mechanisms:

$$N(^2D) + O(^3P) \to N(^4S) + O(^1D) + 0.41\ \text{ýÂ}\,, \quad N(^2D) + O(^3P) \to N(^4S) + O(^3P) + 2.37\ \text{eV}\,.$$

The laboratory measurements of the coefficient of this reaction yield a value of $2 \cdot 10^{-12}$ $cm^3 \cdot sec^{-1}$. Aeronomic evaluations by the measurements using satellites yield a coefficient of this reaction within 10^{-14}–10^{-12} $cm^3 \cdot sec^{-1}$. The quenching of $N(^2D)$ on molecular oxygen leading to the formation of vibrationally excited NO_2 may manifest itself as the glow in the spectrum with wavelengths of 570–750 nm. We have the transition of NO_2 from the $^2\Sigma_u^+$ state to the ^2B_i state by the reaction

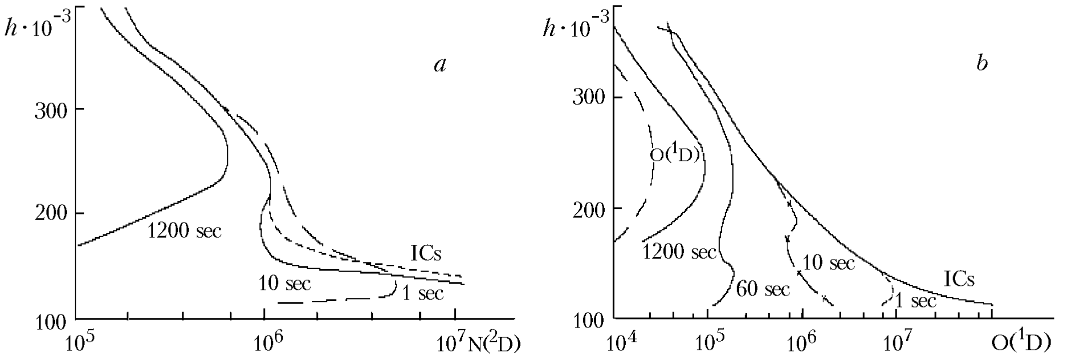

Fig. 3. Altitude-time behavior of electron-excited atomic nitrogen N(^{2}D) (a) and oxygen O(^{1}D) and O(^{1}S) (b).

$$N(^2D) + O_2 \rightarrow NO_2 \rightarrow NO_2 + \hbar\nu \, .$$

The forbidden transition of N(^{2}P) from the ^{2}P state to the ground state ^{4}S is accompanied by the glow with a wavelength of 346.6 nm. Also, there can be atomic-nitrogen lines in the ultraviolet spectrum: the triplet $^2P \rightarrow {}^2D$ and the quartet $^2P \rightarrow {}^3D$ with wavelengths of 149.3 and 174.4 nm respectively.

The glow of N(^{2}P) with a wavelength of 120 nm is observed in the atmosphere, too. This emission represents a triplet with wavelengths of 119.955, 120.022, and 120.071 nm. The N(^{2}P) sources are the reaction

$$N_2 + e \rightarrow N(^2P) + N(^4S) + 2\ \mathrm{eV}$$

and the dissociative recombination of N_2^+

$$N_2^+ + e \rightarrow N(^2P) + N \, .$$

We have the basic sinks in the reactions with O and O_2

$$N(^2P) + O \rightarrow N(^2D) + O \, , \quad N(^2P) + O_2 \rightarrow NO + O \, .$$

The concentration of the molecules $O_2(^1a\Delta_g)$ during the course of 30 min differs only slightly from the initial disturbed conditions. The transition of $O_2(^1a\Delta_g)$ from the $a^1\Sigma_g$ state to $x^3\Sigma_g$ yields infrared atmospheric bands that, just as the (0, 0) band at a wavelength of 1.27 nm, are strongly absorbed in the atmosphere. Also, there is a (0, 1) band experiencing lower absorption at a wavelength of 1.58 nm.

Of interest is the reaction of energy unification of $O_2(^1a\Delta_g)$, in which two molecules together radiate one quantum of light:

$$O_2\,(a^1\Delta_g) + O_2\,(a^1\Delta_g) \rightarrow O_4^+ \rightarrow 2O_2\,(x^3\Sigma_g) + \hbar\nu \, .$$

The emission corresponding to this reaction consists of bands at wavelengths of 363 nm (both molecules remain in the ground state with $\nu = 0$) and 764 nm (we have $\nu = 0$ for one molecule and $\nu = 1$ for the other).

Conclusions. We have presented the results of numerical calculations of the altitude-time distributions of the concentrations of excited components from the disturbed values to background ones. It has been shown that vibrationally excited molecular nitrogen substantially influences the recombination of the ionospheric plasma for such conditions. We have considered different chemical reactions leading to the formation and quenching of the excited components. The results of solution of the model problem proposed confirm the numerical stability of the constructed model as far as the input data are concerned. They may be used for interpretation of the existing experimental data on both the concentration and the intensity of their glow.

NOTATION

B, magnetic induction, T; D, diffusion coefficient, $m^2 \cdot sec^{-1}$; F, rate of formation of particles, $m^{-3} \cdot sec^{-1}$; g, free-fall acceleration, $m \cdot sec^{-2}$; H, altitude scale, m; h, altitude, m; $\hbar$, Planck constant, J·sec; h_mF2, altitude of the maximum of the F2 layer of the earth's ionosphere, m; I, magnetic inclination, deg; J, photodissociation coefficient; k, Boltzmann constant; k_p, index of geomagnetic activity; L, coefficient of cooling of the gas, $W \cdot sec^{-1}$; m, mass, kg; N, concentration of all the particles, m^{-3}; $N(^4S)$, nitrogen atom in the ground state ^4S; $N(^2D)$, excited nitrogen atom with electron level ^2D; $N(^2P)$, excited nitrogen atom with electron level ^2P; $N_2(A_3\Sigma_u^+)$, nitrogen molecule in the ground state $A^3\Sigma_u^+$; $N_2(x^1\Sigma_g^+)$, excited nitrogen molecule with an electron level $x^1\Sigma_g^+$; $N_2^{(v)}$, excited nitrogen molecule with a vibrational level ν; $NO(A^2\Sigma_u^+)$, excited nitric-oxide molecule with vibrational level $A^2\Sigma_u^+$; N_e, concentration of electrons, m^{-3}; N_mF2, concentration of the maximum of the F2 layer of the earth's ionosphere, m^{-3}; n, concentration, m^{-3}; $O(^1D)$, excited oxygen atom with electron level ^1D; $O(^3P)$, oxygen atom in the ground state ^3P; $O(^1S)$, excited oxygen atom with electron level ^1S; $O^+(^2D)$, excited oxygen ion with electron level ^2D; $O^+(^2P)$, excited oxygen ion with electron level ^2P; $O^+(^4S)$, oxygen ion in the ground state ^4S; $O_2(^1\Delta_g)$, excited oxygen molecule with an electron level $^1\Delta_g$; $O_2(A^3\Sigma_u^+)$, excited oxygen molecule with electron level $A^3\Sigma_u^+$; $O_2(a^1\Delta_g)$, excited oxygen molecule with an electron level $a^1\Delta_g$; $O_2(b^1\Delta_g)$; excited oxygen molecule with an electron level $b^1\Delta_g$; P, pressure of the gas, Pa; p_1 and p_2, probabilities of occurrence of the reactions; Q, coefficient of heating of the gas, $W \cdot sec^{-1}$; R, coefficient of the force of ion-neutral friction, sec^{-1}; S, coefficient of the force of ion-ion friction, sec^{-1}; s, length of the line of force, m; T, temperature of particles, K; t, time, sec; v, velocity of particles, $m \cdot sec^{-1}$; α, coefficient of recombination of particles, sec^{-1}; ε, energy of a photoelectron, eV; θ, characteristic temperature, K; λ, thermal-conductivity coefficient, $W \cdot m^{-2} \cdot K^{-1}$; μ, reduced mass, kg; ν, collision frequency, sec^{-1}; ξ, kinematic-viscosity coefficient, $m^2 \cdot sec^{-1}$; ρ, density of the gas, $kg \cdot m^{-3}$; σ, molecular diameter, m; τ, time step of integration, sec; φ, latitude, deg; Ω, rotational velocity of the earth, $rad \cdot sec^{-1}$. Subscripts: $i = 1$ and 2; $j = 1$ and 2, ions: (1, O^+, 2, H^+ $(i \neq j)$); e, electron; m, maximum; n, neutral; ef, effective; x, y, and z, meridian, zonal, and vertical directions; ν, ζ, No. of the N_2 vibrational level.

REFERENCES

1. B. F. Gordeets, A. I. Osipov, and L. A. Shelenin, *Kinetic Processes in Gases and Molecular Lasers* [in Russian], Nauka, Moscow (1980).
2. K. Smith and R. M. Thompson, *Computer Modeling of Gas Lasers* [Russian translation], Nauka, Moscow (1981).
3. M. R. Torr and D. G. Torr, The role of metastable species in the thermosphere, *Rev. Geophys. Space Phys.*, **20**, No. 1, 91–150 (1982).
4. S. A. Ishanov, K. S. Latyshev, and V. V. Medvedev, Modeling of disturbances of the F2 region of the ionosphere under anthropogenic effects, in: *Models in Nature Management* [in Russian], Collection of Sci. Papers of Kaliningrad University, Kaliningrad (1989).
5. A. E. Hedin, J. E. Salah, J. V. Evans, et al., A global thermospheric model based on mass spectrometer and in coherent scatter data. MSIS 1 density and temperature, *J. Geophys. Res.*, **82**, No. 16, 2148–2178 (1977).
6. J. C. G. Walker, R. S. Stolarski, and A. F. Naby, The vibrational temperature of molecular nitrogen in the thermosphere, *Ann. Geophys.*, **25**, No. 4, 831–839 (1969).
7. G. P. Newton, J. Walker, and P. H. E. Meijer, Vibrationally excited nitrogen in stable auroal red arcs and its effects on ionospheric recombination, *J. Geophys. Res.*, **79**, No. 25, 3807–3818 (1974).
8. A. E. S. Green and R. S. Stolarski, Analytic models of electron-impact excitation cross section, *J. Atmos. Terr. Phys.*, **34**, No. 10, 1703–1718 (1972).
9. T. E. Van Zandt and T. F. O'Malley, Rate coefficient of the reaction of O^+ with vibrationally excited N_2, *J. Geophys. Res.*, **78**, No. 28, 6818–6820 (1973).
10. K. S. Latyshev and V. V. Medvedev, Versions of the method of sweep of the numerical solution of equations of ion diffusion in the problem of ionosphere modeling, in: *Diagnostics and Modeling of Ionospheric Perturbations* [in Russian], Nauka, Moscow (1978), pp. 108–114.
11. I. L. Krinberg and L. V. Tashchilin, *Ionosphere and Plasmasphere* [in Russian], Nauka, Moscow (1984).