Modification of the particle-in-cell method for a slightly ionized plasma

E. A. Rudenchik and A. I. Sukhorukov

Institute of Terrestrial Magnetism, the Ionosphere, and Radio Propagation, Russian Academy of Sciences, 142092 Troitsk, Moscow Province, Russia

P. Stubbe

Max-Planck-Institut für Aeronomie, Katlenburg-Lindau 37191, Germany

(Submitted 14 December 1995)
Zh. Éksp. Teor. Fiz. **110**, 105–113 (July 1996)

An algorithm for numerical modeling of a slightly ionized plasma by the particle-in-cell method is developed on the basis of a statistical description of collisions of electrons with neutral atoms and molecules, including elastic collisions and those associated with the excitation, ionization, and attachment of electrons to neutrals. The algorithm can be used to investigate the dynamics of a highly nonequilibrium plasma on ordinary computers. The penetration of an electromagnetic pulse from a powerful lightning discharge into the lower nighttime ionosphere and significant modification of the latter are modeled. The heating of electrons to several electron-volts and the possibility of strong induced ionization of the lower ionosphere above thunderstorms are confirmed. The self-consistent fields calculated on a time scale of 100 μs exhibit highly nonlinear decay in transmission through the D layer of the ionosphere. [S1063-7761(96)00907-9]

1. INTRODUCTION

The penetration of the lower ionosphere by the electromagnetic fields of lightning discharges is accompanied by the formation of a highly nonequilibrium, slightly ionized plasma. The particle-in-cell (PIC) method provides the most workable means for describing the dynamics of a highly nonequilibrium plasma.[1–3] In its initial form this method can be used to investigate a highly ionized plasma and requires large computer resources. A slightly ionized plasma is simpler to describe, because the collisions of electrons are determined by the external medium (neutral atoms and molecules) in this case, and over sufficiently long times the statistical properties of the medium do not depend on the parameters of the electron gas. The modified particle method is tailored to the description of a slightly ionized plasma. Only collisions of electrons with neutrals are treated within the scope of this method, where the density and temperature of the neutrals are assumed to be given. The modified method retains the main advantages of the conventional particle method but is far simpler to implement and is capable of yielding informative results on everyday computers within a reasonable time period. It can be used to study phenomena associated with strong anisotropy of the distribution function of plasma electrons.

The interaction of a powerful electromagnetic pulse from a lightning discharge in the lower ionosphere poses an especially timely problem in connection with the recent discovery (or reliable confirmation) of a multitude of atmospheric phenomena induced by powerful lightning discharges, specifically the luminous emissions known as *red sprites* and *blue jets*,[4–6] and high-intensity electromagnetic pulses in the F_2 layer of the ionosphere above lightning source points, correlating with upward fluxes of high-energy electrons (of the order of several electron-volts).[7] Important new data have been obtained in studies of the lightning-induced, anomalously early disturbances of guided-wave signals from very low-frequency (VLF) transmitters, probably caused by the heating of electrons and a change in the ionization balance of the D layer,[8–10] as well as cloud-to-stratosphere lightning discharges.[11] A proper calculation of the self-consistent electric fields generated by various types of lightning discharges in the atmosphere on a time scale $<10^{-1}$ s is essential to the unambiguous interpretation of these phenomena. In this article we examine the dynamics of highly nonlinear phenomena in the lower ionosphere in a time interval $<10^{-4}$ s, in the very beginning of which the electrons have a highly anisotropic velocity distribution. A similar problem has been investigated within the framework of the kinetic approach in the approximation of weak anisotropy of the electron distribution function[10] and also in the approximation of electrons preheated to a constant temperature of 6 eV with a conductivity tensor of the form used in hydrodynamic theory, but with additional ionization taken into account on the basis of experimental data for the dependence of the ionization frequency on the amplitude of the electric field.[12]

2. MODIFIED PARTICLE METHOD

As in the conventional PIC method, the electron gas in the modified particle method is regarded as a set of coarse particles ("particles-in-cells") having certain coordinates and velocities. The mass and charge of each particle can be many times the mass and charge of the electron, but the charge-to-mass ratio, the velocity, and the cross section of interaction of a particle with neutrals are the same as for the individual electron. The path of a particle between collisions is determined from the solution of the equations of motion in an alternating electromagnetic field. The current density obtained after statistical averaging is substituted into the Maxwell equations to determine the self-consistent electromagnetic field.

The collisions of electrons with neutrals is modeled by statistical methods. The probability of collision of a particle in time dt is

$$\sum_{i,j} N_i \sigma_j^{(i)} v\,dt = \frac{v\,dt}{l_0},$$

where v is the velocity of the particle, N_i is the density of neutrals of the ith species, $\sigma_j^{(i)}$ is the collision cross section in the jth process, and l_0 is the mean free path. The number of collisions corresponding to this distribution is established as follows. The length l of the path traversed by the particle is determined in each time step of the trajectory calculations. The time step is set to ensure that the ratio $a = l/l_0$ will remain much smaller than unity. As soon as a exceeds a certain value (which is still much smaller than unity, say 0.1), a generator of random numbers distributed uniformly over the interval $[0,1]$ is actuated, and if a random number comes out smaller than a, a collision is assumed to have taken place. After each actuation of the random number generator, irrespective of the outcome, the instantaneous value of l is set to zero. While the resulting time distribution of the collision probability may differ from the theoretical (Poisson) distribution in subtler details (the occurrence of maxima at values of l/l_0 equal to $0.1, 0.2, 0.3, \dots$), numerous tests have confirmed that it has correct values of the mean, variance, skewness, and kurtosis. If a collision takes place, a new random number is generated in the interval $[0,1]$ and, depending on the subinterval in which it lies (each subinterval is proportional to the probability of the process $n_i \sigma_j^{(i)}$), it is ascertained just what process occurs in collision. A random number generator is then used again to determine the particle scattering angle (and the energy of the secondary particle in the event of ionization). The modulus of the postcollision particle velocity is determined by the energy loss $E_j^{(i)}$ which is assumed to be known for each process.

The current density can always be calculated with allowance for symmetry of the problem. In the one-dimensional problem (depending only on z), to determine the current in the interval Δz, it is necessary to sum over all particles with different coordinates x and y. Since the particle velocities are clearly independent of x and y, this procedure is of a formal nature. The current density $\mathbf{j}(t, z_n)$ at a given node z_n is determined by summing over all particles situated in the two intervals of the computational grid adjacent to the given node:

$$\mathbf{j}(t, z_n) = \frac{1}{2}[\mathbf{j}(t, n-1) + \mathbf{j}(t, n)].$$

Here $\mathbf{j}(t,n)$ is the current density in the grid intervals (z_n, z_{n+1}):

$$\mathbf{j}(t,n) = \frac{1}{\Delta z} \sum_{k \in K(t,n)} q_k \mathbf{v}_k(t), \tag{1}$$

where $K(t,n)$ is the set of indices of particles belonging to the interval (z_n, z_{n+1}) at time t, and q_k and $\mathbf{v}_k$ are the charge and velocity of the kth particle.

The initial coordinates and charge of the particles stipulate the initial charge density distribution of the electrons. This is achieved in two ways in the given algorithm. At low electron densities the charge of the particles is assumed to be fixed. Its value is determined by requiring that the plasma frequency corresponding to a single particle in a grid interval be much smaller than the characteristic frequencies of the problem. However, as the electron density increases, the number of such particles can become unrealistically large. The density of particles is then fixed, and the correct charge density distribution is established by a variable particle charge.

The initial particle velocity distribution is specified by a random number generator that establishes a Maxwell velocity distribution with a known initial temperature.

3. ENERGY CONVERSION

To gain insight into the energy conversion processes and to check the conservation of total energy, we determine the energy density and energy flux of the field, the kinetic energy of the electrons, and the energy imparted from electrons to neutrals. We consider the following quantities:

$$\mathscr{E}(t,n) = \frac{m}{2e} \sum_{k \in K(t,n)} q_k v_k^2(t),$$

$$\mathscr{D}(t,n) = \frac{m}{2e}\left(\sum_{k \in K(t-\Delta t,n)} q_k u_k^2(t,\Delta t) - \sum_{k \in I(t,\Delta t,n)} q_k v_k^2(t) \right),$$

$$\mathscr{Q}(t,n) = \frac{m}{2e}\left(\sum_{k \in K(t,n) \setminus K(t-\Delta t,n)} q_k v_k^2(t) - \sum_{k \in K(t-\Delta t,n) \setminus K(t,n)} q_k v_k^2(t) \right).$$

Here $K(t,n)$, q_k, and v_k are defined in (1), $I(t,\Delta t,n)$ is the set of indices of particles formed by ionization in the interval $(t-\Delta t, t)$ and belonging to the interval (z_n, z_{n+1}) at time t, $u_k^2(t,\Delta t)$ is the total variation of the square of the velocity of the kth particle in inelastic collisions in the interval $(t-\Delta t, t)$ (the final velocity is assumed to be zero in the event of attachment), $\mathscr{E}(t,n)$ is the kinetic energy of the particles at time t, $\mathscr{D}(t,n)$ is the energy imparted from particles to neutrals, and $\mathscr{Q}(t,n)$ is the difference in the energies of particles entering and leaving the interval (z_n, z_{n+1}) during the time Δt.

In zero electric field

$$u_k^2(t,\Delta t) = v_k^2(t-\Delta t) - v_k^2(t),$$

and the energy conservation law has the form

$$\mathscr{E}(t_m, n) - \mathscr{E}(0,n) + \sum_{l=1}^{m} [\mathscr{D}(t_l, n) - \mathscr{Q}(t_l, n)] = 0, \tag{2}$$

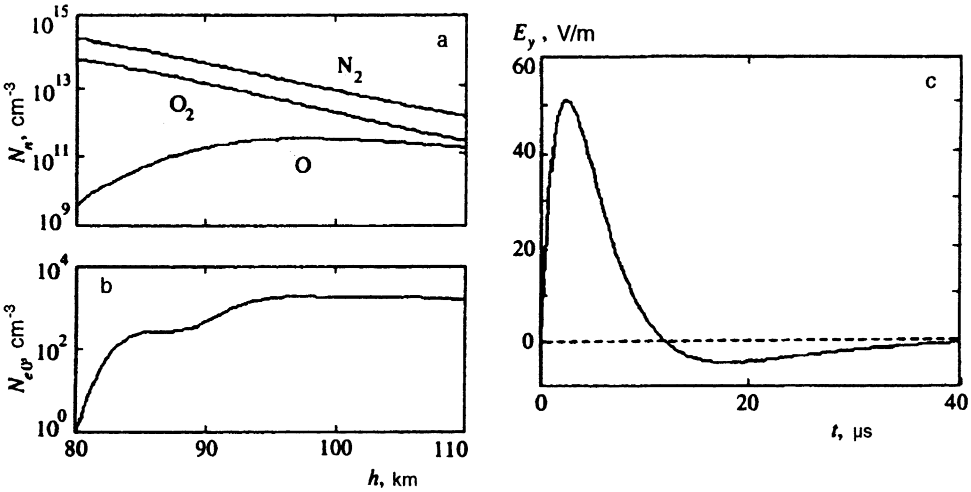

FIG. 1. Initial distributions of the density of neutral components N_n (a), the electron density N_{e0} (b), and the amplitude of the electric field of the incident wave E_y (c).

where t_m are the nodes of the time grid $(t_{m+1}-t_m=\Delta t)$. We call attention to the fact that in zero electromagnetic field this conservation law must be satisfied with machine precision, which is a test of the algorithm. The same is true in the presence of a static magnetic field when one uses an algorithm that provides exact conservation of energy during motion of the particles between collisions (we have recruited such an algorithm from Ref. 3).

In an electromagnetic field the left-hand side of Eq. (2) is equal to the work done by the field. The law of conservation of total energy assumes the form

$$\mathscr{E}_f(t_m,n)+\mathscr{E}(t_m,n)-\mathscr{E}(0,n)+S(t_m,z_n)-S(t_m,z_{n+1})+\sum_{l=1}^{m}[\mathscr{D}(t_l,n)-\mathscr{Q}(t_l,n)]=0,$$

where $\mathscr{E}_f(t,n)$ is the energy of the electromagnetic field,

$$S(t,z)=\int_0^t s(\tau,z)d\tau,$$

and $s(t,z)$ is the energy flux density of the field.

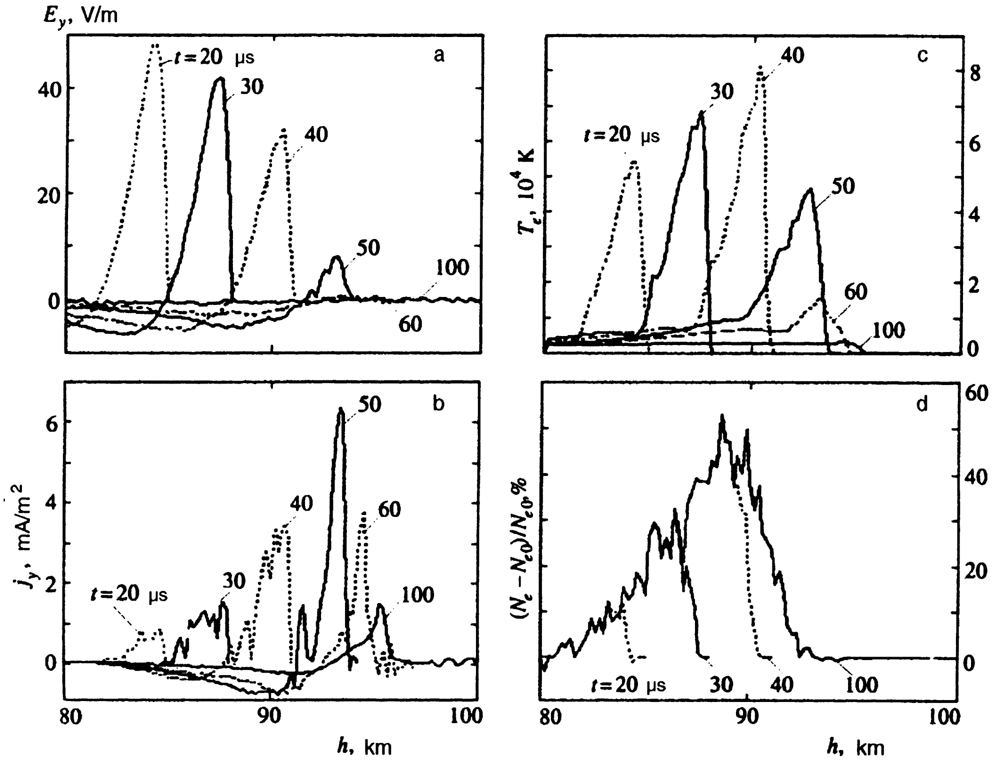

FIG. 2. Height (h) variations of the y-component of the electric field E_y (a), the y-component of the current density j_y (b), the effective electron temperature T_e (c), and the relative variation of the electron density $(N_e-N_{e0})/N_{e0}$ (d) at various times t.

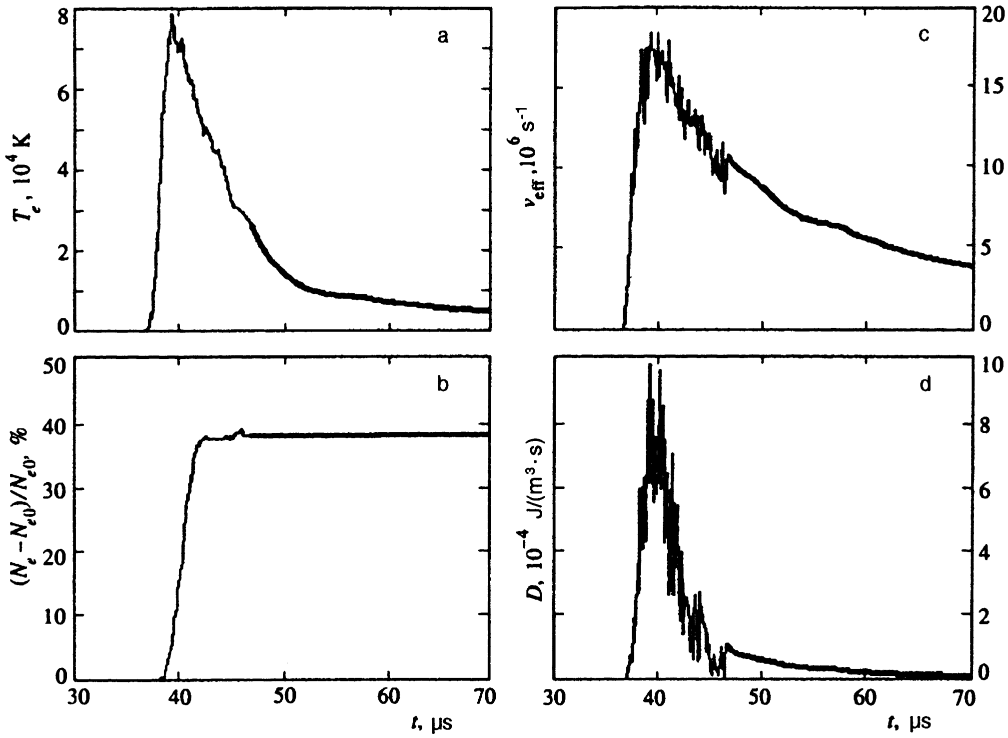

FIG. 3. Time (t) variations of the electron temperature T_e (a), the relative variation of the electron density $(N_e-N_{e0})/N_{e0}$ (b), the effective collision frequency $\nu_{\rm eff}$ (c), and the rate of energy transfer from electrons to neutrals D (d) at height $h=90$ km. The heavy lines represent the results of calculations based on hydrodynamic theory.

4. RESULTS OF THE CALCULATIONS

The above algorithm for the modified particle method has been applied to the problem of interaction of a high-intensity electromagnetic pulse from a lightning discharge with the lower ionosphere. We model this process by the one-dimensional problem of vertical propagation of a plane electromagnetic wave through a horizontally stratified ionosphere.

The initial distributions of the electron density N_{e0} and the density of neutrals N_n corresponding to a nighttime ionosphere model are shown in Fig. 1. The upper boundary in the model is the leading edge of a pulse moving at the speed of light c. The lower boundary is located at a height $h=79$ km, where the amplitude of an incident linearly polarized pulse (E_y, B_x) is specified. The profile of the pulse modeling the electric field of a strong lightning discharge is also shown in Fig. 1. The geomagnetic field is assumed to have a strength of 0.3 G and to be directed horizontally along the y axis. An explicit scheme of second-order precision (''hopscotch'' scheme[1,3]) is used to solve the system of Maxwell equations numerically.

Two separate parts can be discerned in the pulse incident on the ionosphere: a leading part of duration of the order of one to several tens of microseconds, where the electric field is strong (up to 10^2 V/m for the most powerful discharges), and a trailing part, where the amplitude of the field is comparatively low. This field structure is preserved as long as the currents are fairly small.[13] Rapid heating of the electron gas and the ionization of neutrals take place during passage of the leading part of the pulse. During passage of the trailing part of the pulse, the heating of electrons by the electric field is not as strong, and the electrons cool as a result of the excitation of lower energy levels of the neutrals.

Of utmost interest is the process in the leading part of the pulse, where the modified particle method is also used, whereas in the trailing part the current density is calculated by hydrodynamic theory,[14] i.e., the system of ordinary differential equations for the electron temperature and the current density is solved at each node of the spatial z-grid. The initial values of these quantities are determined by matching with the modified particle method. The error limits of the calculation of the trailing part of the pulse do not affect the leading part, which moves with the speed of light.

Data on the collision cross sections are taken from Refs. 15–17, and 18. The excitation of vibrational and optical levels, the ionization of neutrals, and the attachment of electrons are taken into account.

The results of the calculations are represented by graphs of the electric field $\mathbf{E}$, the magnetic field $\mathbf{B}$, the current density $\mathbf{j}$, the effective electron temperature t_e, the electron density N_e, the effective collision frequency $\nu_{\rm eff}$, and the electron energy dissipation rate D as functions of the height $h=z+z_0$ and the time t. Within the framework of the modified particle method, the values of these quantities at a particular node of the computational grid are determined by averaging over particles located in the two intervals adjacent to that node. As in the case of the current density $\mathbf{j}$ (1), we have

$$N_e(t,z_n)=\frac{1}{2\Delta z e}\left(\sum_{k\in K(t,n)} q_k+\sum_{k\in K(t,n+1)} q_k\right),$$

$$T_e(t,z_n)=\frac{2}{3}\frac{1}{2\Delta z N_e(t,z_n)}[\mathscr{E}(t,n)+\mathscr{E}(t,n+1)],$$

$$D(t,z_n)=\frac{1}{2\Delta z\Delta t}[\mathscr{D}(t,n)+\mathscr{D}(t,n+1)].$$

We use the following definition for the effective collision frequency in the modified particle method:

$$\nu_{\text{eff}}(t,z_n)=\frac{1}{\Delta t}\frac{1}{\mathscr{E}(t,n)+\mathscr{E}(t,n+1)}[\tilde{\nu}(t,n)+\tilde{\nu}(t,n+1)],$$

where

$$\tilde{\nu}(t,n)=\frac{m}{2e}\sum_{k\in K(t,n)}q_k\sum_{t_{\text{st}}\in(t-\Delta t,t)}v_k^2(t_{\text{st}})(1-\cos\theta_{\text{st}}),$$

t_{st} denotes the collision times of the kth particle, $v_k(t_{\text{st}})$ is the precollision particle velocity, and θ_{st} is the angle between the velocity vectors before and after particle collision.

The calculations are carried out in the interval $t=(0,\ 100\ \mu\text{s})$ for a grid spacing $\Delta z=50$ m ($\Delta z=200$ m in the derivation) and 100 particles per grid interval. Control calculations for 255 and 400 particles per grid interval have demonstrated the required convergence of the results. The results are shown in Figs. 2 and 3. Figure 2 shows the evolution of a pulse as it penetrates the ionosphere at time intervals $\Delta t=20,30,\dots,,100\ \mu\text{s}$ after the instant at which the leading edge of the incident pulse is located at a height $h=79$ km. For the chosen parameters of the initial pulse the electron density increases 40–50%, and the electron temperature reaches $\sim 8\cdot 10^4$ K in the vicinity of heights ~ 90 km. The time variations of the ionization-induced electron temperature, the effective electron collision frequency, and the rate of energy transfer from electrons to neutrals are shown separately for a height of 90 km in Fig. 3. An analysis of the energy balance shows that a large part of the field energy is spent in the excitation and ionization of neutrals in the range of heights up to ~ 93 km. It is evident from Fig. 3 that in the trailing part of the pulse, hydrodynamic theory gives somewhat excessive values of the energy losses and collision frequencies.

5. CONCLUSION

The modified particle method is an effective tool for the investigation of processes in a slightly ionized plasma. Its application is especially productive in problems associated with rapidly changing and highly anisotropic distribution functions, as in the rapid heating of electrons by a strong electric field. We note that other methods, as a rule, are inapplicable in this situation. On the other hand, if a problem involves transition from a highly transient to a quasisteady state, the modified particle method can be coordinated with other methods such as hydrodynamic theory[14] or the kinetic equation method.[10]

The modified particle method has demonstrated its effectiveness in solving the problem of the penetration of the electromagnetic fields of lightning discharges into the lower ionosphere. A modeling study has confirmed the theoretical conclusion[10] that impulsive heating of electrons to several electron-volts and strong additional ionization at altitudes of 80–95 km are induced by powerful lightning discharges.

This work has been supported by the International Science Foundation (Grant RIK000) and the Russian Fund for Fundamental Research (Grant 94-05-16095a).

[1] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, IOP Publ. Ltd., Bristol, England (1988).
[2] H. Matsuoto and Y. Omura, *Computer Space Plasma Physics: Simulation Techniques and Software*, Terra Sci. Publ., Tokyo (1993).
[3] Yu. A. Berezin and V. A. Vshivkov, *The Particle Method in Rarefied Plasma Dynamics* [in Russian], Nauka, Novosibirsk (1980).
[4] D. D. Sentman, E. M. Wescott, D. L. Osborne *et al.*, Geophys. Res. Lett. **22**, 1205 (1995).
[5] D. D. Sentman and E. M. Wescott, Phys. Plasmas **2**, 2514 (1995).
[6] E. M. Wescott, D. Sentman, D. Osborne *et al.*, Geophys. Res. Lett. **22**, 1209 (1995).
[7] W. J. Burke, T. L. Aggson, N. C. Maynard *et al.*, J. Geophys. Res. **97**, 6359 (1992).
[8] U. S. Inan, T. F. Bell, and J. V. Rodriguez, J. Geophys. Res. **18**, 705 (1991).
[9] U. S. Inan, J. V. Rodriguez, and V. P. Idone, J. Geophys. Res. **20**, 2355 (1993).
[10] Y. N. Taranenko, U. S. Inan, and T. F. Bell, J. Geophys. Res. **20**, 1539 (1993).
[11] R. L. Dowden, C. D. D. Adams, J. B. Brundel *et al.*, J. Atm. Terr. Phys. **56**, 1513 (1994).
[12] H. L. Rowland, R. F. Fernsler, J. D. Huba *et al.*, J. Geophys. Res. **22**, 361 (1995).
[13] A. I. Sukhorukov, MPAE-W-100-95; J. Atm. Terr. Phys. **57** (1995), to be published.
[14] A. V. Gurevich, *Nonlinear Phenomena in the Ionosphere*, Springer-Verlag, New York (1978).
[15] T. Murphy, *Los Alamos National Laboratory Report* No. La-11288-MS (1988).
[16] M. H. Ress, *Physics and Chemistry of the Upper Atmosphere*, Cambridge Univ. Press, Cambridge (1989).
[17] Y. Itakawa, M. Hayashi, A. Ichimura *et al.*, J. Phys. Chem. Ref. Data **15**, 985 (1986).
[18] Y. Itakawa, A. Ichimura, K. Onda *et al.*, J. Phys. Chem. Ref. Data **18**, 23 (1989).

Translated by James S. Wood