The Auroral Ionosphere: Comparison of a Time-Dependent Model With Composition Measurements

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A time-dependent model of the auroral ionosphere including the odd nitrogen species, NO, $N(^2D)$, and $N(^4S)$, is used for comparison with data from a coordinated rocket-satellite measurement of an auroral event. The chemical scheme and the adopted rate coefficients have been shown to be compatible with daytime mid-latitude ionospheric chemistry. The electron flux and neutral atmospheric parameters measured on the satellite are used to compute the appropriate ionization and dissociation rates. The calculated NO^+, O_2^+, O^+, Ne, and NO densities agree well with the rocket measurements. The calculated N_2^+ densities are larger than the measured densities by a factor of 3 at most altitudes. The calculations show that the nitric oxide content of the aurora ($\sim 1.2 \times 10^9$ NO molecules/cm^3 at 105 km) is below the saturation value.

INTRODUCTION

During the last decade, several measurements of the composition of the auroral ionosphere have been made using rocket-borne mass spectrometers. They have been recently reviewed by *Swider and Narcisi* [1977] and generally show that the amount of NO^+ ions in the E region is enhanced by a variable factor with respect to the daytime mid-latitude conditions. The high NO^+/O_2^+ ratio measurement by *Donahue et al.* [1970] led them to speculate that charge exchange of O_2^+ ions with enhanced amounts of nitric oxide or atomic nitrogen may be responsible for the increase of the NO^+ density. Subsequently, measurements of this ratio during steady state auroral conditions have been used to infer the amount of nitric oxide present in the auroral E region [*Swider and Narcisi*, 1974; *Narcisi and Swider*, 1976; *Swider and Narcisi*, 1977]. Satellite measurements of the intensity of the nitric oxide γ band resonance scattering in twilight have also indicated that the amount of NO is higher and more variable at high latitudes than at mid-latitude [*Rusch and Barth*, 1975] and that the NO density responds to the auroral activity during severe magnetic storms [*Gerard and Barth*, 1977].

Various models have been developed to examine how the odd nitrogen densities are affected by particle precipitation in the E region [*Jones and Rees*, 1973; *Vallance-Jones*, 1975; *Hyman et al.*, 1976; *Gerard and Barth*, 1977; *Roble and Rees*, 1977]. They show that significant buildup of nitric oxide may be obtained provided the atomic nitrogen atoms resulting from the increased ionization and dissociation of N_2 are mainly produced in the metastable $N(^2D)$ state. However, the results of these calculations could not be tested quantitatively against actual observations, since simultaneous determination of the precipitated electron spectrum as well as the neutral and ionic composition was missing. Such a requirement on the fraction of $N(^2D)$ produced is in agreement with the analysis of the daytime $N(^2D)$ and No densities [*Frederick and Rusch*, 1977; *Cravens et al.*, 1979].

In this study we take advantage of a successfully coordinated measurement of the electron spectrum, electron temperature, and neutral composition by experiments on board the Atmosphere Explorer C satellite and simultaneous rocket measurements of ion composition and airglow reported by *Rees et al.* [1977] and *Sharp et al.* [1979]. Our aim is to determine whether the observed ionosphere and the nitric oxide may be modeled adequately by a time-dependent calculation using the daytime chemistry and being constrained by a large number of observed quantities. The nitric oxide density was inferred from a measurement of the NO_2 continuum on the same flight [*Sharp*, 1978].

MODEL

The launch conditions of the rocket whose data will be analyzed here have been described in detail by *Rees et al.* [1977] and will not be repeated here. Suffice it to say that the rocket launch was coordinated with a pass of the AE-C satellite over Fort Churchill at an altitude of 490 km. During the period the intensity of the N_2^+ first negative band at 3914 Å was 4 kR, but a brighter display had been observed prior to the launch. The aurora remained relatively time invariant during the flight as could be judged from the ground-based and rocket measurements of the 3914-Å intensity. The energy spectrum of the precipitated electrons was measured by the low-energy electron detector (LEE) [*Hoffman et al.*, 1973] on the AE-C satellite. The neutral atmospheric composition was measured by the open source mass spectrometer [*Nier et al.*, 1973] on the satellite between 470 and 200 km and showed only small latitudinal gradients as determined by comparisons of downleg to upleg data.

At lower altitudes the densities are obtained by extrapolating downward assuming diffusive equilibrium. The density profiles obtained agree well with those inferred from the photometric rocket data down to near the base of the aurora [*Sharp et al.*, 1979] and are listed in Table 1. This atmospheric composition is remarkable in that it shows an unusually large O_2/O ratio at all altitudes. For example, it is 3 times richer in O_2 and 3 times poorer in O at 200 km than the MSIS model [*Hedin et al.*, 1977] corresponding to the observed N_2 profile. There is no indication from either the rocket or the satellite data of any unusual structure in the neutral density profiles. Surely, the unusually large O_2/O ratio indicates that the atmosphere is adjusting to auroral heating and induced vertical winds. It is not the purpose of this paper to quantitatively examine the neutral density profiles. Suffice it to say that vertical winds would tend to produce an O_2/O ratio larger

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TABLE 1. Neutral Atmosphere, 4278 Emission, and Ion Production Rates

Z, km	T_n, °K	N_2, cm^{-3}	O, cm^{-3}	O_2, cm^{-3}	I_{4278}, photons cm^{-3} s^{-1}	I_{N_2}, cm^{-3} s^{-1}	I_O, cm^{-3} s^{-1}	I_{O_2}, cm^{-3} s^{-1}
90	187	4.9(13)	7.9(10)	1.3(13)	23.0	8.8(3)	9.2(1)	1.8(2)
100	195	8.7(12)	1.4(11)	1.9(12)	914	3.5(4)	4.0(3)	7.3(3)
102.5	204	5.6(12)	1.2(11)	1.1(12)	952	3.6(4)	4.2(3)	7.3(3)
105	213	3.6(12)	1.1(11)	7.0(11)	881	3.3(4)	3.9(3)	6.4(3)
110	250	1.6(12)	7.4(10)	2.7(11)	58.1	2.2(3)	2.7(3)	3.8(3)
130	529	1.3(11)	1.5(10)	1.8(10)	95.2	3.6(3)	5.4(2)	4.9(2)
150	716	3.6(10)	5.5(9)	4.3(9)	31.1	1.2(3)	2.0(2)	1.4(2)
170	826	1.4(10)	2.5(9)	1.5(9)	13.3	5.0(2)	9.4(1)	5.3(1)
190	890	6.3(9)	1.4(9)	6.0(8)	6.4	2.4(2)	5.1(1)	2.3(1)
210	927	3.0(9)	8.3(8)	2.6(8)	3.3	1.3(2)	3.1(1)	1.1(1)
230	949	1.5(9)	6.6(8)	1.2(8)	1.9	7.1(1)	2.1(1)	5.5(0)

Read 4.9(13) as 4.9×10^{13}.

than normal and that the measurements are consistent with this expectation.

The ionization rate profile is calculated by using a method developed by *Lazarev* [1967] for the case of a monodirected-monoenergetic beam. This formula gives an analytical expression for the total ionization rate as a function of the penetration depth and depends on the energy of the primary electrons and the local mass density [*Gerard*, 1970]. To illustrate its validity, Figure 1 shows the altitude distribution of the total ionization rate for a unit flux of incident electrons of three different energies. It is compared with the profile calculated by *Berger et al.* [1970] using a Monte-Carlo calculation for the degradation of the electrons. In this comparison, the same neutral composition is used, the *Jacchia* [1971] model for an exospheric temperature of 1050°K. The agreement between the two methods is very good, both in shape and in magnitude for 20-keV electrons; it is within 30% for a 2-keV precipitation. Consequently, we feel confident that this method yields reliable auroral ionization profiles. To model the particular event we are analyzing, the electron spectrum measured by LEE at universal time 15368 s is used as input, together with the neutral atmospheric composition listed in Table 1. The ionization rate is integrated over the energy spectrum, and an isotropic pitch angle distribution from 0° to 80° is assumed, in agreement with the pitch angle distribution measured by the detectors. Because of the shape of the measured electron energy spectrum, there is reason to believe that high-energy electrons are present beyond the instrument threshold of 25 keV. We have therefore performed two calculations: one extrapolating the LEE energy spectrum to higher energies than was done by *Rees et al.* [1977], and the other assuming no flux above 25 keV. The volume emission rate of the λ3914-Å band of the N_2^+ first negative system, $\eta(3914)$, is calculated from the total ionization rate q by using

$$\eta(3914) = q\frac{0.88[N_2]}{0.88[N_2] + 0.5[O] + [O_2]}\frac{1}{14.7}$$

[*Vallance-Jones*, 1975]. The resulting distribution of the vertical column emission rate is shown in Figure 2 and compared with the rocket photometer measurement. The two curves agree very well at high altitude, but the calculated intensity progressively exceeds the measurements as altitude decreases. At 90 km the ratio of the calculated to the measured intensity is approximately 2 for the extrapolated flux and 1.4 for the case when no extrapolation was made. A similar problem was encountered by *Rees et al.* [1977], whose calculated 3914-Å intensity is approximately twice the observed intensity at all altitudes. No satisfactory interpretation can be given to the discrepancy except that the correlation between the satellite and the rocket was only realized when the latter was at 217 km. The electron spectrum or pitch angle distribution may have been different when the rocket entered the auroral ionization peak. Since a better agreement with the measured 3914-Å profile was obtained from the actual electron measurement, it will be used in the following calculation. The calculated ionization rates for N_2, O_2, and O are shown in Table 1.

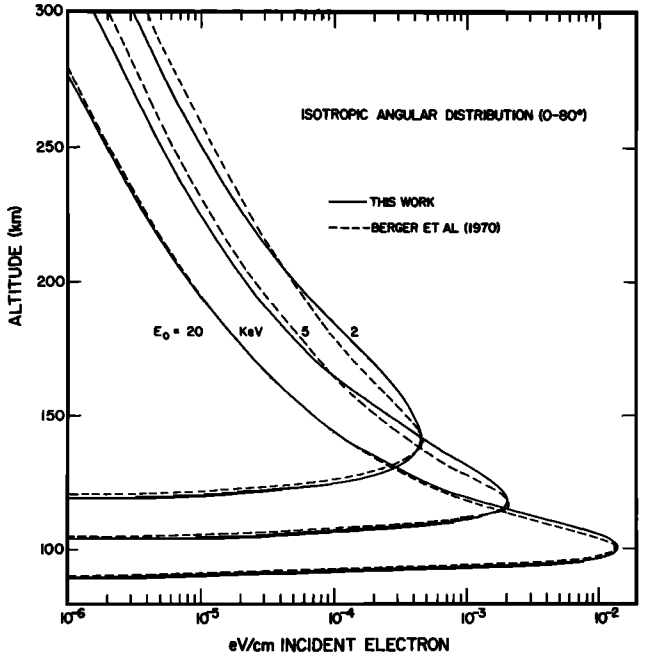

Fig. 1. Comparison of the total ionization rate versus altitude for a unit flux of incident electrons for 2, 5, and 20 keV between this work and *Berger et al.* [1970].

The production rates of individual ions are obtained from the total ion production rate q following the method described by *Vallance-Jones* [1975]. The relative production of O^+ ions in the three lower levels ^4S, ^2D, and ^2P is 0.48, 0.32, and 0.20 of the total O^+ production, respectively.

The ion and odd nitrogen densities are calculated by using a time-dependent model described by *Rusch et al.* [1977*a*] and *Cravens et al.* [1979]. The program uses a general second-order differential equation solver developed at the National Center for Atmospheric Research by *Hastings and Roble* [1977]. The continuity equations are solved for N_2^+, NO^+, O_2^+, N^+, O^+

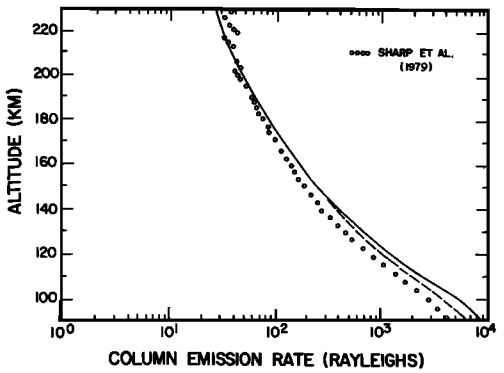

Fig. 2. The vertical column emission rate of 3914-Å emission versus altitude for this work compared to the measurement of *Sharp et al.* [1979].

(^4S), $O^+(^2D)$, $O^+(^2P)$, $N(^2D)$, $N(^2P)$, $N(^4S)$, and NO with the chemical reactions listed in Table 2. The NO and $N(^4S)$ calculations include molecular and eddy diffusion and appropriate flux conditions at the lower (50 km) and upper (250 km) boundaries. Most of the reaction rates and their temperature dependence used in the calculations have been measured in the laboratory, and their values have been confirmed by the analysis of the *AE* measurements of the thermospheric ion composition [*Torr and Torr*, 1978]. However, a few branching ratios and quenching rates have not been experimentally determined, and a choice must be made guided by our knowledge of the odd nitrogen daytime chemistry. The reaction of N_2^+ with O (reaction (R7)) is assumed to produce only $N(^2D)$ atoms, and the dissociation of N_2 by fast electron impact yields 75% of $N(^2D)$ and 25% of $N(^4S)$ in the model. The values are in agreement with the [N I] 5200-Å airglow analysis by *Frederick and Rusch* [1977] and give satisfactory agreement with the nitric oxide densities observed in the mid-latitude lower thermosphere [*Cravens et al.*, 1979].

Results

As was mentioned earlier, the enhanced dissociation and ionization of N_2 due to the particle precipitation produced an increase of the nitric oxide sources in the *E* region. Consequently, in an atmosphere subject to constant particle flux, the nitric oxide density increases with time until a saturation is reached.

In Figure 3 the results of three time-dependent calculations are shown. Case 1 (solid lines) shows the NO buildup and development of the NO^+/O_2^+ ratio using the ionization rate profile described in the text at all times. Case 2 (dashed lines) uses a two-step ionization rate such that the initial ionization rate is 10 times the measured one for the first 2×10^9 s of computation. The ionization rate is then decreased to the measured value with a 10-s exponential decay and then held constant. Case 3 (dotted lines) represents a calculation similar to case 2 except that the time is for the larger flux in 3×10^9 s. Starting from 2×10^7 cm^{-3}, the NO density in case 1 varies little during the first 10^8 seconds but increases to 2×10^9 cm^{-3}

TABLE 2. Reactions and Reaction Rates

No.	Reaction	Reaction Rate*	Source
(R1)	$O + e \rightarrow O^+(^4S, ^2D, ^2P) + 2e$	see text†	f's from *Torr and Torr* [1978]
(R2)	$O_2 + e \rightarrow O_2^+ + 2e$	see text	
(R3)	$O_2 + e \rightarrow O + O^+(^4S, ^2D, ^2P) + 2e$	see text‡	
(R4)	$N_2 + e \rightarrow N_2^+ + 2e$	see text	
(R5)	$N_2 + e \rightarrow N(^4S) + N(^2D, ^2P) + e$	see text	
(R6)	$N_2 + e \rightarrow N(^4S, ^2D, ^2P) + N^+ + 2e$	see text	
(R7)	$N_2^+ + O \rightarrow NO^+ + N(^2D)$	$1.4 \times 10^{-10}(T/300)^{-0.44}$	*McFarland et al.* [1974]
(R8)	$N_2^+ + O_2 \rightarrow O_2^+ + N_2$	$5 \times 10^{-11}(T/300)^{-0.8}$	*Lindinger et al.* [1974]
(R9)	$N_2^+ + e \rightarrow N(^4S) + N(^2D)$	$1.8 \times 10^{-7}(T/300)^{-0.39}$	*Mehr and Biondi* [1969]
(R10)	$O^+ + N_2 \rightarrow NO^+ + N(^4S)$	5×10^{-13}	*Lindinger et al.* [1974]
(R11)	$O^+ + O_2 \rightarrow O_2^+ + O$	$2 \times 10^{-11}(T_n/300)^{-0.4}$	*McFarland et al.* [1974]
(R12)	$O_2^+ + NO \rightarrow NO^+ + O_2$	4.4×10^{-10}	*Lindinger et al.* [1974]
(R13)	$O_2^+ + N(^2D) \rightarrow NO^+ + O$	1.8×10^{-10}	*Goldan et al.* [1966]
(R14)	$O_2^+ + e \rightarrow O + O$	$1 \times 10^{-6} T_e^{-0.7}$	*Torr et al.* [1976a]
(R15)	$N^+ + O_2 \rightarrow NO^+ + O$	2.75×10^{-10}	*McFarland et al.* [1973]
(R16)	$NO^+ + e \rightarrow N(^4S, ^2D) + O$	$4.2 \times 10^{-7}(T_e/300)^{-0.85}$	*Walls and Dunn* [1974]
(R17)	$N(^4S) + O_2 \rightarrow NO + O$	$2.4 \times 10^{-11} \exp(-3975/T_n)$	*Wilson* [1967]
(R18)	$N(^2D) + O_2 \rightarrow NO + O$	6×10^{-13}	*Lin and Kaufman* [1971]
(R19)	$N(^2D) + e \rightarrow N(^4S) + e$	$6 \times 10^{-10}(T_e/300)^{0.5}$	*Frederick and Rusch* [1977]
(R20)	$N(^2D) + O \rightarrow N(^4S) + O$	5×10^{-13}	*Frederick and Rusch* [1977]
(R21)	$N(^4S) + NO \rightarrow N_2 + O$	2.1×10^{-11}	*Phillips and Schiff* [1962]
(R22)	$N(^2D) \rightarrow N(^4S) + h\nu_{5200}$	$A_{^2D} = 1.07 \times 10^{-5}$ s^{-1}	*Garstang* [1956]
(R23)	$O^+(^2D) + N_2 \rightarrow N_2^+ + O$	1×10^{-9}	*Rutherford and Vroom* [1971]
(R24)	$N(^2P) + O \rightarrow N(^2D) + O$	1×10^{-11}	*Young and Dunn* [1975]
(R25)	$N(^2P) + e \rightarrow N(^2D) + e$	$6 \times 10^{-10}(T_e/300)^{0.5}$	Assumed
(R26)	$N(^2P) \rightarrow N(^2D) + h\nu$	$A = 0.079$ s^{-1}	*Garstang* [1956]
(R27)	$N(^2P) \rightarrow N(^4S) + h\nu$	$A = 0.005$ s^{-1}	*Garstang* [1956]
(R28)	$O^+(^2P) + O \rightarrow O^+(^2D) + O$	5.2×10^{-11}	*Rusch et al.* [1977]
(R29)	$O^+(^2P) + e \rightarrow O^+(^2D) + e$	$1.89 \times 10^{-7}(T_e/300)^{-0.5}$	*Henry et al.* [1970]
(R30)	$O^+(^2P) \rightarrow O^+(^2D) + h\nu$	$A = 0.17$ s^{-1}	*Seaton and Osterbrook* [1957]
(R31)	$O^+(^2P) \rightarrow O^+(^4S) + h\nu$	$A = 0.048$ s^{-1}	*Seaton and Osterbrook* [1957]
(R32)	$O^+(^2P) + N_2 \rightarrow N_2^+ + O$	4.8×10^{-10}	*Rusch et al.* [1977]
(R33)	$N(^2D) + NO \rightarrow N_2 + O$	7×10^{-11}	*Black et al.* [1969]
(R34)	$N(^2P) + O_2 \rightarrow NO + O$	2.6×10^{-12}	*Husain et al.* [1974]

*Rates are in units of cm^3 s^{-1} unless otherwise noted.
†$f(^4S) = 0.484$, $f(^2D) = 0.323$, $f(^2P) = 0.194$.
‡$f(^4S)$, $f(^2D)$, $f(^2P)$, same as for (R1).

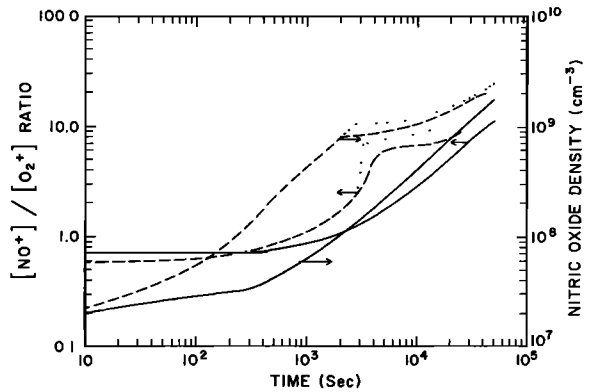

Fig. 3. Nitric oxide density and NO^+/O_2^+ ratio versus time. The solid lines correspond to the ionizing flux measured by LEE. The dashed lines correspond to a flux of 10 times the measured one for 2×10^3 s and then a decay to the measured flux. The dotted lines correspond to a flux of 10 times the measured one for 3×10^3 s and then a decay to the measured flux.

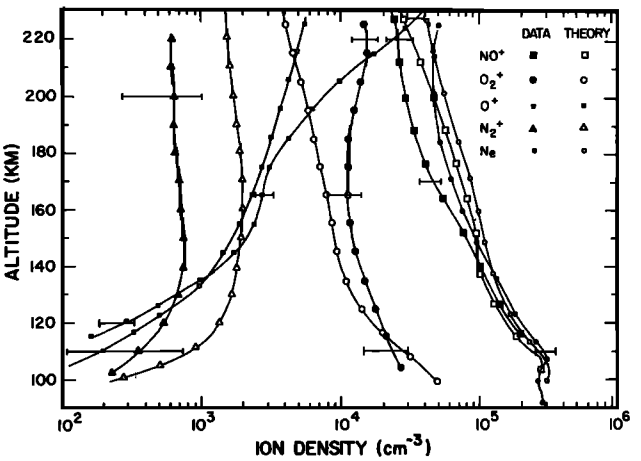

Fig. 4. Comparison between the calculated and observed ionospheric densities at $t = 5 \times 10^4$ s using the NO^+ dissociative recombination rate of *Walls and Dunn* [1974].

after 5×10^4 s. As a consequence, O_2^+ ions are progressively converted into NO^+ through reaction (R12), and the NO^+/O_2^+ ratio increases from 0.7 to 12. The ratio of NO^+/O_2^+ observed at 105 km by the rocket mass spectrometer is observed in the model after about 3×10^4 s.

We recognize that the assumption of a constant precipitation during a time period of several times 10^4 seconds is unrealistic. However, a more intense electron flux could produce the same result in a shorter time, since the density of NO depends only on the total integrated energy flux and the fraction of $N(^2D)$ and $N(^4S)$ atoms produced by reactions (R5), (R6), (R7), and (R16). In fact, a strong breakup period preceded this aurora and was probably able to generate in a few minutes most of the NO present in this aurora. Cases 2 and 3 are attempts to simulate this situation. The energy deposition in the atmosphere above Fort Churchhill was nearly constant for about 1000 s before the rocket launch and remained constant during the upleg portion of the flight. Previous to this, the large breakup deposited an average energy of nearly 10 times the energy at launch for several thousand seconds (W. E. Sharp, private communication, 1978).

In case 2 the measured NO^+/O_2^+ ratio is achieved after 1.6×10^4 s and in case 3 after 3.1×10^3 s. In case 3 most of the nitric oxide owes its existence to the larger flux. In each case, however, the electron density is present in response to the low flux. The time constant for the ionosphere to come into equilibrium with the incident flux is about 500 s at 190 km and about 60 s at 110 km. Thus all three cases produce essentially the same ion density profiles at the time when the NO^+/O_2^+ ratio is equal to the measurement, and the observed electron density is consistent with the measured ionization rate. In case 3 the observations produce the NO^+/O_2^+ ratio in less than 1 hour. We realize that minor constituents are subject to transport by vertical and horizontal winds and will be transported out of the vicinity of their creation, possibly with very short time constants. A horizontal wind of 30 m/s would remove the nitric oxide generated in a 1° wide auroral arc in 1 hour. While we do not claim to have exactly represented the time history of this particular aurora, we do, however, feel that the results are consistent with the scenario adopted and that (1) nitric oxide densities of several times $10^9/cm^3$ can be generated in auroral arcs and the agreement between the calculated NO density at 110 km (see Figure 6) indicates that the time constant for this buildup was less than the time constant for its horizontal or vertical dispersion and (2) the agreement between the measured and calculated ion densities (see Figure 5) shows that the electron density resulted from the measured ionization rate. We illustrate the calculated ion composition at that time in Figures 4 and 5. It may be seen that a good agreement with the observations is obtained for most ions. The detailed comparison will be discussed in the next section.

The altitude distributions of $N(^2D)$, $N(^4S)$, and NO are shown in Figure 6 for the time when the NO^+/O_2^+ ratio was in agreement with the measurement. In this case the $N(^2D)$ and $N(^4S)$ densities are nearly equal, in contrast to the daytime situation, where $[N(^4S)] \sim 20[N(^2D)]$ at 180 km. The NO densities are enhanced with respect to mid-latitude conditions by more than an order of magnitude. The NO density at 110 km derived by *Sharp* [1978] from the intensity of the NO_2 continuum measured on the same flight is also indicated in Figure 6. The agreement between the two methods strongly supports the validity of the deduced NO density.

Discussion and Conclusions

We have used a time-dependent model of the auroral ionosphere which includes a detailed calculation of the odd nitrogen chemistry to compare it with a comprehensive set of coordinated rocket and satellite measurements. The absolute densities of NO^+, O_2^+, O^+, and N_2^+ are compared at the time

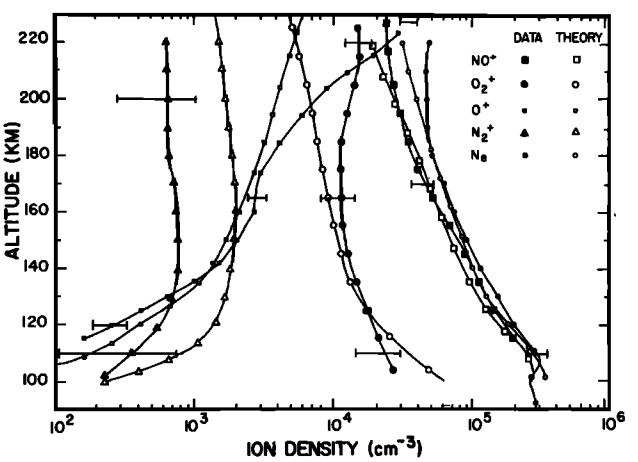

Fig. 5. Same as Figure 4 except that the *Huang et al.* [1975] rate is adopted for the NO^+ recombination rate.

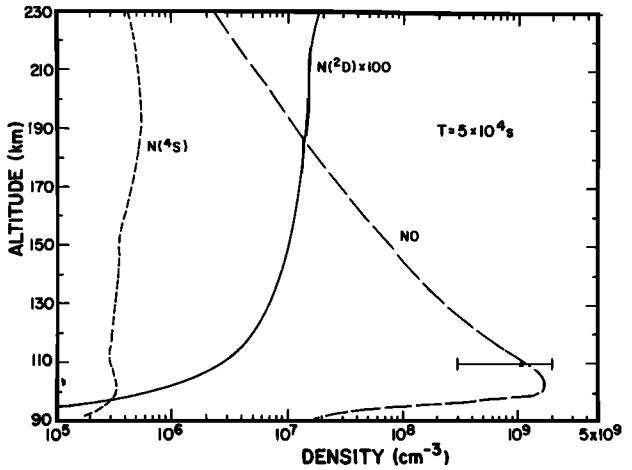

Fig. 6. The calculated altitude distributions of NO, N(^2D), and N(^4S). The measurement of *Sharp* [1978] is included for comparison.

when the model predicts the NO^+/O_2^+ ratio. The comparison between the calculated and measured NO^+, O_2^+, and O^+ densities is excellent, especially at low altitudes, and the calculated NO density agrees well with that determined from the measured NO_2 continuum emission [*Sharp*, 1978]. Note that the NO density at the time of the measurement is well below its saturation value.

The calculated and measured O^+ densities agree well below 190 km. The major source of O^+ at low altitudes ($Z < 150$ km) is dissociative ionization of O_2, and we have assumed that the O^+ ions produced by this reaction are found in metastable states in the same proportion as direct impact ionization of O. Thus less than 50% of the O^+ ions are formed in the ground state. Metastable O^+ ions are lost far more rapidly than ground state O^+ (see Table 2), and this accounts in part for the excellent agreement.

Two difficulties remain: The measured ion densities diverge from the theory at high altitudes, and the calculated N_2^+ densities are nearly a factor of 3 higher at most altitudes.

The detailed comparison between the calculated and measured 3914-Å emission is instructive in the first case. In the work of *Rees et al.* [1977] the measured 3914-Å emission changes slope above 180 km and indicates an increased ionization rate. This would account for the increased ion density at high altitudes.

The N_2^+ problem is more difficult to understand. In each of the models the calculated N_2^+ is a factor of 3 higher than the measurements at most altitudes and approaches the measured N_2^+ at low altitudes.

The chemistry of N_2^+ is straightforward, the loss processes being charge exchange with O_2 at low altitude and the ion atom interchange reaction with O at high altitude. Also it appears that the higher recombination rate for NO^+ of *Huang et al.* [1975] better describes the NO^+ density distribution. This recombination rate is not consistent with the mid-latitude studies of *Torr et al.* [1976*b*] and may be deceiving inasmuch as the NO^+ is produced mainly by $N_2^+ + O$ at high altitudes. The NO^+ density may be too large in Figure 4 as a direct result of the high N_2^+. The *Huang et al.* [1975] rate is probably correct for vibrationally excited NO^+ and if applicable to the aurora would imply that NO^+ is vibrationally excited. But the sources of NO^+ ions in the aurora are the same as those in the dayglow, and so we should not expect NO^+ to be found in an enhanced vibrational state. Also, in recent calculations, *Swider and Narcisi* [1977], *Narcisi and Swider* [1976], and *Swider and Narcisi* [1974] appear to have the same problem with the calculated N_2^+ densities when the neutral atmosphere adopted is one of relatively low atomic oxygen concentration.

We stress further need for broad-based measurements of auroral conditions which can serve as constraints on model calculations.

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