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The Solar Flare of 18 August 1979

*Incoherent Scatter Radar Data and
Photochemical Model Comparisons*

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by

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ABSTRACT

Measurements of electron density at seven D-region altitudes were made with the Arecibo radar during a Class-X solar flare on 18 August 1979. Measurements of solar x-ray fluxes during the same period were available from the GOES-2 satellite (0.5–4 Å and 1–8 Å) and from ISEE-3 (in four bands between 26 and 400 keV). From the x-ray flux data we computed ionization rates in the D-region and the associated chemical changes, using a coupled atmospheric chemistry and diffusion model (with 836 chemical reactions and 19 vertical levels). The computed electron densities matched the data fairly well after we had adjusted the rate coefficients of two reactions, viz:

and

We discuss the hierarchies among the many flare-induced chemical reactions in two altitude ranges within the D-region and the effects of adjusting several other rate coefficients.

I. INTRODUCTION

A sequence of ionospheric D-region incoherent scatter measurements was in progress using the Arecibo radar at the time of onset of a Class-X solar flare on 18 August 1979. The D-region response to the flare was recorded. This paper describes the first detailed analysis of the data.

Both the total backscattered power over a bandwidth of 250 kHz and the spectra of the signal with a bandwidth of 1 kHz were recorded. The altitude resolution was 600 m, and the time resolution was about 1.8 minutes. The data cover the altitude range 60 to 90 km, and the time coverage extends from 20 minutes before commencement of the flare until about 3 hours after. The data have been analyzed to give electron concentrations at seven discrete altitudes, each separated by about 5 km. These electron concentrations are plotted in Fig. 1. A discussion of the data analysis and an estimation of errors are given in Appendix A. The absolute electron densities vs altitude are believed to be accurate to within $\pm 20\%$, whereas the relative electron densities vs time are within $\pm 5\%$.

Fig. 1. Measured values of electron densities as functions of time for several altitudes.

The ionospheric effects of a solar flare are caused by the flare-enhanced emissions of solar x rays (Rowe *et al.*, 1970; Deshpande *et al.*, 1972; Mitra, 1974). At the time of the event, in August 1979, the solar x-ray fluxes were monitored continuously in altogether six wavelength bands by the GOES-2 and ISEE-3 satellites. Figure 2 shows the fluxes measured by GOES-2 during the 18 August flare in the 0.5-4-Å and 1-8-Å bands, together with the 0.29-0.48-Å flux measured by ISEE-3. From the measured x-ray fluxes we computed ionization rates, as shown in Fig. 3.

We have also made a detailed comparison of the electron density data with theoretical predictions based on a Los Alamos ionospheric chemistry computer model. This paper stresses the model and the comparisons, which are described in Section II. We also identify certain key chemical reactions for which we must adjust the rate coefficients to obtain agreement with the data. Further details are in Appendices B and C.

Fig. 2. Solar x-ray flux data from the GOES-2 and ISEE-3 satellites. Curve A: 0.29-0.48 Å; curve B: 0.5-4 Å; curve C: 1-8 Å.

Fig. 3. Contours of computed ion-pair production rates before and during the solar flare, at altitudes between 60 and 90 km.

II. COMPUTATIONAL MODEL

A. General Features

The computer model is an extension of the time-dependent 1-D chemistry and diffusion model whose general structure was described by Zinn *et al.*, 1982. The photochemical and photoelectron-collisional rate coefficients are computed interactively as functions of altitude and time, based on the time-varying solar output spectrum and solar zenith angle and the varying column densities of absorbers. For D-region computations the chemical reaction set was expanded to include 8 species of negative ions and 23 positive ions (see Appendix B). The code computes the full set of ion and electron and neutral species concentrations (56 species in all) interactively over a range of altitudes between 50 and 1300 km (19 levels, with 5-km spacing between 50 and 120 km and coarser spacing above), including diffusion and transport terms.

To compute ion-electron production rates associated with the deposition of solar x rays, we use the x-ray fluxes measured by the satellites GOES-2 (two wavelength bands, 0.5–4 Å and 1–8 Å) and ISEE-3 (0.29–0.48-Å band). (See Fig. 2.) Additional x-ray flux data for three higher energy bands were also provided by the ISEE-3 satellite. However, the fluxes of the higher-energy x rays were too small to be significant in the D-region, and they are not included in the ionization rate computations.

To compute x-ray deposition rates and ionization rates from the three-band x-ray flux data, we fit the flux data at each time-point with a spectrum described by two separate power laws in λ (the wavelength) that join continuously at $\lambda = 1.9$ Å. Thus at each instant the spectral flux is described by three parameters, which are fitted to the three measured bandwise flux integrals. The fitting procedure and the computation of ionization rates are described in Appendix C. Results of numerical experiments with other spectral shape functions are also described. Uncertainties in the relative ionization rates vs altitude associated with uncertainties in the flare x-ray spectral distribution are estimated to be less than 15%.

The x-ray deposition is assumed to produce ionization at a rate of one ion-electron pair for each 35 eV of energy deposited. The computed ion-electron production rates vs time for seven D-region altitudes are plotted in Fig. 3. In addition, for each ion-electron pair, a definite number of atoms (or ions or molecules) of N, O, $N(^2D)$, $O(^1D)$, $N_2(A^3\Sigma)$, $O_2(^1\Delta)$, N_2^+ , O_2^+ , N^+ , and O^+ is produced (Appendix B).

To set up the solar flare computation, the geographic, geomagnetic, and solar coordinates, and the solar and geomagnetic activity indices were set to values appropriate to Arecibo, PR, at 0000 hours (LST) on 16 August 1979. The concentrations of N_2 , O_2 , H_2 , CO_2 , H_2O , O, He, Ar, H, CO, NO, NO_2 , N_2O , and O_3 at all altitudes were initialized to values based on experimental data. The initial concentrations of other species were set to zero. The model computation was then run for the 59 hours up to and including the solar flare, with the solar zenith angles, temperatures, E-fields, vertical winds, and solar/magnetic activity indices updated every 30 minutes. At times before the start of the flare, the chemical and photochemical rate coefficients and ion-pair production rates were also updated every 30 minutes. However, after commencement of the flare, they were updated once per minute.

Some of the computed results for the flare period are plotted in Figs. 4 and 5. Figure 4 is a set of computed electron density vs time plots for altitudes between 60 and 90 km in steps of 5 km. Figure 5 is a corresponding composite plot of negative ion densities.

It will be noted that the computed electron densities in Fig. 4 are in fair agreement with the measured electron densities in Fig. 1. This suggests that the model probably includes most of the important chemical reactions and a reasonable representation of the flare x-ray spectrum.

The largest component of the computer model is the chemistry subroutine. It is described below.

Fig. 4. Computed electron concentrations before and during the solar flare, at the indicated altitudes.

Fig. 5. Computed negative ion concentrations.

B. Chemistry Subroutine

The chemistry model was designed for computing electron and ion densities during a solar flare or other strong ionospheric disturbance. The ion and neutral species included in the model are listed in Table I. The species set does not include all of the complex positive ions that are known to be important in the D-region under normal (nonflare) conditions, such as $\text{H}_3\text{O}^+ \cdot (\text{H}_2\text{O})_n$ with $n \geq 3$. For the negative ions we have ignored OH^- , HCO_3^- , and all negative ion hydrates. The terminal negative ion is nominally NO_3^- . The omitted species are not expected to be important within the brief time duration of a solar flare.

The ion reaction rate coefficients that we have used are all derived from either the DNA Reaction Rate Handbook (Bortner and Baurer, 1978) or the compendium by Albritton (1978), with a few exceptions which are explicitly noted. The more important reactions and their rate coefficients are listed in Appendix B.

TABLE I
SPECIES INCLUDED IN THE MODEL^a

Electrons

O^- O_2^- O_3^- O_4^- CO_3^- CO_4^- NO_2^- NO_3^-
 O^+ N^+ H^+ He^+ $\text{O}^+(\text{2D})$
 N_2^+ O_2^+ NO^+ OH^+
 H_2O^+ O_4^+ H_3O^+ N_4^+ $\text{O}_2^+ \cdot \text{N}_2$ $\text{NO}^+ \cdot \text{N}_2$
 $\text{O}_2^+ \cdot \text{W}$ $\text{NO}^+ \cdot \text{CO}_2$ $\text{NO}^+ \cdot \text{W}$ $\text{NO}^+ \cdot \text{W}_2$ $\text{NO}^+ \cdot \text{W}_3$ $\text{H}_3\text{O}^+ \cdot \text{W}$ $\text{H}_3\text{O}^+ \cdot \text{W}_2$ $\text{H}_3\text{O}^+ \cdot \text{OH}$
 N O H He Ar $\text{N}(\text{2D})$ $\text{O}(\text{1D})$ $\text{O}(\text{1S})$
 N_2 O_2 H_2 CO NO OH $\text{N}_2(\text{A}^3\Sigma)$ $\text{O}_2(\text{a}^1\Delta)$ $\text{O}_2(\text{b}^1\Sigma)$
 H_2O NO_2 N_2O CO_2 HO_2 O_3

^a "W" means " H_2O ".

III. COMPUTATIONS AND COMPARISONS WITH THE DATA

The computations show that during the flare the negative ions are unimportant above 70-km altitude. On the other hand, at 60 km the negative ion concentrations are slightly larger than the electron concentrations. The predominant negative ion species is CO_3^- since there is insufficient time for conversion to NO_3^- .

During the flare the precursor positive ions are mainly N_2^+ and O_2^+ . Below 80 km these simple ions are converted rapidly to $\text{H}_3\text{O}^+ \cdot \text{W}_n$ and $\text{NO}^+ \cdot \text{W}_m$. However, above 85 km the conversion to complex ions is slow, and the predominant positive ion species are O_2^+ and NO^+ . The electron-ion recombination coefficients of polyatomic ions are much larger than those of diatomic ions; therefore, the degree of conversion of the positive ions from O_2^+ and NO^+ to larger complexes has an important effect on the electron concentrations. The solar flare electron density data indicate that complex positive ions are dominant at altitudes up to 85 km and diatomic ions are dominant above.

During the period of peak solar x-ray flux, the rates of ionization are changing relatively slowly, so the electron-ion concentrations, n_{ei} , can be approximated fairly accurately with the simple steady-state expression $n_{ei} = \sqrt{Q/\alpha_{eff}}$, where Q is the ionization rate ($\text{cm}^{-3} \text{s}^{-1}$) and α_{eff} is the species-weighted average recombination rate coefficient. Conversely, $\alpha_{eff} = Q/n_{ei}^2$. From the measured electron concentrations, together with the ion-pair production rates computed from the GOES-2 and ISEE-3 x-ray flux data, we can calculate a set of "empirical" values of α_{eff} (at altitudes where negative ion concentrations are small in comparison with n_e). The values of α_{eff} thus obtained for the time of maximum solar x-ray deposition (14:16–14:18 UT) are listed in Table II. At 70–80 km the values of α_{eff} in Table II correspond to a positive ion composition that consists mainly of polyatomic complexes. At 90 km, on the other hand, the positive ions are mostly O_2^+ and NO^+ .

TABLE II
VALUES OF α_{eff}
DERIVED FROM THE DATA
(AT FLARE MAXIMUM)

Altitude (km)	α_{eff} (cm ³ /s)
70	2.6×10^{-6}
75	2.3×10^{-6}
80	1.6×10^{-6}
85	1.1×10^{-6}
90	2.8×10^{-7}

According to the computer model results, the most important reaction paths for positive ions and negative ions in the D-region during a flare are as diagrammed in Fig. 6(a,b). Figure 6(a,b) is similar in many respects to a pair of diagrams by Mitra and Rowe (1972), but there are several differences. The most important difference is the inclusion in our reaction scheme of two reactions of negative ions with O₂(¹Δ).

We ran several sets of model computations. The first was run with chemical rate coefficients that were all taken from published literature, with no adjustments or insertions. Also, we assumed a nominal water vapor profile. We obtained approximate quantitative agreement with the measured electron concentrations in Fig. 1, but there were some significant discrepancies. At 60- and 65-km altitude the computed peak electron densities were too low by 40%; at 80 and 85 km they were too high by 40%; and at 90 km it was too low by 20%. We proceeded then to examine the hierarchies of the various chemical reaction rates in each altitude range to see if there were plausible adjustments of rate coefficients, within the ranges of their estimated error bars, that could lead to better agreement between the computed electron densities and the data.

At 60- and 65-km altitude the dominant reactions of free electrons are three-body attachment to O₂;

in approximate quasi equilibrium with detachment from O₂⁻ by encounters with O₂(¹Δ);

The attachment rate coefficient k_1 (for $T = 250$ K and $M = \text{air}$) is probably known to within $\pm 30\%$. (See Phelps, 1969.) However, k_2 is described as uncertain within a range of (+900%, -90%) (Fehsenfeld et al., 1969). We found that we could improve the agreement between the computed and measured peak n_e by increasing the assumed value of k_2 from 2×10^{-10} cm³/s to 1×10^{-9} .

The adjustment of k_2 did not completely remove the discrepancy between the computed and measured n_e at 60 km; the computed electron density was still low by about 18%. At 65 km it was still low by 35%. The response of n_e to changes in k_2 is nonlinear and tends to saturate for large values of k_2 . There is a close coupling between the rates of attachment/detachment, ion-electron recombination, and the quasi equilibria between O₂⁻ and complex negative ions. Further details are discussed in Section IV.

Because of Reaction (2), the electron density is also sensitive to the O₂(¹Δ) concentration. This is computed interactively within the model, using rate coefficients that are well determined. However, the O₂(¹Δ) concentration is somewhat sensitive to the H₂O concentration, which can exhibit large fluctuations (see Elsasser et al., 1980). We have assumed a water concentration of 4.15 ppmv at 60 km, close to the center of the range of the Elsasser et al. measured values.

Fig. 6A. Diagram of the dominant reaction paths for positive ions.

Fig. 6B. Dominant reaction paths for negative ions.

At 80 and 85 km the computed peak electron densities were too high. At those altitudes, the n_e are largely controlled by the concentration ratio of complex positive ions to diatomic ions, which determines the effective recombination coefficient α_{eff} . This ratio is influenced by reactions that control the quasi equilibria between O_2^+ , $\text{O}_2^+\cdot\text{N}_2$, and O_4^+ and the rate of conversion of O_4^+ to $\text{O}_2^+\cdot\text{H}_2\text{O}$. The most important of these are

and

The rate coefficients k_3 , k_4 , and k_5 all have substantial error bars (Albritton, 1978). Moreover, the measurements of k_4 and k_5 were at room temperature, whereas the temperature at 80-km altitude is about 190 K.

The rate of Reaction (3) (at $T = 190$ K with $\text{M} = \text{air}$), along with the parallel indirect reaction path involving $\text{O}_2^+\cdot\text{N}_2$, is probably uncertain by $\pm 50\%$ (see Albritton, 1978; Bortner and Baurer, 1978). Nevertheless, we used the Bortner and Baurer values without adjustments.

With respect to Reaction (4), the rate coefficient was measured by Fehsenfeld et al., 1971, and by Howard et al., 1972, the two measured values differing by a factor of ~ 1.5 . We chose the larger (Fehsenfeld et al.) value. Another significant uncertainty is in the water vapor concentrations, which also affect the rate of Reaction (4). The H_2O concentration used in the model at 80 km (2.5 ppmv) was consistent with the concentration at 60 km, according to the constraints of photochemical/diffusive equilibrium and therefore consistent with the measurements of Elsasser et al., 1980.

With respect to Reaction (5), which impedes the process of conversion of diatomic ions to complex hydrates, the rate coefficient was measured to be $(3 \pm 2) \times 10^{-10} \text{ cm}^3/\text{s}$ at 295 K (Fehsenfeld and Ferguson, 1972). At 80 and 85 km (where $T \approx 190$ K), the largest value of k_5 that can be accommodated by the flare n_e data is $1 \times 10^{-10} \text{ cm}^3/\text{s}$ —i.e., lower than the Fehsenfeld/Ferguson measured 295 K values but within their estimated error range. However, the overall rate of Reaction (5) also depends on the atomic oxygen concentration, which exhibits large quasi-random fluctuations (Offermann et al., 1981). The computed O concentration at 80-km altitude shows a regular diurnal variation of a factor of 4, with a minimum before dawn and a maximum in late afternoon. However, it also depends on the eddy diffusion coefficients K_{zz} , which are highly uncertain and/or variable. Various recommended K_{zz} profiles are given by Ailen et al., 1981; Brasseur and Offermann, 1986; Garcia and Solomon, 1983; Bjarnason et al., 1987; and others. We ran separate 24-hour pre-flare computations with the Allen et al., K_{zz} profile and the Brasseur/Offermann profile, and the computed daytime O concentrations at 80 km differed by a factor of 2 between the two computations. We conclude that our computed O concentrations can be in error by a factor of 2 or more, and therefore our value of $k_5(190 \text{ K})$ is uncertain by a similar factor. That is, $k_5(190 \text{ K}) = 1.0 \times 10^{-10} \text{ cm}^3/\text{s}$ (+100%, -50%). The computed O concentrations are within the range of measured values reported by Offermann et al., 1981.

The computed electron and negative ion densities plotted in Figs. 4 and 5 were computed with the adjusted rate coefficients. A numerical comparison of the computed and measured values of n_e at the peak of the solar flare is in Table III. One will note from Table III that there are still significant discrepancies at 65 and 85 km.

We have also compared the computed and measured time variations of n_e and find modest agreement. The times of the two n_e maxima and the minimum agree to within 1 minute between the computations and the data, except at 85 km where there is a 2-minute discrepancy. The relative heights of the maxima and minimum are also in fair agreement, with the worst disagreement appearing again at 85 km.

TABLE III
COMPARISON OF COMPUTED
MAXIMUM ELECTRON DENSITIES
VS MEASURED ONES

Altitude (km)	Maximum n_e (cm^{-3})	
	Measured	Computed
60	5.3×10^3	4.5×10^3
65	1.3×10^4	9.6×10^3
70	1.7×10^4	1.6×10^4
75	2.4×10^4	2.4×10^4
80	3.5×10^4	3.5×10^4
85	5.2×10^4	7.0×10^4
90	1.26×10^5	1.1×10^5

Other studies of D-region chemistry during solar flares have been reported by Mitra and Rowe (1972), Deshpande and Mitra (1972), and Deshpande *et al.* (1972). They have noted that the effective recombination rate coefficients α_{eff} at 70–80 km are reduced during a flare, compared with nonflare conditions. Our results in Table II support this conclusion. The model computations at 80 km at the flare maximum indicate that 40% of the positive ions are O_2^+ and NO^+ , there being insufficient time for complete conversion to complex ions. Before the flare, essentially all the positive ions at 80 km were polyatomic, consisting mainly of hydrated H_3O^+ complexes, with recombination rate coefficients close to $3 \times 10^{-6} \text{ cm}^3/\text{s}$.

Determinations of α_{eff} in the midlatitude D-region under moderately disturbed conditions have been reported by Larsen *et al.*, 1976. Below 80-km altitude their values of α_{eff} are substantially larger than our values in Table II. Again the difference is attributable to the reduced concentrations of large complex ions existing during the solar flare as contrasted with the predominant proportions of large complexes that occur under more normal conditions.

Large amounts of NO and atomic N are produced by the flare. The increment in NO concentration at 75 km was computed to be 10^6 cm^{-3} , and at 100 km it was 10^7 cm^{-3} . The increment of N concentration was about 10^6 between 80 and 100 km. Over the next few hours the extra N atoms and some of the NO are consumed in the reaction

However, much of the extra NO still remains after 24 hours.

IV. DISCUSSION

We have adjusted, or expressed an opinion on, the values of three rate coefficients [Reactions (2), (4), and (5)] and also the concentration of H_2O , based on the measured maximum electron densities at seven altitudes. Even with the adjusted rate coefficients, the computed electron densities do not fit the data perfectly, and one could ask to what extent the adjustments are to be believed. The answer varies from case to case, but we can proceed as follows: Upon request, at each altitude, the computer code lists out the rates ($\text{cm}^{-3}\text{s}^{-1}$) of each of the most important reactions for electrons and for each ion species. For a given altitude and time, with these listings for guidance, one can

construct an approximate steady-state model leading to a set of algebraic equations for a set of species concentrations. With these equations one can then estimate the sensitivity of the computed n_e to changes in specific rate coefficients, or to specific neutral species concentrations such as H_2O , $\text{O}_2(^1\Delta)$, or O . The results can be checked later by running the full numerical model.

With respect to the sensitivity of n_e at 60 to 65 km to changes in k_2 , it is found that reducing k_2 from 1×10^{-9} to $5 \times 10^{-10} \text{ cm}^3/\text{s}$ leads to a 17% reduction of n_e . A factor-of-2 reduction of $\text{O}_2(^1\Delta)$ concentration would produce the same effect. As noted previously, the computed $\text{O}_2(^1\Delta)$ depends somewhat on the assumed H_2O concentration. However, it is probably still reliable to within a factor of 2. A rocket measurement of $\text{O}_2(^1\Delta)$ at 60 km gave a concentration of 2.3 ppmv (in late afternoon at White Sands, New Mexico; Evans and Llewellyn, 1970), which is 13% lower than our computed value.

We investigated several other reactions that might affect the electron densities at 60 to 65 km. One was

which was found by Fehsenfeld *et al.* to be slow compared with

(See Bortner and Baurer, 1978.) Fehsenfeld (1987) estimated an upper limit of k_6 to be $2 \times 10^{-11} \text{ cm}^3/\text{s}$. With this upper limit we found that Reaction (6) did not have a significant effect on the n_e .

The electron concentrations at 60–65 km could also be affected by reactions that convert O_2^- to complex negative ions (O_4^- , O_3^- , CO_4^- , CO_3^-), or the reverse. Not all of the possible exothermic reactions in this class have been studied. We arbitrarily assumed the existence of three reactions,

and

all with the same nominal rate coefficient of $1 \times 10^{-10} \text{ cm}^3/\text{s}$. With this assumed rate coefficient they produced only an insignificant effect on the n_e . We have also included the processes of photodetachment from CO_3^- , CO_4^- , and NO_3^- , using rate coefficients derived from the cross-section measurements of Hodges *et al.*, 1980. These photodetachment reactions turn out to be quite important in the lower D-region before the flare (see also Thomas and Bowman, 1986) but unimportant during the flare.

For the 80- to 85-km regime we need to know the sensitivity of n_e to hypothetical changes in k_4 , k_5 , and the H_2O and O concentrations. The result of the analytic steady-state model showed that at 80 km a 50% reduction of the product of k_4 times $n_{\text{H}_2\text{O}}$ results in a 12% increase of n_e . At 85 km a factor-of-2 increase in the product of k_5 times n_{O} produces an 8% increase of n_e . To improve agreement between the computed and measured n_e , we chose the larger of the two measured values of k_4 (that of Fehsenfeld *et al.*, 1971), and we adjusted the rate constant k_5 . The sensitivity of n_e to either of these adjustments individually was fairly weak, and both were required simultaneously. The adjustments of k_4 and k_5 led to good agreement at 80 km, but there is a persistent discrepancy at 85 km.

Two other reactions that could affect electron densities in the 80–90-km range are

and

To our knowledge Reaction (10) has never been observed directly nor its rate coefficient measured. We would expect it to be relatively fast so that at 85 km it could contribute significantly to the net rate of conversion of "impermanent" and/or photodecomposable complex ions, such as O_4^+ and $O_2^+ \cdot H_2O$, to "permanent" complex ions such as $H_3O^+ \cdot W_n$. We have assumed $k_{10} = 1 \times 10^{-9}$ cm^3/s . With its assumed rate coefficient, Reaction (10) does contribute to the conversion of the impermanent complex ions to permanent ones, but it does not produce a noticeable change in electron densities.

With respect to Reaction (11), only an upper limit has been determined for the rate coefficient, namely $k_{11} \leq 1 \times 10^{-15}$ cm^3/s (Ferguson et al., 1965). Bortner and Baurer (1978) list the "estimate" $k_{11} = (1) [-16_{-3}^{+1}]$ cm^3/s , where the bracket indicates the power of 10 with error bars. If $k_{11} = 1 \times 10^{-16}$, Reaction (11) is the fastest process for forming NO^+ at 80 to 90 km during the flare and has a substantial influence on the relative proportions of NO^+ and O_2^+ and their respective families of complex ions. It can therefore affect the effective recombination coefficient α_{eff} , although the functional dependency is weak. The value $k_{11} = 1 \times 10^{-16}$ cm^3/s is reasonably consistent with the flare n_e data at 80-90 km. Increasing k_{11} to 1×10^{-15} cm^3/s would lead to a bad discrepancy at 90 km. Reducing k_{11} to 1×10^{-17} cm^3/s leads to a 4% increase in n_e at 90 km and slightly better agreement with the data. The computed n_e at 90 km are still 15% lower than the data, and this discrepancy could be attributable to our possible underestimate of the flare x-ray flux beyond 8 Å. (See Appendix C, Table C-I.)

To summarize, we believe that the 60- to 65-km data give a rather clear indication of the need for an increased value of k_2 (i.e., 1×10^{-9} cm^3/s). The 80- to 85-km data indicate a need for choosing the larger value of k_4 and for adjusting k_5 downward. Our other rate coefficient adjustments were more in the realm of speculation.

The flare n_e data do not suggest a clear preference for water vapor concentrations either above or below the nominal mesospheric average values. A larger-than-normal H_2O concentration would lead to better agreement at 85 km, but a smaller-than-normal concentration would be preferable at 60 to 65 km.

There are still fairly conspicuous discrepancies between the computed and measured n_e at 65 km and 85 km, which we have not been able to fix with any plausible adjustments of rate coefficients, H_2O concentrations, eddy diffusion coefficients, or NO concentrations.

Thus far the experimental radar backscatter data have been analyzed only to the point of providing electron densities. In principle, the data also contain information on the mean ion mass, on the temperature ratio T_e/T_i , and on negative ion densities. (See Ganguly *et al.*, 1979; Ganguly 1984a,b; Ganguly and Coco, 1982 and 1987; Mathews, 1986.) Experimental knowledge of these quantities would be useful as further checks on our computer model.

It will be observed that the computer model we have used contains some details that are of minor importance within the limited ranges of time and altitude of interest for the solar flare problem. Some of these are (1) the full treatment of diffusion and vertical transport, (2) inclusion of the F-region and topside ionosphere (19 layers extending to 1300 km), and (3) the full treatment of the neutral chemistry (55 species and 836 reactions). On the other hand, parts of the neutral chemistry model were necessary for setting up the initial conditions for the flare problem [e.g., for computing $O_2(^1\Delta)$ and atomic O concentrations]. Moreover, our long-term objective is the development and testing of a self-consistent mesosphere-thermosphere-ionosphere computer model, and this solar flare analysis is a part of that program.

V. CONCLUSIONS

We have made a detailed set of measurements of electron density vs time at several D-region altitudes during a large solar flare. Solar x-ray flux data were also available for the same time period in several wavelength bands from which we computed ionization rates vs time and altitude. From the ionization rates and a chemistry model we computed electron densities that could be compared with the electron density data. We found that fairly good agreement between the computations

and the data could be obtained after adjusting the values of three rate coefficients that were not otherwise well known [Reactions (2), (4), and (5)].

The data and computations both show a transition from complex positive ions to diatomics at about 85-km altitude. During the flare, negative ions are important below 65-km altitude and unimportant above.

We believe that the present combined set of solar flare ionospheric data and x-ray flux data is the most complete set available to date. They were complete enough to warrant a major theoretical analysis effort, which we have attempted to describe.

VI. ACKNOWLEDGMENTS

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APPENDIX A

ANALYSIS OF THE INCOHERENT SCATTER DATA

The analysis of the incoherent scatter data was based on now-standard techniques that were designed originally by Ganguly (Ganguly *et al.*, 1979) and are described elsewhere (Mathews, 1986; Mathews *et al.*, 1982; Ganguly 1984a,b, 1985; Coco, 1981; Ganguly and Coco, 1987.)

Because of the rapidly changing conditions during the solar flare the backscatter signal-integration time was reduced to 100 seconds, where 30 minutes is more common for D-region measurements. Use of the short integration time was possible because of the substantially enhanced electron densities that occurred in the D-region during the flare. The associated uncertainties in signal power $\Delta P_s/P_s$ at the time of the flare peak were close to 1% at all D-region altitudes. At any given altitude the uncertainties in relative electron densities as functions of time were probably less than 5%.

In determining absolute electron densities from the data we applied the antenna beam pattern correction factors (G') computed by Breakall and Mathews (1982). The correction is largest at the lowest altitude (60 km), where it amounts to 11%. However, at D-region altitudes there may exist additional fine-scale (kilometer-size) interference fringe effects not accounted for in the Breakall-Mathews analysis, and it is possible that these fringe effects could introduce errors of 10 to 20% in the absolute electron densities vs altitude.

In deriving electron densities from backscatter power it was assumed that the electron and ion temperatures were equal, as is customary for D-region measurements. However, it is conceivable that this assumption could break down in the upper D-region at the peak of the solar flare. We hope to examine this question in the future.

APPENDIX B

CHEMISTRY

The chemistry module includes 836 reactions in all. Most of these are reactions between neutral species and are not of particular importance for flare ionization chemistry. Of the 836 reactions, 570 involve ions and/or electrons, but of these only a subset of about 150 are important for determining electron densities in the D-region, particularly during a solar flare. We instructed the computer to identify those reactions, and they are listed in Table B-I, along with their rate coefficients and literature references and occasional notes. The notation for Table B-I appears at the end of the table.

In addition to the set of ordinary reaction rate coefficients, it is also necessary to specify the fractional number of each species of ion, atom, or excited molecule that is produced in direct association with each x-ray-induced ionization event. In the D- and E-regions the rate of production of species i can be written as

$$Q_i = Q(a_{i,N_2}n_{N_2} + a_{i,O_2}n_{O_2} + a_{i,O}n_O)/(n_{N_2} + n_{O_2} + n_O), \quad (B-1)$$

where Q is the ionization rate due to x rays or energetic electrons ($\text{cm}^{-3}\text{s}^{-1}$); the n_{N_2} , n_{O_2} , and n_O are number densities of N_2 , O_2 , and O , respectively; and the a_{i,N_2} , a_{i,O_2} , and $a_{i,O}$ are coefficients whose values are listed in Table B-II. The a_{i,N_2} and a_{i,O_2} entries in Table B-II are all derived from the computations of Myers and Schoonover (1976), except for the $N(^2D)$ entry, which is derived from experimental data by Green *et al.* (1984).

Since the computed ion chemistry is strongly influenced by the computed neutral composition, we show in Fig. B-1 an altitude profile of the neutral composition computed for 1328 GMT, just before commencement of the flare. The computation was run with eddy diffusion coefficients from Allen *et al.*, 1981.

TABLE B-1
DOMINANT ELECTRON AND ION REACTIONS WITH RATE COEFFICIENTS AND REFERENCES^{a, b}

Reactants		Products		A	B	C	Reference
e	O	O ⁻	+ hv	1.30E-15	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	O ₂	O ₂ ⁻	+ hv	2.00E-19	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	NO ₂	M[1.1E+17] NO ₂ ⁻		3.50E-28	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	O ₂	M O ₂ ⁻		1.14E-30	0.0	273.	Bortner and Baurer, 1978 (DNA 1948H)
e	O ₃	O ⁻ O ₂		9.00E-12	1.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	e W ₂ H ₃ O ⁺	e H	3H ₂ O	7.00E-20	-4.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	WNO ⁺ M	H ₂ O NO	M	6.00E-27	-2.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	W ₂ NO ⁺ M	NO 2H ₂ O	M	6.00E-27	-2.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	OH ₂ NO ⁺ M	2H ₂ O M		6.00E-27	-2.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	W ₃ NO ⁺ M	NO 3H ₂ O	M	6.00E-27	-2.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	W ₂ H ₃ O ⁺ M	H 3H ₂ O	M	6.00E-27	-2.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	NOCO ₂ ⁺	NO CO ₂		1.50E-06	-0.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	WNO ⁺	NO H ₂ O		1.50E-06	-0.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	W ₂ O ⁺	2O H ₂ O		1.50E-06	-0.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	H ₃ O ⁺	H H ₂ O		1.30E-06	-0.7	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	W ₂ NO ⁺	NO 2H ₂ O		3.00E-06	-0.2	0.	Estimate
e	OH ₂ NO ⁺	H ₂ O H	OH	2.00E-06	-0.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	WH ₃ O ⁺	H 2H ₂ O		2.50E-06	-0.1	0.	Huang et al., 1978
e	W ₃ NO ⁺	NO		3.00E-06	-0.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	W ₂ H ₃ O ⁺	H 3H ₂ O		3.00E-06	-0.1	0.	Huang et al., 1978
e	NO ⁺	O N(2D)		4.00E-07	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	N ₂ ⁺	2N(2D)		1.80E-07	-0.4	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	O ₂ ⁺	O O(1D)		1.89E-07	-0.6	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	O ₂ ⁺	O O(1S)		2.10E-08	-0.6	0.	Bortner and Baurer, 1978 (DNA 1948H)
e	O ₄ ⁺	2O O ₂		2.00E-06	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
CO ₃ -	W ₂ NO ⁺ [1.5E+19]	NO CO ₂	O 2H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
CO ₃ -	OH ₂ NO ⁺ [1.5E+19]	CO ₂ O	2H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
CO ₃ -	W ₃ NO ⁺ [1.5E+19]	CO ₂ O NO	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
CO ₄ -	W ₃ NO ⁺ [1.5E+19]	CO ₂ O ₂ NO	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
CO ₃ -	W ₂ H ₃ O ⁺ [1.5E+19]	CO ₂ O H	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
CO ₄ -	W ₂ H ₃ O ⁺ [1.5E+19]	CO ₂ O ₂ H	2H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ⁻	NOCO ₂ ⁺ [1.5E+19]	O CO ₂ NO		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ₂ -	NOCO ₂ ⁺ [1.5E+19]	O ₂ CO ₂ NO		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
CO ₃ -	NOCO ₂ ⁺ [1.5E+19]	2CO ₂ O NO		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ⁻	WNO ⁺ [1.5E+19]	NO O H ₂ O		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
NO ₃ -	WNO ⁺ [1.5E+19]	NO ₂ O NO	H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ⁻	W ₂ NO ⁺ [1.5E+19]	NO O	2H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ₂ -	W ₂ NO ⁺ [1.5E+19]	NO O ₂ 2H ₂ O		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
NO ₃ -	W ₂ NO ⁺ [1.5E+19]	NO ₂ O NO	2H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ⁻	OH ₂ NO ⁺ [1.5E+19]	O 2H ₂ O		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ₂ -	OH ₂ NO ⁺ [1.5E+19]	O ₂ 2H ₂ O		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
NO ₃ -	WH ₃ O ⁺ [1.5E+19]	NO ₂ OH	2H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ⁻	W ₃ NO ⁺ [1.5E+19]	O NO	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ₂ -	W ₃ NO ⁺ [1.5E+19]	O ₂ NO	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
NO ₃ -	W ₂ H ₃ O ⁺ [1.5E+19]	NO ₂ OH	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ⁻	W ₂ H ₃ O ⁺ [1.5E+19]	O H	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ₂ -	W ₂ H ₃ O ⁺ [1.5E+19]	O ₂ H	3H ₂ O	6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
NO ₃ -	O ₂ ⁺ [1.0E+19]	NO ₂ O O ₂		1.30E-07	-0.5	(3.E-25)	Bortner and Baurer, 1978 (DNA 1948H)
NO ₃ -	O ₄ ⁺ [1.5E+19]	2O ₂ O NO ₂		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
NO ₂ -	NO ⁺ [1.0E+19]	2NO O		1.00E-07	-0.5	(3.E-25)	Bortner and Baurer, 1978 (DNA 1948H)
NO ₃ -	NO ⁺ [1.0E+19]	NO ₂ O NO		9.00E-08	-0.5	(3.E-25)	Bortner and Baurer, 1978 (DNA 1948H)
O ⁻	N ₂ NO ⁺ [1.5E+19]	NO O N ₂		6.90E-08	-0.4	(2.E-25)	Smith and Church, 1977
O ₂ -	O ₂ (DL)	e 2O ₂		1.00E-09	0.0	0.	See Text
O ⁻	CO	e CO ₂		6.00E-10	-0.3	0.	Bortner and Baurer, 1978 (DNA 1948H)
CO ₃ -	O	e O ₂ CO ₂		2.00E-11	0.0	0.	Upper limit, Fehsenfeld et al., 1979
O ⁻	H ₂	e H ₂ O		6.00E-10	-0.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
O ⁻	O	e O ₂		2.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O ⁻	O ₂ (DL)	e O ₃		3.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O ₂ -	O	e O ₃		1.50E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O ₃ -	O	e 2O ₂		1.00E-11	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
W ₂ O ₂ ⁺	O ₂ (DL)	O ₂ ⁺ H ₂ O O ₂		1.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
N ⁺	O ₂	O ₂ ⁺ N		2.00E-10	0.0	0.	Albritton, 1978; O'Keefe et al., 1986
N ⁺	O ₂	O ₂ ⁺ N(2D)		8.40E-11	0.0	0.	Albritton, 1978; O'Keefe et al., 1986
O ₂ ⁺	NO	NO ⁺ O ₂		4.50E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
N ₂ ⁺	O	O ⁺ N ₂		1.00E-11	-0.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
N ₂ ⁺	O ₂	O ₂ ⁺ N ₂		5.00E-11	-0.8	0.	Bortner and Baurer, 1978 (DNA 1948H)
N ₄ ⁺	O ₂	O ₂ ⁺ 2N ₂		2.50E-10	0.0	0.	Albritton, 1978
O ⁺	O ₂	O ₂ ⁺ O		2.00E-11	-0.4	0.	Bortner and Baurer, 1978 (DNA 1948H)
O ₄ ⁺	O ₂ (DL)	O ₂ ⁺ 2O ₂		1.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
NOCO ₂ ⁺	H ₂ O	WNO ⁺ CO ₂		1.00E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
N ₂ NO ⁺	CO ₂	NOCO ₂ ⁺ N ₂		1.00E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O ⁺	CO ₂	O ₂ ⁺ CO		1.10E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)

TABLE B-I (Continued)

Reactants	Products	A	B	C	Reference
N2O2+ H2O	WO2+ N2	4.00E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
N2NO+ H2O	WNO+ N2	1.00E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
WNO+ N2	N2NO+ H2O	4.19E-11	-1.4	5267.	Reverse
O4+ H2O	WO2+ O2	2.20E-09	0.0	0.	Albritton, 1978
WNO+ OH	H3O+ NO2	6.00E-11	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
WNO+ HO2	H3O+ NO	5.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
WO2+ H	H3O+ O2	1.00E-09	0.0	0.	See Text
WO2+ H2	H3O+ HO2	3.00E-10	0.0	0.	Estimate
WO2+ H2O	H3O+ OH	5.71E-07	0.0	2266.	Bortner and Baurer, 1978 (DNA 1948H)
WO2+ H2O	OHH3O+ O2	1.00E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
OHH3O+ H2O	WH3O+ OH	1.40E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
W3NO+ H2O	W2H3O+ OH	7.00E-11	0.0	0.	Albritton, 1978; (Products altered)
N+ O2	NO+ O	5.00E-11	0.0	0.	Albritton, 1978; O'Keefe et al., 1986
N+ O2	NO+ O(1L)	2.00E-10	0.0	0.	Albritton, 1978; O'Keefe et al., 1986
N+ O2	O+ NO	2.80E-11	0.0	0.	Albritton, 1978; O'Keefe et al., 1986
O+ N2	NO+ N	1.20E-12	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
N2+ O	NO+ N(2D)	1.30E-10	-0.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2+ N2	NO+ NO	1.00E-17	0.0	0.	See Text
N2O2+ O2	O4+ N2	1.00E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O4+ N2	N2O2+ O2	7.54E-09	0.2	1897.	Reverse
O4+ O	O2+ O3	1.00E-10	0.0	0.	See Text
CO4- O2(DL)	O2- CO2	4.00E-10	0.0	0.	See Text
CO4- O3	O3- O2	1.30E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2- NO2	NO2- O2	1.20E-09	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2- O	O- O2	1.50E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O- O3	O3- O	5.30E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2- O3	O3- O2	4.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O4- O3	O3- 2O2	3.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
CO3- NO	NO2- CO2	1.10E-11	-1.1	0.	Bortner and Baurer, 1978 (DNA 1948H)
CO3- NO2	NO3- CO2	2.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
CO3- O	O2- CO2	1.10E-10	0.0	0.	Albritton, 1978
CO4- O	CO3- O2	1.50E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O3- CO2	CO3- O2	5.50E-10	-0.5	0.	Bortner and Baurer, 1978 (DNA 1948H)
CO3- O2	O3- CO2	3.70E-11	0.6	4043.	Reverse
CO3- O2(DL)	O3- CO2	1.00E-10	0.0	0.	See Text
O4- CO2	CO4- O2	4.30E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
CO4- O2	O4- CO2	7.72E-12	0.1	2433.	Reverse
CO3- O3	O2- CO2	1.00E-10	0.0	0.	See Text
O3- NO2	NO3- O2	2.00E-11	0.0	0.	Bortner and Baurer, 1975 (DNA 1948H)
NO2- O3	NO3- O2	1.80E-11	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O3- O	O2- O2	3.20E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O4- O	O3- O2	4.00E-10	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
H3O+ H2O	WH3O+ N2	3.40E-27	-4.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
H3O+ H2O	WH3O+ O2	3.70E-27	-2.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
WH3O+ H2O	W2H3O+ N2	2.30E-27	-2.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
WH3O+ H2O	W2H3O+ O2	2.00E-27	-4.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
NO+ CO2	NOCO2+ M	4.40E-29	-6.0	0.	Smith, Adams and Grief, 1977
NO+ H2O	WNO+ M	1.50E-28	-2.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2+ H2O	WO2+ M	2.80E-28	-2.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
WNO+ H2O	W2NO+ M	1.10E-27	-4.7	0.	Bortner and Baurer, 1978 (DNA 1948H)
W2NO+ H2O	W3NO+ M	1.60E-27	-4.7	0.	Bortner and Baurer, 1978 (DNA 1948H)
H3O+ OH	OHH3O+ M	5.39E-25	-0.7	0.	Reverse
O+ N2	NO+ N	6.00E-29	-2.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2+ N2	N2O2+ M	9.00E-31	-2.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
NO+ N2	N2NO+ M	4.00E-31	-4.4	0.	Smith, Adams and Grief, 1977
N2+ N2	N4+ M	5.00E-29	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2+ O2	O4+ M	3.90E-30	-3.2	0.	Bortner and Baurer, 1978 (DNA 1948H)
NOCO2+ M	NO+ CO2	9.20E-06	-7.0	5500.	Smith, Adams and Grief, 1977
W2NO+ M	WNO+ H2O	9.04E-03	-5.7	8100.	Bortner and Baurer, 1978 (DNA 1948H)
W3NO+ M	W2NO+ H2O	1.00E-02	-5.7	6800.	Bortner and Baurer, 1978 (DNA 1948H)
W2H3O+ M	WH3O+ H2O	2.00E-03	-5.0	10000.	Bortner and Baurer, 1978 (DNA 1948H)
N2O2+ M	O2+ N2	3.32E-06	-1.1	2857.	Reverse
N2NO+ M	NO+ N2	2.00E-08	-5.4	2100.	Smith, Adams and Grief, 1977
O4+ M	O2+ O2	2.42E-05	-4.2	5400.	Bortner and Baurer, 1978 (DNA 1948H)
O- O2	CO3- + hv	1.00E-17	0.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O- CO2	CO3- M	3.10E-28	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2- CO2	CO4- M	2.00E-29	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O- O2	O3- M	1.10E-30	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O2- O2	O4- M	3.50E-31	-1.0	0.	Bortner and Baurer, 1978 (DNA 1948H)
O4- M	O2- O2	2.20E-05	-1.0	6300.	Bortner and Baurer, 1978 (DNA 1948H)
NO + hv	NO+ e	2.25E-06			Huebner, 1979
N2 + hv	N2+ e	8.94E-07			Huebner, 1979
O2 + hv	O2+ e	1.30E-06			Huebner, 1979

TABLE B-I (Continued)

Reactants		Products		A	B	C	Reference
CO3-	+ hv	e	CO2	0	1.01E-02		Hodges et al., 1980
CO4-	+ hv	e	CO2	O2	3.79E-02		Hodges et al., 1980
NO2-	+ hv	e	NO2		3.83E-02		Hodges et al., 1980
NO3-	+ hv	e	NO	O2	3.83E-02		Hodges et al., 1980
O-	+ hv	e	O		1.16E+00		Lee and Smith, 1979; Hodges et al., 1980
O2-	+ hv	e	O2		3.43E-01		Lee and Smith, 1979; Hodges et al., 1980
O4-	+ hv	e	O2		2.10E-01		Lee and Smith, 1979; Hodges et al., 1980
WO2+	+ hv	O2+	H2O		5.72E-01		Smith and Lee, 1978
O4+	+ hv	O2+	O2		2.97E-01		Smith and Lee, 1978
CO3-	+ hv	O-	CO2		1.67E-01		Smith et al., 1979
CO4-	+ hv	O2-	CO2		1.40E-02		Bortner and Baurer, 1978 (DNA 1948H)
O4-	+ hv	O2-	O2		1.96E-01		Smith et al., 1979

^aHere "W" denotes H₂O, as in the complex ions WNO⁺ and WO₂⁺ (i.e., NO⁺·H₂O and O₂⁺·H₂O).

^bMost of the reaction rate coefficients are expressed in the form

$$k = A(T/300)^B \exp(-C/T),$$

and the quantities A, B, and C are listed in Table B-I. However, there are a few exceptions, as noted below.

A different format is used in the case of ion-ion recombination reactions. These reactions are all exoenergetic and have no activation energy. However, they proceed by parallel two-body and three-body reaction paths. For the general ion-ion recombination reaction $X^+ + Y^- \rightarrow \text{products}$, we represent the rate coefficient as

$$k = A(T/300)^B + C(T/300)^{(B-2.1)}[M],$$

where [M] is the third-body concentration. To emphasize the different connotation of "C" for these reactions, it is listed in Table B-I as a quantity in parentheses. Most of the entries for these reactions are generalizations from the data of Smith and Church (1977).

Some three-body reactions approach a second-order limit, as [M] is increased, beyond which a further increase in [M] does not increase the rate. For such reactions the limiting value of [M] is given in square brackets next to the reactants.

For photon reactions the rate coefficient values shown are as evaluated at the top of the atmosphere.

Rate coefficients referenced as "reverse" were computed from their opposite counterparts assuming detailed balance.

TABLE B-II
THE COEFFICIENTS FOR EQ. (B-1)

Species	a_{i,N_2}	a_{i,O_2}	$a_{i,O}$
e_-	0.9625	1.15	1
N_2^+	0.7875	0	0
N^+	0.175	0	0
N	0.55	0	0
$N(^2D)$	0.675	0	0
N_2	-2.310	0	0
$N_2(A^3\Sigma)$	0.738	0	0
O_2^+	0	0.80	0
O^+	0	0.35	1
O	0	1.15	-1
$O(^1D)$	0	0.65	0
$O_2(^1\Delta)$	0	3.85	0
$O_2(^1\Sigma)$	0	0.55	0
O_2	0	-6.275	0

Fig. B-1. Vertical profiles of computed neutral composition for 0900 LST (1328 GMT), just before onset of the flare.

APPENDIX C

COMPUTATION OF IONIZATION RATES FROM THE GOES-2 AND ISEE-3 FLUX DATA

Let λ be the wavelength in Angstroms and $F_\lambda(t, \lambda)$ the solar x-ray flux at the top of the atmosphere at time t per unit interval of λ (units of $\text{erg}/\text{cm}^2 \cdot \text{s} \cdot \text{\AA}$). For wavelengths below the nitrogen K absorption edge $\lambda_K \approx 31 \text{ \AA}$, the effective linear photoabsorption coefficient of air of number density n for photons of wavelength λ is

$$\bar{n}\bar{\sigma} = (n_{N_2}a_{N_2} + n_{O_2}a_{O_2} + n_O a_O)\lambda^3 \equiv (\bar{n}\bar{a})\lambda^3 \text{ cm}^{-1}, \quad (\text{C-1})$$

where n_{N_2} , n_{O_2} , and n_O are number densities (cm^{-3}) and a_{N_2} , a_{O_2} , and a_O are the photoabsorption cross sections (cm^2) for $\lambda = 1 \text{ \AA}$ for the species N_2 , O_2 , and atomic O. For a given altitude, solar zenith angle, and photon energy, the effective atmospheric optical thickness is

$$\tau = (N_{N_2}a_{N_2} + N_{O_2}a_{O_2} + N_O a_O)\lambda^3 \equiv (\bar{N}\bar{a})\lambda^3, \quad (\text{C-2})$$

where N_{N_2} , N_{O_2} , and N_O are the column densities (cm^{-2}) of N_2 , O_2 , and O along the line of sight to the sun. The 1- $\text{\AA}$ absorption cross sections are $a_{N_2} = 7.3 \times 10^{-23}$, $a_{O_2} = 1.14 \times 10^{-22}$, and $a_O = 5.7 \times 10^{-23} \text{ cm}^2$. Beyond the K edge ($\lambda > 31 \text{ \AA}$) the same expressions for $\bar{n}\bar{\sigma}$ and τ still apply, but a_{N_2} , a_{O_2} , and a_O are each reduced by a factor of 18. The local ion-pair production rate at altitude z and time t due to solar x rays with wavelengths shorter than $40 \text{ \AA}$ is

$$Q(z, t) = 1.78 \times 10^{10} (\bar{n}\bar{a}) \int_0^{40} \lambda^3 F_\lambda \exp(-\bar{N}\bar{a}\lambda^3) d\lambda \text{ cm}^{-3}\text{s}^{-1}, \quad (\text{C-3})$$

assuming that each ion pair requires the deposition of 35 eV of energy. The upper integration limit of $40 \text{ \AA}$ is arbitrary; photons of longer wavelength make a negligible contribution. We will assume that the solar x-ray spectral flux during the flare, $F_\lambda(t, \lambda)$, can be represented by a two-segment function composed of two power laws in λ that join continuously at $\lambda = 1.87 \text{ \AA}$ (the wavelength of the strong eXXV line that is commonly observed in solar flares). That is,

$$F_\lambda(t, \lambda) = \begin{cases} a_1 \lambda^{n_1} & \text{for } \lambda \leq 1.87 \text{ \AA} \\ a_2 \lambda^{n_2} & \text{for } \lambda \geq 1.87 \text{ \AA} \end{cases} \quad (\text{C-4a})$$

where a_1 , a_2 , n_1 , and n_2 are all functions of time, and they are to be determined from the GOES-2 and ISEE-3 flux data. Coefficients a_1 and a_2 are also related by the continuity condition

$$a_1 (1.87)^{n_1} = a_2 (1.87)^{n_2}. \quad (\text{C-4b})$$

Now let Φ_a , Φ_b , and Φ_c be the three measured flux integral values for the nominal wavelength bands 0.29–0.48 $\text{\AA}$, 0.5–4 $\text{\AA}$, and 1–8 $\text{\AA}$, respectively, at a given instant of time (in units of $\text{erg}/\text{cm}^2 \cdot \text{s}$). Φ_a is measured by satellite ISEE-3, and Φ_b and Φ_c are measured by GOES-2. To fit the spectral parameters a_1 and a_2 , n_1 and n_2 to the data Φ_a , Φ_b , and Φ_c , we equate

$$\Phi_a = \int_{0.29}^{0.48} F_\lambda d\lambda = A_1 (0.48^{n_1} - 0.29^{n_1}) \quad (\text{C-5a})$$

$$\Phi_b = \int_{0.5}^4 F_\lambda d\lambda = A_1 (1.87^{n_1} - 0.5^{n_1}) + A_2 (4^{n_2} - 1.87^{n_2}) \quad (\text{C-5b})$$

$$\Phi_c = \int_1^8 F_\lambda d\lambda = A_1 (1.87^{n_1} - 1^{n_1}) + A_2 (8^{n_2} - 1.87^{n_2}) \quad (\text{C-5c})$$

where

$$\begin{aligned} m_1 &\equiv n_1 + 1, \quad m_2 \equiv n_2 + 1, \\ A_1 &\equiv a_1/m_1, \quad \text{and} \quad A_2 \equiv a_2/m_2. \end{aligned} \quad (\text{C-5d})$$

Also, from Eq. (C-4b),

$$A_2 m_2 (1.87)^{m_2} = A_1 m_1 (1.87)^{m_1}. \quad (\text{C-5e})$$

Equations (C-5a) through (C-5c) and (C-5e) constitute four equations for the four unknowns A_1, A_2, m_1 , and m_2 (or, alternatively, a_1, a_2, n_1 , and n_2). For each set of Φ_a, Φ_b , and Φ_c , they are solved iteratively with the computer.

We used this two-power-law representation of the x-ray spectrum in all the computations that we have described, with the results that were shown in Figs. 3-5. One may object that this representation was totally arbitrary, and we could have used any of an infinite variety of other spectral forms, all consistent with the given Φ_a, Φ_b , and Φ_c . It is known, for instance, that a flare x-ray spectrum contains many discrete coronal emission lines in addition to the continuum (although the continuum is dominant). To address the question of the sensitivity of the computed ionization rates $Q(z, t)$ to the assumed spectral form, we can at least examine the range of wavelengths that gives the largest contribution to $Q(z, t)$ at each given altitude. That is, we can evaluate the integral in Eq. (C-3), namely

$$\frac{dQ}{d\lambda}(z, t) = 1.78 \times 10^{10} (\bar{n}a) \lambda^3 F_\lambda \exp(-\bar{N}a\lambda^3), \quad (\text{C-6})$$

and look for the maxima. Some results for the case of the two-power-law spectrum at the time when the 1-8-Å flux Φ_c is maximum are shown in the second column of Table C-I for each of four altitudes.

TABLE C-I
WAVELENGTHS CORRESPONDING TO MAXIMUM $dQ/d\lambda$
AND FRACTIONAL CONTRIBUTION TO Q FROM WAVELENGTHS BEYOND 8 Å

Altitude (km)	$\lambda(\text{max } dQ/d\lambda)$ (Å)	Fraction of Q from $\lambda > 8 \text{ Å}$
60	1.7	0.0
70	2.1	0.0
80	3.7	0.00002
90	6.8	0.30

The results in Table C-I show that the wavelengths making the largest contribution to Q at the altitudes of interest are well within the spectral range covered by the x-ray detectors. (In fact, they are within the range covered by the GOES-2 detectors alone.) This fact helps to assure that the computed $Q(z, t)$ between 60 and 90 km should be fairly insensitive to the detailed shape of the assumed spectrum, as long as the flux integrals fit the measured Φ_a, Φ_b , and Φ_c (or even Φ_b and Φ_c alone).

Another test of the sensitivity of the $Q(z, t)$ to the spectrum F_λ is to examine the value of the fractional contribution to the $Q(z, t)$ integral [in Eq. (C-3), for given z and t] that comes from photons of wavelength greater than 8 Å, since 8 Å is the longest wavelength for which the GOES-2 or ISEE-3 x-ray detectors give any coverage. This fraction is tabulated in the third column of Table C-I. The results show that at 90 km, the $Q(z, t)$ are fairly sensitive to the longer wavelengths $\lambda > 8 \text{ Å}$, where the fluxes are unknown; below 90 km, they are not.

To further explore the question of sensitivity of the computed results to the assumed form of the spectrum, we made a separate set of computations using the "free-free-bound-free" (FFBF) spectrum described by Culhane and Acton (1970), viz:

$$F_{\lambda} = A \exp(-hc/\lambda kT) / \left[T^{0.2} \lambda^{1.7} \left\{ 1 - (7.1\lambda)^{-2.8 \times 10^{-4} T} \right\} \right], \quad (C-7)$$

where T is a parameter representing the coronal electron temperature (in degrees Kelvin). (See also Dere *et al.*, 1974.) The two parameters A and T (both functions of time) can be fitted to the GOES-2 measured fluxes Φ_b and Φ_c (without using the ISEE-3 flux data). When this was done and the ionization rates $Q(z,t)$ were computed, we found that at the times of flare flux maxima, at all altitudes between 60 and 90 km, the $Q(z,t)$ values computed with the Culhane-Acton spectrum agreed to within 10% with the values computed with the two-power-law function. Larger discrepancies were found at the time of the flux minimum. It was nevertheless encouraging to find that such a large change in spectral functional form produced such a small change in the $Q(z,t)$.

Figure C-1 shows a comparison of the fitted two-power-law spectrum vs the Culhane-Acton FFBF spectrum, both at the time of maximum Φ_C . The two are in fairly close agreement for $\lambda < 8 \text{ \AA}$, but they deviate above $8 \text{ \AA}$. Also shown are two measured x-ray flare spectra from the flares of 21 December 1967 and 26 October 1967, respectively (Culhane *et al.*, 1969). The two measured spectra showed a stronger λ -dependence in the 1-8- $\text{\AA}$ region than did the flare of 18 August 1979, but they were also considerably less intense.

Fig. C-1. Comparison of two fitted spectral flux functions for the time of maximum 1-8- $\text{\AA}$ flux. Curve A: two-power-law fit; Curve B: Culhane-Acton FFBF function ($T = 1.7\text{E}+7 \text{ K}$). Also shown are measured spectral flux data for two solar flares (Culhane *et al.*, 1969). Curve C: the flare of 21 December 1967; Curve D: the flare of 10 October 1967.

The spectral response functions of the two GOES-2 x-ray detectors, and their method of calibration, are described by Donnelly *et al.* (1977). The data from the two detectors (designated *b* and *c*) are reported as x-ray flux integrals $\Phi_b^o \equiv \Phi^o(0.5-4 \text{ \AA})$ and $\Phi_c^o \equiv \Phi^o(1-8 \text{ \AA})$. They are obtained from measurements of detector currents I_b and I_c , together with detector sensitivity coefficients $\bar{G}_b^o$ and $\bar{G}_c^o$, which are given by Donnelly *et al.* (1977) (their Table 3.3). That is,

$$\Phi_b^o = I_b / \bar{G}_b^o \quad (\text{C-8a})$$

and

$$\Phi_c^o = I_c / \bar{G}_c^o. \quad (\text{C-8b})$$

The standard sensitivity coefficients are based on an assumed standard normalized flare-like x-ray spectrum ϕ_λ^o . That is, they are computed as

$$\bar{G}_b^o = \int_0^\infty G_b(\lambda) \phi^o(\lambda) d\lambda / \int_{0.5}^4 \phi^o(\lambda) d\lambda \quad (\text{C-9a})$$

and

$$\bar{G}_c^o = \int_0^\infty G_c(\lambda) \phi^o(\lambda) d\lambda / \int_1^8 \phi^o(\lambda) d\lambda \quad (\text{C-9b})$$

where $G_b(\lambda)$ and $G_c(\lambda)$ are the instrumental response functions for the two detectors as determined in the laboratory. [The functions $G_b(\lambda)$, $G_c(\lambda)$, and $\phi^o(\lambda)$ are tabulated by Donnelly *et al.*]

Now for an actual or assumed solar x-ray spectrum $\phi(\lambda)$ that differs from the standard spectrum $\phi^o(\lambda)$, the standard detector sensitivity coefficients are not applicable, and we must compute new ones, namely

$$\bar{G}_b = \int_0^\infty G_b(\lambda) \phi(\lambda) d\lambda / \int_{0.5}^4 \phi(\lambda) d\lambda \quad (\text{C-10a})$$

and

$$\bar{G}_c = \int_0^\infty G_c(\lambda) \phi(\lambda) d\lambda / \int_1^8 \phi(\lambda) d\lambda. \quad (\text{C-10b})$$

Then from the measured detector currents the integrated x-ray fluxes can be determined, as

$$\Phi_b = I_b / \bar{G}_b \quad (\text{C-11a})$$

and

$$\Phi_c = I_c / \bar{G}_c. \quad (\text{C-11b})$$

The x-ray flux data are actually reported in terms of the standard integrated fluxes $\Phi^o(0.5-4)$ and $\Phi^o(1-8)$, instead of the detector currents I_b and I_c . However, combining Eqs. (C-8a,b) and (C-11a,b), we obtain

$$\Phi_b = \Phi_b^o \bar{G}_b^o / \bar{G}_b \quad (\text{C-12a})$$

and

$$\Phi_c = \Phi_c^o \bar{G}_c^o / \bar{G}_c. \quad (\text{C-12b})$$

That is, after we have determined a fitted spectrum $\phi(\lambda)$ [$\phi(\lambda)$ is to be identified with $F_\lambda(\lambda)$ in Eq. (C-3) et seq.], we can compute the correction factors $\bar{G}_b^o / \bar{G}_b$ and $\bar{G}_c^o / \bar{G}_c$ that must be applied to the reported flux values Φ_b^o and Φ_c^o to take account of the fact that the spectrum $\phi(\lambda)$ is not identical to the standard spectrum $\phi^o(\lambda)$. In practice we have found that the correction factors are very close to 1.

The ISEE-3 satellite also measures x-ray fluxes in several higher energy bands beyond the 0.29–0.48- $\text{\AA}$ band that we have used. We found that during the 18 August 1979 flare the fluxes in these bands were too low to contribute significantly to the air ionization above 55 km.

For about 5 minutes at the peak of the solar flare, the GOES-2 0.5–4- $\text{\AA}$ detector went into saturation (see Fig. 2). Before computing the ionization rates Q , shown in Fig. 3, we manually smoothed the 0.5–4- $\text{\AA}$ flux-vs-time curve to correct (approximately) for the saturation, as indicated by the dashed curve in Fig. 2(B).

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