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On Formulating a Simple D-Region Model

WILLIAM SWIDER



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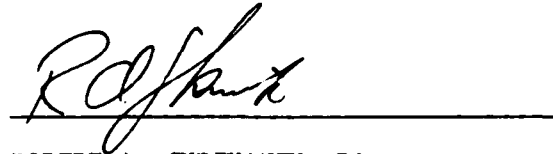
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<p>The ionization production rate q must be known and incorporated into the chemistry of the D-region to determine electron concentrations $\langle e \rangle$ as a function of altitude. There is some D-region research which supports a simple way to determine $\langle e \rangle$ once q is known. Thus, the daytime effective recombination coefficient, Ψ, appears to be relatively insensitive to q and can provide for the determination of $\langle e \rangle$. $\langle e \rangle = (q/\Psi)^{1/2}$ under steady-state conditions. For steady-state conditions at night, an equation exists which yields $\langle e \rangle$ with reasonable accuracy.</p>					
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Preface

This report was performed in support of an experimental program funded in part by the Defense Nuclear Agency (DNA). This report focuses on a body of work that suggests that the effective recombination coefficients in the daytime D-region are fairly invariant and thus lead to a rather simple solution for the electron concentrations. In addition, a quadratic expression is available for the estimation of electron concentrations at night.

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On Formulating a Simple D-Region Model

1. INTRODUCTION

The D-region is the smallest portion of the ionosphere by far. The vertical electron content of this layer is less than 0.01 percent that of the entire ionosphere, which is nominally $6 \times 10^{13} \text{ cm}^{-2}$ at mid-latitudes during daytime. Even for very disturbed conditions, the fractional content of the D-region does not exceed 1.0 percent. Nevertheless, the D-region is responsible for LF and VLF propagation, "survivable" communication modes. Furthermore, radio wave absorption can be appreciable in the disturbed D-region at higher frequencies like HF and VHF. It is well known for example, that HF radio waves can be totally absorbed during a Solar Proton Event (SPE), hence, the earlier common name, Polar Cap Absorption (PCA) event.

The large neutral but low charged particle concentrations of the D-region have made observations of this region difficult. Thrane¹ and Sechrist² have discussed these difficulties, plus the uncertainties associated with the various types of electron concentration measurements.

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1. Thrane, E. V. (1974) Methods of measurements and results of lower ionospheric structure, Akademie-Verlag, Berlin, pp. 3-21.
2. Sechrist, C.F., Jr. (1974) Comparison of techniques for measurements of D-region electron densities, Radio Sci. 9:137-149.

The D-region, with its attendant large neutral gas concentrations is much more difficult to model than the other (higher) layers of the ionosphere. Three-body processes are important. The composition of negative and positive ions is not simply related to the major gases, because minor species can play a role in three-body ion chemistry. (The chemistry of the higher ionospheric layers is limited to binary processes.)

Models of the D-region prior to about 1965 dealt with a very limited number of ionic species, like O_2^+ , NO^+ and O_2^- . The pioneering positive ion measurements of the D-region [Narcisi and Bailey³] showed that the dominant species were proton hydrate (PH) ions, $H_3O^+ \cdot (H_2O)_n$. Major negative ions include CO_3^- , HCO_3^- and NO_3^- [Arnold et al;⁴ Narcisi et al⁵]. The degree of hydration of these ions in the D-region is not great, especially for the first two of these ions [Keesee et al⁶]. Temperature and water vapor concentrations are key factors in the hydration level of these ions.

Models of the D-region are very complex since the distribution of minor species like NO and H_2O must be known. Temperatures are also required. Many of the ionic reactions depend strongly upon the temperature. Other minor species that participate in the chemistry of the D-region include O, O_3 , NO_2 , and CO_2 . Global models of these species and the temperature field are extremely difficult to formulate, although Brasseur and DeBaets⁷ have constructed a 2-D model of the D-region. However, an accurate, predictive model of the D-region is difficult to formulate and is cumbersome since so many parameters are required. Constant monitoring of the various minor species is impractical, although real time monitoring of energetic precipitating particles and/or x-rays must be undertaken for the modelling of disturbed events.

3. Narcisi, R.S., and Bailey, A.D. (1965) Mass spectrometric measurements of positive ions at altitude from 64 to 112 kilometers, J. Geophys. Res. 70:3687-3700.
4. Arnold, F., Kissel, J., Krankowsky, D., Wieder, H., and Zahringer, J. (1971) Negative ions in the lower ionosphere: A mass spectrometric measurement, J. Atmos. Terr. Phys. 33:1169-1175.
5. Narcisi, R.S., Bailey, A.D., Wlodyka, L.E., and Philbrick, C.R. (1972) Ion composition measurements in the lower ionosphere during the November 1966 and March 1970 solar eclipses, J. Atmos. Terr. Phys. 34:647-668.
6. Keesee, R.G., Lee, N., and Castleman, A.W., Jr. (1979) Atmospheric negative ion hydration derived from laboratory results and comparison to rocket-borne measurements in the lower ionosphere, J. Geophys. Res. 84:3719-3722.
7. Brasseur, G., and De Baets, P. (1986) Ions in the mesosphere and lower thermosphere: A two-dimensional model, J. Geophys. Res. 91:4025-4046.

Based upon all the knowledge gained over the last two decades particularly, and in view of the complexities for physically modelling the D-region, it will be argued here that this region may be equally well and much more simply modelled by the use of a bulk electron loss coefficient for the daytime and an analytical expression for nighttime. This approach is probably best for predictive purposes. This argument derives from a considerably rapid ion chemistry and a low level of ionization, that is, a fairly "frozen" chemistry [Swider⁸]. Charged particle concentrations never approach more than about 10^{-9} the total neutral particle concentrations.

2. EFFECTIVE RECOMBINATION COEFFICIENT OF THE DAYTIME D-REGION

The effective recombination coefficient of the D-region as derived from the continuity equation for electrons under steady state conditions and in the absence of transport processes is:

$$\Psi = (\alpha_D + \lambda\alpha_i)(1+\lambda) = q/[e]^2 \quad (1)$$

where α_D is the mean dissociative recombination coefficient, α_i is the mean ion-ion recombination coefficient, λ is the ratio of negative ions to electrons, q is the total ion-electron pair production rate, and $[e]$ is the electron concentration. The notation of Adams and Masley,⁹ Ψ for α_{eff} , has been adopted. They suggested that Ψ varies only with altitude. It appears that this suggestion is most likely to be true if minor neutral species are not involved with the ion chemistry, that is, if all chemistry is frozen (fast). However, Ψ does depend somewhat on q , $[H_2O]$, and temperature. (Some changes in certain significant minor neutral species concentrations are believed to occur for large ionization production rates [Swider and Keneshea,¹⁰ Solomon et al¹¹].)

8. Swider, W. (1988) Electron loss and the determination of electron concentrations in the D-region, PAGEOPH, in press.
9. Adams, G. W., and Masley, A. J. (1965) Production rates and electron densities in the lower ionosphere due to solar cosmic rays, J. Atmos. Terr. Phys. 27:289-298.
10. Swider, W., and Keneshea, T. J. (1973) Decrease of ozone and atomic oxygen in the lower mesosphere during a PCA event, Planet. Space Sci. 21:1969-1973.
11. Solomon, S., Reid, G. C., Rusch, D. W., and Thomas, R. J. (1983) Mesospheric ozone depletion during the solar proton event of July 13, 1982, Part II. comparison between theory and experiment, Geophys. Res. Lett. 10:257-260.

For the quiet D-region, the photo-ionization of NO by HLy α is the main source of electrons in the daytime. A rapid sequence of temperature-dependent three-body and "switching" reactions leads from NO⁺ ions to NO⁺·(H₂O)₃ ions and thence to proton-hydrate (PH) ions, H₃O⁺·(H₂O)_n, with the n = 2 ion formed first. Thus, water concentrations must be known as well as temperatures.

For disturbed conditions, O₂⁺ ions are the principal precursor ions for PH ions. (The more abundantly formed N₂⁺ ions are unobservable since charge transfer with O₂ is virtually instantaneous at D-region altitudes.) The sequence of three-body and "switching" reactions is much like that for NO⁺ in the quiet D-region, except that the n = 1 PH ion is now generated first. Another important difference is that an intermediate ion in the sequence, O₄⁺, reverts to O₂⁺ upon reaction with O, inhibiting the overall ion transition scheme somewhat.

At the top of the D-region, nominally 90 km, the major positive ions are usually O₂⁺ and NO⁺, and negative ion concentrations are negligible. Hence, the range for the effective recombination coefficient is rather limited,

$$\alpha(\text{O}_2^+) < \Psi (90 \text{ km}) < \alpha(\text{NO}^+) . \quad (2a)$$

The dissociative recombination coefficients of these ions are not very different. For a temperature of 190° K, approximate numerical values are:

$$3 \times 10^{-7} \text{ cm}^3 \text{ sec}^{-1} < \Psi (90 \text{ km}, 190^\circ \text{K}) < 6 \times 10^{-7} \text{ cm}^3 \text{ sec}^{-1} . \quad (2b)$$

At a somewhat lower height, as discussed below, an ionic scheme that begins with O₂⁺ and NO⁺ ions and ends with PH ions, H₃O⁺·(H₂O)_n becomes operative. The relative distribution of these ions comes into thermodynamic equilibrium at some lower height, roughly 65 km.

The transition altitude, where [NO⁺] + [O₂⁺] \approx \sum_n [H₃O⁺·(H₂O)_n], is principally a function of the parameters q, [H₂O] and T. For the quiet D-region, this altitude generally is near 82 km in the daytime and near 86 km at night [Narcisi¹²]. This altitude becomes lower, 5-10 km at most, as q is enhanced. The transition altitude decreases as q increases because with an increase of q (and [e]), dissociative recombination of NO⁺ and O₂⁺ increases, but not their rate of conversion to PH ions.

12. Narcisi, R.S. (1974) Ion and neutral composition measurements in the lower ionosphere in Lower Ionosphere Studies, Akademie Verlag, Berlin.

In any case, the transition from $\alpha(O_2^+)$ and $\alpha(NO^+)$ to $\alpha(PH)$ is not of very much importance inasmuch as rate coefficients for PH ions are only 4-5 times those for NO^+/O_2^+ ions and depend little upon temperature. Values of α_D are $(3.0 \pm 0.5) \times 10^{-6} \text{ cm}^3 \text{ sec}^{-1}$ for $H_3O^+ - H_7O_3^+$ ions and about $5 \times 10^{-6} \text{ cm}^3 \text{ sec}^{-1}$ for the next two heavier hydrates [Huang et al¹³]. Thus, at 75 km, where negative ions are still insignificant, $\Psi \approx 4 \times 10^{-6} \text{ cm}^3 \text{ sec}^{-1}$ is a good estimate for most conditions. (The heights 80 and 85 km are near the transition level.)

Negative ions become plentiful near 70 km, basically the consensus altitude, $z(\lambda_1)$, for where $\lambda = 1$. Thomson scatter data (Ganguly et al¹⁴) agree with this altitude. Now it is a convenient circumstance that the ion-ion recombination coefficients of D-region ions neither differ substantially from one another [Smith et al¹⁵] nor vary much with temperature, perhaps $T^{-1/2}$ [Smith and Church¹⁶]. (Figure 3 of the latter paper is an excellent summary of α_D and α_i from ground level to 90 km.) Thus, for the lower half of the D-region, the effective recombination coefficient may be expressed as (see Eq. (1)):

$$\Psi = (4 \times 10^{-6} + 6 \times 10^{-8} \lambda)(1 + \lambda) \quad (3)$$

since α_D remains near $4 \times 10^{-6} \text{ cm}^3 \text{ sec}^{-1}$ and α_i is about $6 \times 10^{-8} \text{ cm}^3 \text{ sec}^{-1}$. This equation can provide guidance as to λ , if Ψ is well-determined, that is $\lambda = 1$ where $\Psi \approx 8 \times 10^{-6} \text{ cm}^3 \text{ sec}^{-1}$ and $\lambda = 10$ where $\Psi \approx 5 \times 10^{-5} \text{ cm}^3 \text{ sec}^{-1}$.

Two relatively well-determined profiles for Ψ were deduced from the SPEs of November 1969 and August 1972. The former event was exceptionally well covered with much in-situ data and both satellite and rocket-based observations of the precipitating proton fluxes in a program largely sponsored by DNA. The crosses in Figure 1 represent Ψ for this event from as many as four separate results

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13. Huang, C.-M., Whitaker, M., Biondi, M.A., and Johnsen, R. (1978) Electron-temperature dependence of recombination of electrons with $H_3O^+ \cdot (H_2O)_n$ -series ions, Phys. Rev. A. 18:64-67.
 14. Ganguly, S., Matthews, J.D., and Tepley, C.A. (1979) Thomson scatter radar detection of D-region negative ions at Arecibo, Geophys. Rev. Lett. 6:89-92
 15. Smith, D., Adams, N.G., and Church, M.J. (1976) Mutual neutralization rates of ionospherically important ions, Planet. Space Sci. 24:697-703.
 16. Smith, D., and Church, M.J. (1977) Ion-ion recombination rates in the earth's atmosphere, Planet Space Sci. 25:433-439.

[Swider and Dean;¹⁷ Ulwick¹⁸]. Good agreement with some other results has been noted [Swider and Dean¹⁷], and the data have been matched well with a model [Swider et al¹⁹].

Circles in Figure 1 represent mean Ψ for five instances during the very intense SPE of 3-11 August 1972 [Reagan and Watt²⁰]. Electron concentrations were obtained with backscatter radar. The lowest altitude data may suffer from the neglect of negative ions upon the radar signals.

Shown also in the figure is Gledhill's²¹ least squares fits to all the Ψ -values in the literature for both quiet and disturbed (SPE, SPA, Flare) conditions. These two lines do not differ substantially from one another and underscore that the level of ionization has little bearing upon Ψ , except to shift the simple ion/PH ion transition altitude, which is a function of q , H_2O , and T . The scatter shown in Gledhill's report, particularly in the upper D-region, is much larger than can be tolerated on the basis of the chemistry outlined above. In addition, a least squares fit is somewhat misleading for the lower altitudes where a curved rather than a linear fit is undoubtedly proper. Attachment becomes more important with decreasing altitude and the initial process is dependent on the square of the neutral concentration. The divergence of these curves below 65 km is questionable. On the other hand, the higher Ψ values above 70-75 km for the quiet curve is consistent with the notion that Ψ increases as q decreases since dissociative recombination of electrons with PH ions rather than O_2^+ or NO^+ is more probable as these ions have a greater chance to transition to PH ions prior to dissociative recombination when $[e]$ is low.

17. Swider, W., and Dean, W. A. (1975) Effective electron loss coefficient of the disturbed D-region, J. Geophys. Res. 80:1815-1819.
18. Ulwick, J. C. (1973) Steady state coefficients in the D-region during solar particle events, Space Res. 13:581-586.
19. Swider, W., Keneshea, T. J., and Foley, C. A. (1978) An SPE-disturbed D-region model, Planet. Space Res. 26:883-892.
20. Reagan, J. B., and Watt, T. M. (1976) Simultaneous satellite and radar studies of the D-region ionosphere during the intense solar particle events of August 1972, J. Geophys. Res. 81:4579-4596.
21. Gledhill, J. A. (1986) The effective recombination coefficient of electrons in the ionosphere between 50 and 150 km, Radio Sci. 21:399-408.

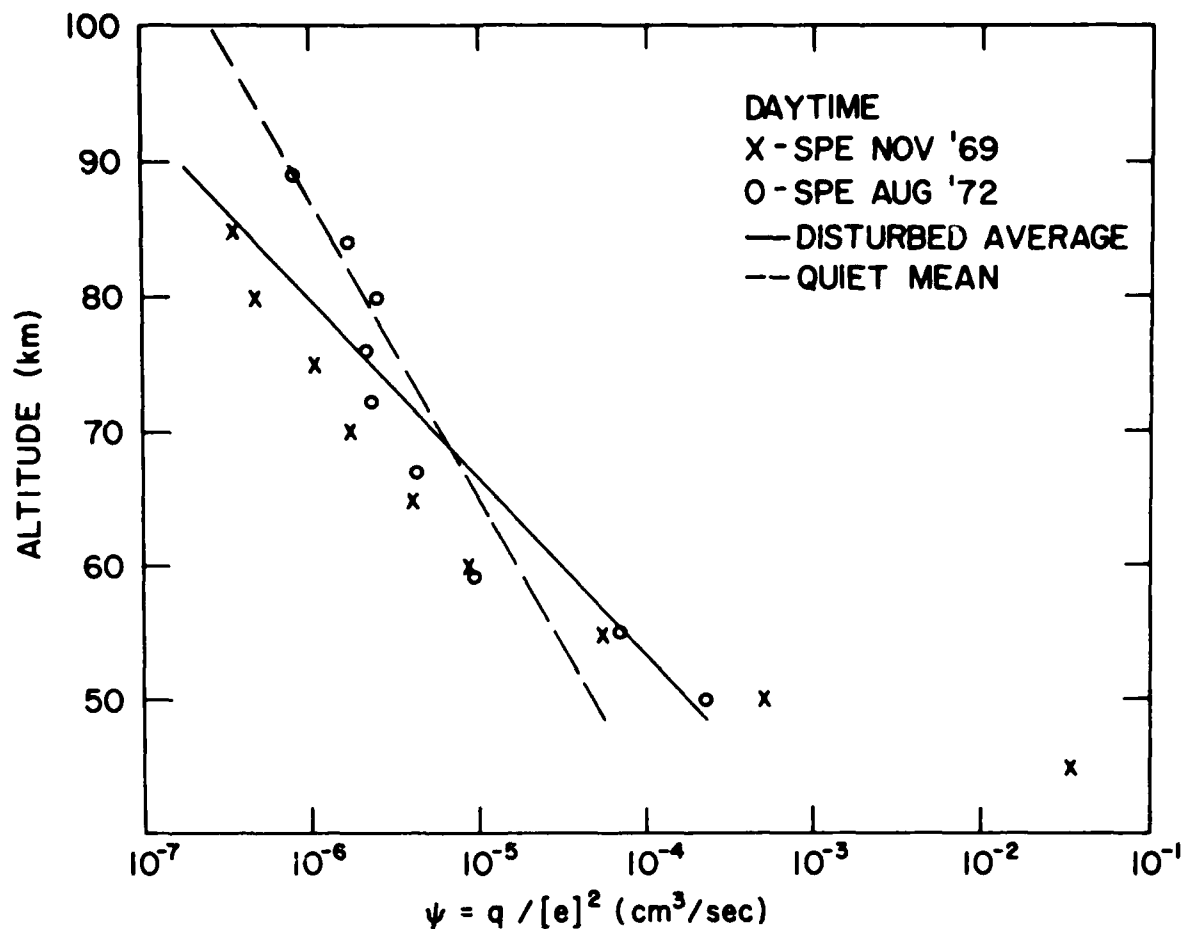


Figure 1. Effective Recombination Coefficients for the November 1969, SPE (crosses) [Swider and Dean]¹⁶ and the August 1972, SPE [Reagan and Watt²⁰] (circles) Compared to a Least Squares Fit of All Such Data for Quiet and Disturbed Conditions [Gledhill²¹]

Recalling from Eq. (3) that $\Psi = 8 \times 10^{-6} \text{ cm}^3 \text{ sec}^{-1}$ at $z(\lambda_1)$, the four curves in Figure 1 yield a range of about 63 to 68 km for $z(\lambda_1)$. It seems reasonable to assume that this altitude should decrease somewhat as q (and $[e]$) increases, since the probability of an electron undergoing dissociative recombination must increase vs attachment which is basically independent of $[e]$. However, the change of $z(\lambda_1)$ is not great. Recall that Swider et al¹⁹ were able to model the November 1969, SPE rather well. Their $z(\lambda_1)$ was 62 km. The same model yielded 63 km for $z(\lambda_1)$ under quiet conditions [Swider²²]. However, both altitudes appear to be a little too low.

22. Swider, W. (1983) Latitudinal influences on the quiet daytime D-region, Adv. Space Res. 2:213-216.

Profiles of the effective recombination coefficient determined for quiet daytime conditions using several different atmospheric (T, M) models [Swider²²] are compared in Figure 2 to the SPE data shown in Figure 1. A larger Ψ for quiet conditions as compared to the November 1969, SPE is expected above about 75 km as already stated. It is somewhat surprising that Ψ from SPE'72 fits the quiet (low q) model so well. These results emphasize that Ψ is a function of [M], the total concentration. This is the reason for the shift among the curves with altitude. There is no difference between curves 1 and 4 (same atmospheric model) except above 70 km, where their NO distributions are different. In any case, the two SPE data sets appear to encompass both disturbed and quiet conditions.

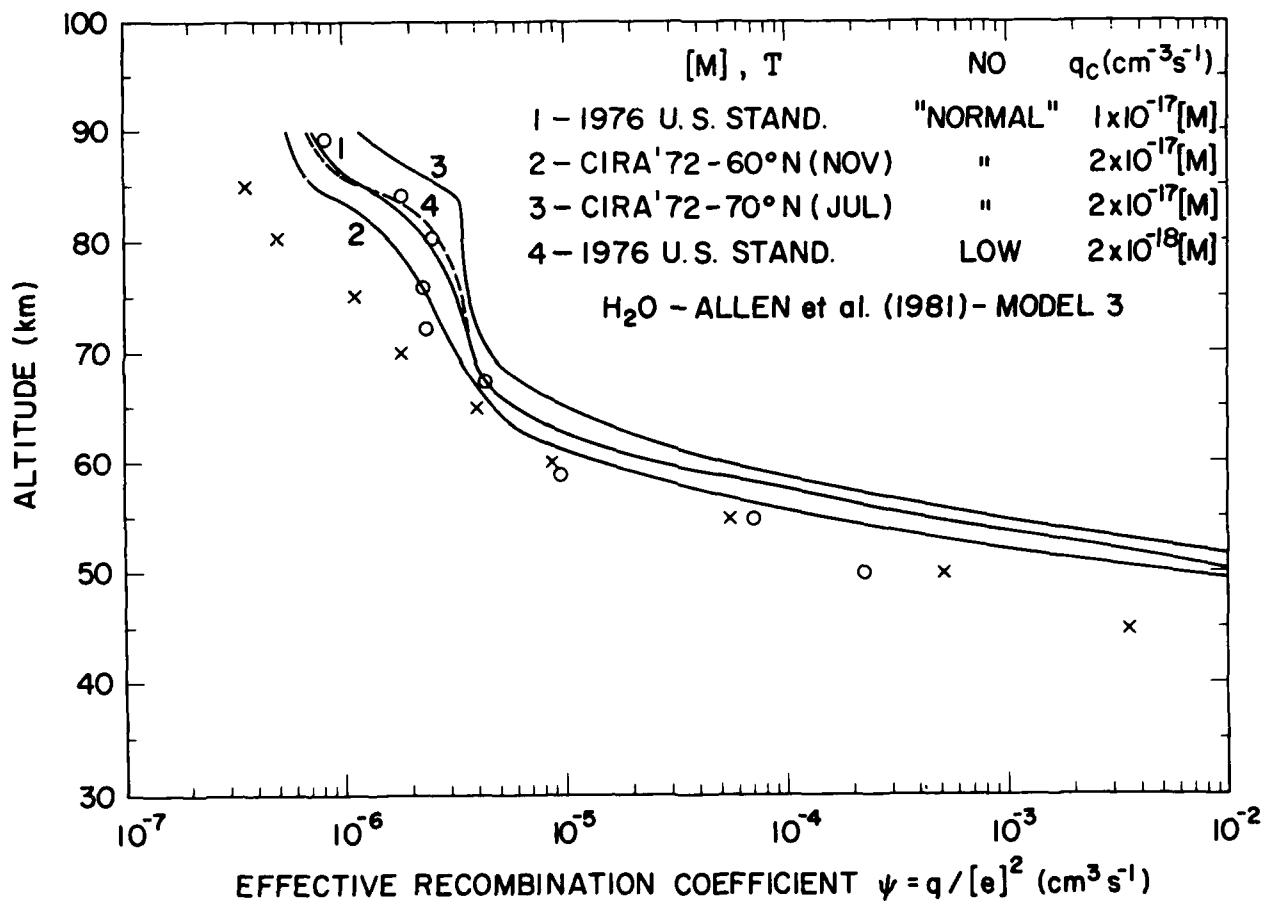


Figure 2. Theoretical Profiles of Effective Recombination Coefficients [Swider²²] for Several Atmospheric Models as Compared to Two SPE Results From the Previous Figure

An example of the use of an empirical Ψ may be illustrated for the 23 September 1978, SPE. Using the q -values listed by Kossey et al.²³ for noon, and the Ψ values of Swider and Dean,¹⁷ the following $[e]$ are deduced: $2.9 \times 10^4 \text{ cm}^{-3}$ (80 km), $1.4 \times 10^4 \text{ cm}^{-3}$ (70 km), $5.1 \times 10^3 \text{ cm}^{-3}$ (60 km), $4.0 \times 10^2 \text{ cm}^{-3}$ (50 km) and about 2.0 cm^{-3} at 40 km. These concentrations were used to calculate the electron conductivity from the formula

$$\sigma_e = \frac{3.27 \times 10^{-10} [e]}{P(\text{Torr})} \text{ mho/m} . \quad (4)$$

The results are plotted (dots) in Figure 3 along with the results obtained from the (extrapolated) inversion of the data and from a detailed model. Clearly, this simple method of determining σ_e from an experimentally derived Ψ which is backed by physical theory [Swider et al.¹⁹], works well.

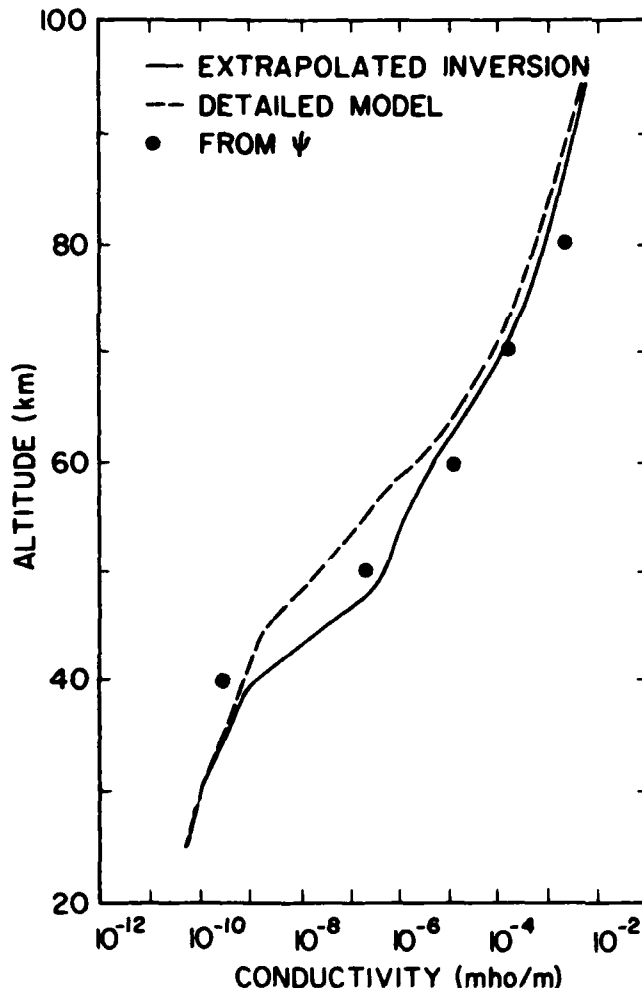


Figure 3. Conductivity as Determined from a Detailed Model and the Inversion of Propagation Data [Kossey et al.],²³ as Compared to a Simple Estimate (dots) Derived From Effective Recombination Coefficients

23. Kossey, P. A., Rasmussen, J. E., Field, E. C., and Warber, C. R. (1985) Conductivity profiles of the disturbed polar ionosphere from VLF reflection data, AGARD-CP-382:8. 1. 1-8. 1. 10.

3. EFFECTIVE RECOMBINATION COEFFICIENT AT NIGHT

Above 80 km, there is little difference between night and day for disturbed conditions (same q day and night). For quiet conditions, $q(\text{day}) \gg q(\text{night})$ and the transition altitude from simple diatomic ions to PH ions is higher at night [Narcisi¹²]. Negative ion formation is minimal both day and night above 80 km where there is considerable [O] to counter the formation of the initial negative ion, O_2^- , by the process $O + O_2^- \rightarrow O_3 + e$.

At night, photo-processes are inoperative and atomic oxygen declines sharply with decreasing height below 80 km. Attachment rapidly becomes the main electron loss process with decreasing altitude below this point. There is a quick switch from $\Psi \approx \alpha_D$ ($z > 80$ km) to $\Psi \approx \lambda \alpha_1 (1 + \lambda)$ for $z < 70$ km. It is convenient to express attachment in terms of the O_2^- formation rate, $L(A) \approx 1.8 \times 10^{-30} [O_2]^2 \text{ sec}^{-1}$. The formula [Swider et al²⁴]

$$[e] = \left\{ \left(\frac{L(A)}{2\alpha_D} \right)^2 + \frac{q}{\alpha_D} \right\}^{1/2} - \left(\frac{L(A)}{2\alpha_D} \right) \quad (5)$$

appears to be quite adequate for disturbed conditions. The equation simplifies to $[e] = (q/\alpha_D)$ near/above 80 km, that is, $\Psi = \alpha_D$, and $[e] = q/L(A)$ near/below 70 km, which yields $\Psi = L(A)^2/q$. Thus, at night, a pure attachment (linear) loss of electrons occurs below this point. The electron concentration is proportional to the production rate. Gledhill²¹ calculated a mean least squares fit for Ψ under nighttime conditions. This result should not be used in view of Eq. (5). The quiet nighttime D-region is basically nonexistent, being only the tail of the lower nighttime E-region [Keneshea²⁵]. However, Eq. (5) should be appropriate for this case too. The recommended value for α_D is $6 \times 10^{-7} \text{ cm}^3 \text{ sec}^{-1}$.

24. Swider, W., Narcisi, R. S., Keneshea, T. J., and Ulwick, J. C. (1971) Electron loss during a nighttime PCA event, J. Geophys. Res. 76:4691-4694.

25. Keneshea, T. J., Narcisi, R. S., and Swider, W. (1970) Diurnal model of the D-region, J. Geophys. Res. 75:845-854.

4. DISCUSSION AND CONCLUSIONS

Distributions of [O], [NO], [H₂O], and T are important factors in formulating physical models of the D-region. Global models of these parameters are mostly incomplete. Other species distributions relevant to the negative ion chemistry, like NO₂, and O₃, are needed also. Rate constants for many of the positive and negative ion reactions are unmeasured. There is evidence [Narcisi et al²⁶] that a layer of heavy negative ions exists near 80 km. Backscatter data [Ganguly²⁷] yield similar evidence about a third of the time. Gas-phase chemistry allows for only a few light negative ions at this altitude.

These and other complexities notwithstanding, the D-region is generally understood. Physical models, while imperfect, provide the basis of this understanding. However, to provide a predictive model of electron concentrations that can match propagation data, parameters like NO, H₂O, and T need be observed virtually in real time. Constant monitoring of these parameters is impractical, although real time monitoring of the particle/X-ray intensity is required for disturbed events. On the other hand, the effective recombination coefficient for electrons in the daytime D-region appears to be much less variable than either [e] or q.

The considerable scatter for Ψ in the literature [Gledhill²¹] probably results from poor measurements of either [e], q, or both as compared to better measured events like the SPE's of November 1969 and August 1972. The parameter Ψ cannot vary that widely on physical grounds. At 65-85 km in the daytime, electrons dissociatively recombine with either simple ions (NO⁺, O₂⁺) or PH ions, H₃O⁺ · (H₂O)_n. The latter ions become proportionally more important with descent. A knowledge of T and H₂O can help refine the value of α_D , although [e] only depends upon the square root of $\Psi \approx \alpha_D$ anyway at these altitudes. The main effect of a larger q is to lower the crossover altitude of simple ions to PH ions a few kilometers since with a greater number of electrons, dissociative recombination with O₂⁺ and NO⁺ ions is enhanced relative to their transition to oxonium ions which have larger dissociative recombination coefficients. At lower altitudes, where negative ions are significant, Ψ is perhaps more nearly invariant (Figures 1, 2, and 3).

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26. Narcisi, R., Bailey, A., Federico, G., Wlodyka, L. (1983) Positive and negative ion composition measurements in the D- and E-region during the 26 February 1979 solar eclipse, J. Atmos. Terr. Phys. 45:461-478.
 27. Ganguly, S. (1984) Observation of large negative ion zones around 88 km, J. Atmos. Terr. Phys. 46:633-636.

Additional data are needed to test this hypothesis. A DNA-sponsored program is underway to do just that. Electrons are quite difficult to measure at low altitudes, but a new technique will be tried. Ambient electrons will be converted to negative ions via a release of SF_6 . Non-ambient SF_6^- ions will be measured by a mass spectrometer relative to the ambient negative ion species.

A daytime profile of Ψ for 50 to 90 km averaged from the crosses and circles shown in Figure 1 is recommended. The circles may be preferable for lower T (summer) and the crosses for winter. The circles also appear to represent quiet conditions best (see Figure 2). At night, Ψ is not invariant, being inversely proportional to q below about 70 km. However, a suitable analytical solution exists for $[e]$ under disturbed conditions, which also should be applicable for quiet conditions.

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