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AERONOMY OF SATURN AND TITAN

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ABSTRACT

The Saturn system presents exciting and unique objects for planetary aeronomy. The photochemistry of H_2 and He leads to the formation of an ionosphere. Methane photolysis results in the formation of spectroscopically detectable amounts of C_2H_6 and C_2H_2 and in the case of Titan, C_2H_4. Density profiles of C_2H_6, C_2H_2, and PH_3 should be indicative of the strength of atmospheric mixing processes.

INTRODUCTION

The Saturn system presents exciting and unique objects for planetary aeronomy. The presence of hydrocarbons on Titan raises interesting possibilities for organic chemistry. Light gases may escape Titan's gravitational field but not the stronger planetary field of Saturn and thus lead to the formation of a gaseous toroidal cloud around Saturn (McDonough and Brice, 1973a, b). From our limited information Saturn's upper atmosphere appears similar in thermal structure, composition, and photochemistry to the Jovian upper atmosphere.

THERMAL STRUCTURE

A distinctive feature of the Saturn system is the thermal IR emission. On Saturn the pronounced emission peak of CH_4 at 7.7 μm suggests a warm stratosphere, T ≥ 130 K, while the same feature on Titan is indicative of temperatures ≥ 160 K. The most plausible interpretation of these emission spectra is the presence of a temperature inversion in their stratospheres similar to the Earth's O_3 layer with solar IR heating in the 3.3 μm CH_4 band balanced by IR cooling in the 7.7 μm CH_4 band, the 12.2 μm C_2H_6 band, and the 13.7 μm C_2H_2 (Gillett *et al.*, 1969; Danielson *et al.*, 1973). Additional heating may be required to achieve these observed "temperatures" and fine absorbing particles which absorb UV and visible sunlight have been suggested (Axel, 1972; Danielson *et al.*, 1973). Since these particles are very small, they are poor emitters and will heat up and collisionally transfer their energy to atmospheric gases.

Strobel and Smith (1973) concluded that the globally averaged vertical temperature contrast in the thermospheres of Saturn and Titan was ~10 K and ~90 K, respectively, for solar EUV heating only. It should be remembered that Pioneer 10 measured a Jovian ionospheric scale height that implied a much warmer thermosphere than solar EUV heating could maintain (Fjeldbo *et al.*, 1975). The above temperature contrast for Saturn's thermosphere should be regarded as a minimum value.

PHOTOCHEMISTRY OF H_2

Molecular hydrogen, the major constituent of the outer planets, has a dissociation continuum below 845 Å and an ionization continuum below 804 Å (Cook and Metzger, 1964). Discrete absorption in the Lyman and Werner bands can lead to fluorescent dissociation of H_2 (cf. Field *et al.*, 1966; Stecher and Williams, 1967). The deposition of solar EUV radiation in a H_2 atmosphere results initially in the production of primarily H_2^+ ions, which react with H_2 to produce H_3^+ + H and break a H_2 bond. If He is present the production of He^+ ions will result in the dissociation of H_2 by ion-molecule reactions. For each H_2 molecule and He atom ionized at least two H atoms will be produced. Three body recombination of H atoms is exceedingly slow in the ionosphere and consequently there is a large downward flux of H atoms on Saturn from this region. For Saturn the globally averaged downward H atom flux is $\sim 2 \times 10^8$ cm^{-2} s^{-1} (Strobel, 1973c).

The planetary albedo at Ly-α is in simple terms a measure of the H atom column density above the absorbing CH_4 layer. This column density is a sensitive function of the eddy diffusion coefficient, K, in the vicinity of the turbopause

(Hunten, 1969; Wallace and Hunten, 1973). The recent rocket measurement of Ly-α from the Saturn system by Weiser *et al.* (1977) gave ~700 R for the disk. This is comparable to a 2kR signal from Jupiter and, based on Wallace and Hunten (1973), would suggest an eddy diffusion coefficient near the turbopause of $10^{(6-7)}$ cm^2 s^{-1}. In addition Weiser *et al.* (1977) detected ~200 R of Ly-α in the vicinity of Saturn which may be indicative of a hydrogen atmosphere associated with the ring system. Measurements of the Ly-α brightness around the satellites will provide important information on processes that produce the gaseous toroidal clouds discussed in the Introduction.

The formation of an ionosphere H_2-dominated atmosphere has been most recently discussed by Atreya and Donahue (1975). Of particular importance are the major sources of H^+ ions as a H^+ plasma can only recombine radiatively at a slow rate (~7×10^{-12} cm^3 s^{-1}). The H_3^+ ions produced by the reaction $H_2^+ + H_2$ dissociatively recombine rapidly (~4×10^{-7} cm^2 s^{-1}). Thus H^+ will be the major ion down to a level where the three body reaction $H^+ + H_2 + H_2 \rightarrow H_3^+ + H_2$ proceeds rapidly. This behavior is illustrated in Figure 1 for Saturn. In the lower ionosphere ($\leq$ 125 km, Figure 1) hydrocarbon ions, produced by hydrogen ions (H^+, H_2^+, H_3^+) reacting with CH_4 and photoionization of CH_3 radicals (Prasad and Tan, 1974), dominate. They dissociatively recombine an order of magnitude faster than H_3^+ and would lead to lower electron densities (up to a factor of 3) in this region than illustrated in Figure 1. Ionospheric models have also been developed for Titan by Whitten *et al.* (1977).

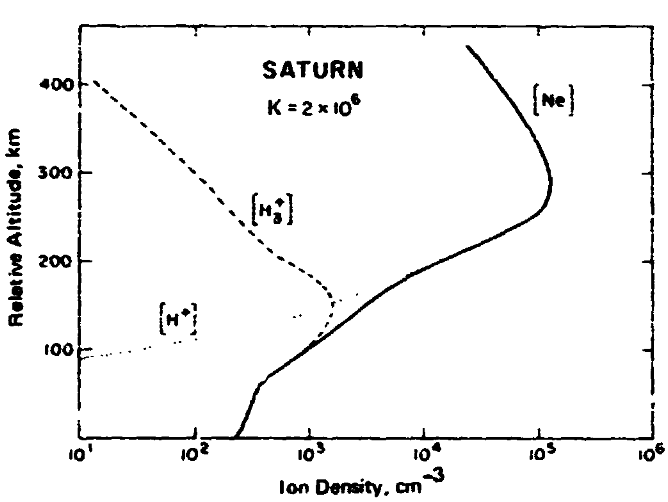

Figure 1. A Model for Saturn's ionosphere with $K = 2 \times 10^6$ cm^{2}s^{-1}, and He mixing ratio of 0.24. The vertical scale gives the height above a reference level where the H_2 density is 1×10^{16} cm^{-3}. (after Atreya and Donahue, 1975).

PHOTOCHEMISTRY OF HYDROCARBONS

The principal hydrocarbon in the outer solar system is CH_4. C_2H_6 has been detected in the atmospheres of Saturn, and Titan (Ridgway, 1974; Gillett and Forrest, 1974; Gillett *et al.*, 1973). Hydrocarbons in the presence of UV radiation can form polymers. Based on photochemical models for the outer planets Strobel (1975) concluded that only a small percentage of dissociated CH_4 molecules are converted to complex hydrocarbons. To first order a closed photochemical model can be constructed; the principal reactions are schematically presented in Figure 2. Approximately 70% of the solar photons which dissociate CH_4 are at Ly-α where the primary processes are (Rebbert and Ausloos, 1972; Ausloos, 1972)

$$CH_4 + h\nu\,(\text{Ly-}\alpha) \rightarrow {}^1CH_2 + H_2 \quad 92\%$$
$$CH + H + H_2 \quad 8\% \qquad (1)$$

where ${}^1CH_2$ denotes the singlet state of CH_2.

The only chemical means (other than energetic photons) for breaking the bond of two C atoms is the reaction sequence: $H + C_2H_4 \rightarrow C_2H_5$, $H + C_2H_5 \rightarrow 2CH_3$. For this destruction to be important a large H atom concentration is required at pressures ~10 mbar. As a consequence there is some production of higher hydrocarbons. To conserve C atoms a downward flow of C_2H_6 and C_2H_2 is balanced by an upward flow of CH_4. It is postulated that a deep circulation is present in Saturn that transports higher hydrocarbons to the hot, dense interior where they undergo thermal decomposition to produce fresh CH_4 which is transported upwards to replenish the CH_4 destroyed in photolysis.

The photochemical model is most sensitive to the $[CH_4]/[H_2]$ mixing ratio, the escape rate of H atoms from the atmosphere, and the atmospheric mixing rate (eddy diffusion coefficient). From Figure 2 it is evident that as the $[CH_4]/[H_2]$ ratio increases, the production rates of C_2H_4 and C_2H_2 will increase. The fate of the CH_3 radical depends on the $[H]/[CH_3]$ ratio and determines the rate at which CH_4 is recycled. Although the escape rate of H atoms from Saturn is negligible, it can be substantial from the satellites and actually control the H atom density distribution. A large escape rate depresses the H concentration and results in large conversion rates of CH_4 to C_2H_6 and C_2H_2 (>90% for Titan (Strobel, 1974a)). Also large concentrations of C_2H_2 will efficiently remove H atoms by catalytic recombination as illustrated in Figure 2, $H + C_2H_2 \rightarrow C_2H_3$, $H + C_2H_3 \rightarrow H_2 + C_2H_2$ (Strobel, 1973a).

The most abundant hydrocarbons produced in CH_4 photolysis are C_2H_6 and C_2H_2. They have vertical density distributions of the form (Strobel, 1974b):

$$n = c \exp\left[\frac{-z}{H_{av}}\right] + \frac{\phi_0}{K}\left[\frac{1}{H_{av}} - \frac{1}{H_k}\right]^{-1} \quad (2)$$

where $K = K_0 \exp(z/H_k)$, H_{av} is the atmospheric scale height, C is an integration constant, and ϕ_0 is the downward flux approximately equal to the column production rate. Typical hydrocarbon densities are illustrated in Figure 3 for Saturn. C_2H_6 is a stable molecule in a cold, reducing atmosphere. If the interior conditions do not require rapid downward flow, then the C_2H_6 density profile is given approximately by the first term of (2), i.e., C_2H_6 is mixed. For rapid downward flow the C_2H_6 density profile will exhibit the scale height of K and be represented by the second term of Equation (2). For C_2H_2 some chemical removal occurs when the ratio $[H]/[H_2]$ is very small. A large downward flux is required to balance this loss. Consequently its density profile is represented by the second term of Equation (2). The

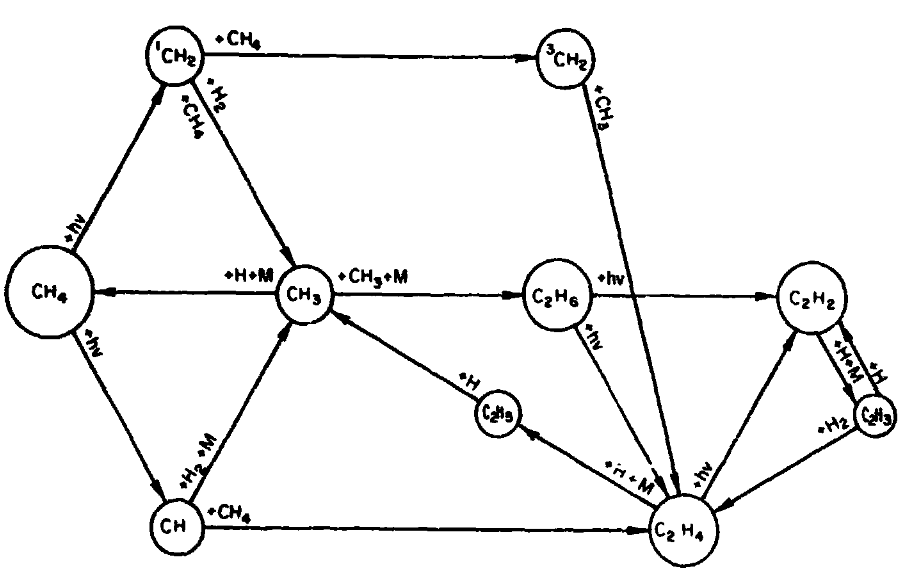

Figure 2. Principal reactions of hydrocarbon photochemistry in the outer solar system atmosphere (after Strobel, 1975).

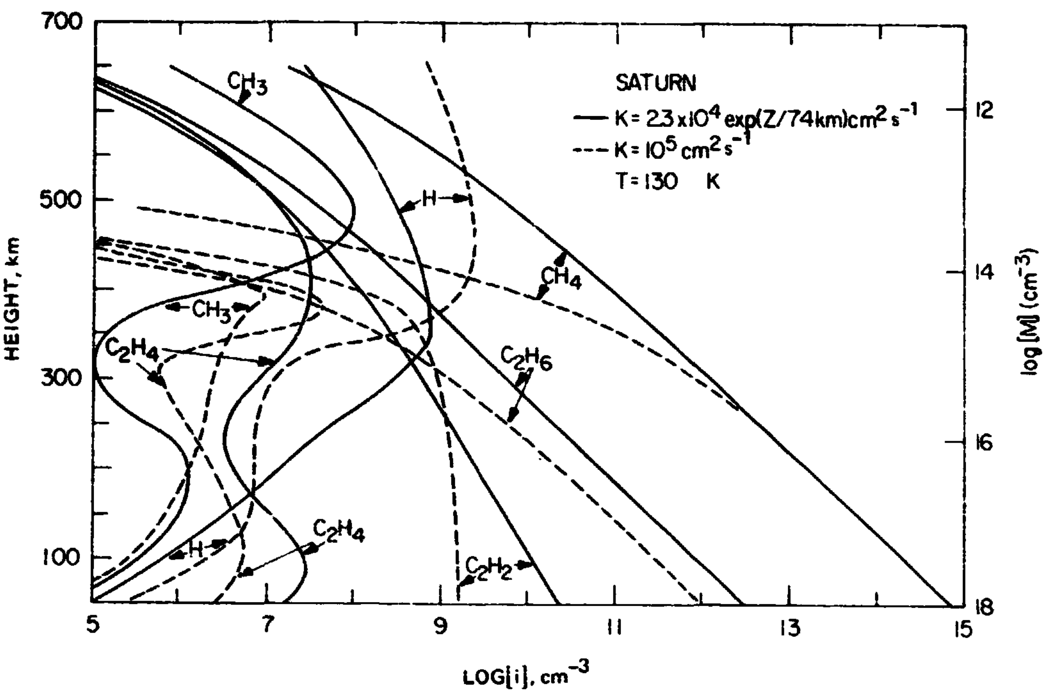

Figure 3. Hydrocarbon density profiles for the Saturnian atmosphere with indicated eddy diffusion profile. Solid line. $K \propto \{M\}^{-0.5}$, dashed lined: $K = 10^5 cm^2 s^{-1}$, where $\{M\}$ = number density of atmospheric gas. Lower boundary condition for C_2H_6 is a small downward flux (see Strobel, 1973a).

rapid decrease in the H concentration below 200 km is due to catalytic removal by C_2H_2 (Strobel, 1973a). It should be noted that for C_2H_2 (and C_2H_6 if rapid downward flow is required) that the very rapid mixing characteristic of the troposphere will result in a substantial decrease in the number density below the tropopause (on the order of the eddy diffusion coefficient ratio).

Products of CH_4 photolysis on Titan are removed by condensation at a cold tropopause and possibly dissolve on the cold surface. As a consequence a large downward flux of photolysis products is anticipated ($\sim 10^{10}$ cm^{-2} s^{-1}, primarily C_2H_6 and C_2H_2). Over the age of the solar system this would represent an accumulation of 30 kg cm^{-2}. Photochemical models for Titan predict observable amounts of C_2H_6 and C_2H_2 for slow mixing rates in the lower stratosphere (eddy diffusion coefficients $\leq 10^5$ cm^2 s^{-1}) as illustrated in Figure 4. Their density profiles are represented by the second term of Equation (2), from which it follows that large densities are associated with slow mixing. The other essential features of the model are that the C_2H_6 abundance is sensitive to the eddy diffusion coefficient, the composition of Titan's atmosphere, and the net escape rate of H atoms from the exobase, whereas the C_2H_2 abundance is principally sensitive to the eddy diffusion coefficient.

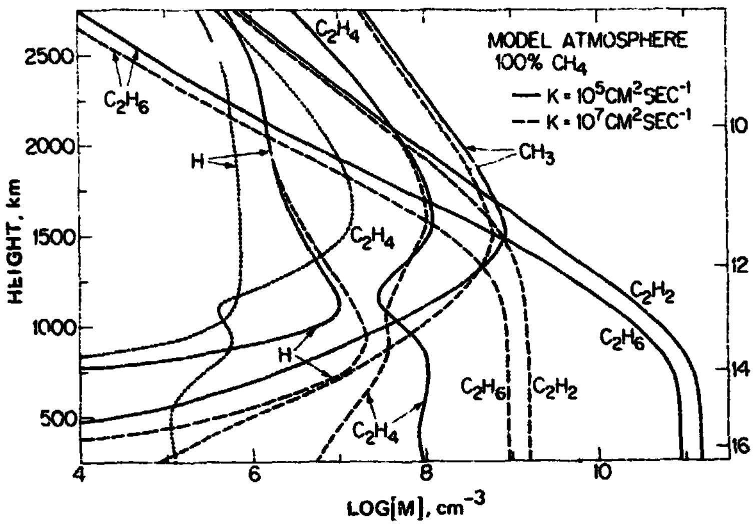

Figure 4. Hydrocarbon densities as a function of the eddy diffusion coefficient for a pure CH_4 atmosphere on Titan. The dotted lines represent a model with $K = 10^5 cm^2 s^{-1}$ and a negligible reaction rate for $CH_2 + CH_3 \rightarrow C_2H_4 + H$.

PHOTOCHEMISTRY OF PH_3 AND NH_3

On Saturn and Titan the cold trap temperatures at the tropopause are sufficiently low and restrict the NH_3 mixing ratio above this level to less than 10^{-12}. As a consequence only the more abundant PH_3 on Saturn is aeronomically important. The Prinn and Lewis (1975) model is applicable with the addition of the reaction $H + PH_3 \rightarrow PH_2 + H_2$, which effectively doubles the dissociation rate (Lee *et al.*, 1976; Strobel, 1977). One questionable feature of this model is the absence of any direct mechanism for partial recycling of PH_3 in the photolysis region. Each absorbed UV photon by PH_3 leads to irreversible conversion to P_4 (red phosphorus).

The vertical PH_3 density profile is given by

$$[PH_3] \propto \exp\left[-\frac{z}{2H_{av}}\left(1 + \sqrt{1 + r}\right)\right] \tag{3}$$

where $r = \frac{4 H_{av}^2 \epsilon J}{K}$, J is the PH_3 dissociation rate and $\epsilon \sim 2$ as discussed above. For sufficiently slow mixing, this expression reduces to

$$[PH_3] \propto \exp\left[- z \sqrt{\frac{\epsilon J}{K}} \right]$$

For Saturn $\epsilon J \sim 2 \times 10^{-7}$ s^{-1} and if $K \sim 10^4$ cm^3 s^{-1}, then the effective PH_3 scale height is ~2 km, i.e. PH_3 is confined to the lower stratosphere. The vertical distribution of $[PH_3]$ is thus indicative of K(z) in the lower stratosphere.

SUMMARY

The photochemistry of H_2 and He leads to the formation of the main ionosphere and, through ion chemistry and recombination, H atoms. Observations of electron density and ion composition will yield information on the chemistry and structure of the ionosphere. H atoms can be observed by Ly-α emission and interpretation of the data should yield the mixing rate near the turbopause. CH_4 photolysis leads principally to the formation of C_2H_6 and C_2H_2. C_2H_6 is a photochemically stable molecule and, depending on the lower boundary condition, is either quasi-mixed or K $[C_2H_6]$ is quasi-conserved above the tropopause. Also K $[C_2H_2]$ is quasi-conserved in this region. Thus observations of the C_2H_2 and C_2H_6 density profiles can yield information on K(z) and the magnitude of the downward C_2H_6 flow to the interior in the case of Saturn. The extent of catalytic removal of H atoms by C_2H_2 requires a measurement of H density profile. The models predict $[C_2H_4]/[C_2H_2] \ll 1$ and that C_2H_4 can only be detected on Titan where its scale height is an order of magnitude larger than on Saturn. Attempts to observe C_2H_4 would serve as a useful internal check on the models.

NH_3 should be frozen out below the tropopause on Saturn and Titan and thus be aeronomically unimportant. On Saturn the vertical PH_3 density profile should be indicative of K(z) in the lower stratosphere in a similar manner as the NH_3 profile on Jupiter (Strobel, 1973b).

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DISCUSSION

S. CHANG: If a probe went into Jupiter's atmosphere or Saturn's atmosphere and actually found significant amounts of ethane in the troposphere, would you conclude that some process other than methane photochemistry is responsible?

STROBEL: That would be one possible interpretation. The other is that thermodynamically there were large amounts in the deep interior and that the mixing was violent enough to carry it up to the observable region.

A. TOKUNAGA: Is there any evidence that the eddy diffusion coefficient is different at the poles relative to the equator? If that were the case, the ethane mixing ratio might vary with latitude.

D. STROBEL: The eddy diffusion coefficient works best when it is regarded as a global average. As one tries to ascribe to it horizontal variations, I think one is stretching the use of the concept. It's a convenient factor to use as a first estimate of what's going on in the atmosphere, but when the subject becomes sufficiently mature, one should use actual dynamical equations to calculate the transport.

J. POLLACK: Didn't Don Hunten once nickname it the eddy confusion coefficient?

D. HUNTEN: The straight answer to Alan's question is that there could be large variations in vertical transport rates with latitude on a planet like Saturn, very large.

D. STROBEL. Especially if the vertically propagating waves are the cause of the phenomena and depending on where they are excited.

D. HUNTEN: George Siscoe was quite interested in hydrogen production rates and, of course, they can be derived implicitly from these computations. The vertical curves at the bottom right of Figure 4 give a downward flux of the things left over, once you've made hydrogen. The corresponding hydrogen is escaping, and the rate is 9×10^9 cm^{-2} s^{-1}.

D. STROBEL: Right. I should emphasize that the atmosphere is considerably larger than the solid body, and therefore captures more solar photons than you might think.