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CHEMISTRY OF THE INNER COMA: A PROGRESS REPORT

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The composition of the inner coma is modeled assuming that about 30 chemical species composed of H, C, and O undergo reactions. Ionization and dissociation by solar radiation and over 100 forward and reverse reactions between atoms, molecules, and ions are considered in the kinetics. Vaporization from a simple H_2O *-* CO_2 *nucleus provides the initial composition of the gas near the surface.*

The formation of a comet is closely connected to the composition of its nucleus. Until we have more direct evidence from space probes we must deduct the composition from spectral observations of the coma. The accumulation of identified atomic, molecular, and ionic species suggests chemical modeling of the nucleus. However, chemical reactions may have a strong influence on the observed composition of the inner coma (see, *e.g.*, Donn and Urey 1957; Jackson and Donn 1968; Biermann and Diercksen 1974). Oppenheimer's (1975) investigation of the steady state indicates that ion chemistry plays an important role and may lead to predictions consistent with observations. More recently Biermann (1976) has investigated production mechanisms for CO. He finds that dissociative recombination of CO_2^+ or some other ions containing the CO radical may be responsible for the large amounts of CO necessary to explain the observed emissions out of the triplet states.

Here I want to report on the progress that is being made on a large-scale computer program that takes the time dependence of all of the above processes into account simultaneously for a large number of reactants. The objective is to determine the chemical composition of the nucleus from the products one can predict and observe in the inner coma. In particular the program considers the influence of wavelength dependent solar flux on dissociation, ionization, and dissociative ionization, and gas phase chemistry on neutral and ionized species. In all cases the inverse reactions are considered. At the present this results in 136 different reactions with species listed in Table I. Reaction rates are taken primarily from Fergusen (1973) and Herbst and Klemperer (1973).

Assuming an H_2O - CO_2 icy conglomerate and a production rate and outstreaming velocity typical at 1 AU heliocentric distance the particle density at the surface of a R_0 = 1 km radius nucleus is about 3 x 10^{13} cm^{-3} for CO_2 and 1.5 x 10^{13} cm^{-3} for H_2O. If the particle density decreases as $(R_0/r)^2$, where r is the distance from the center of the nucleus, then for an optically thin coma several neutral species attain their maximum density about 10 sec after leaving the surface. Typically H and OH are several 10^8 cm^{-3}, O and CO several 10^7 cm^{-3},

TABLE I

SPECIES

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H		H^+	H_2	H_2^+	
C		C^+	C_2		
O	$O(^1D)$	O^+	O_2	O_2^+	O_3
CH		CH^+			
OH		OH^+			
CO		CO^+			
H_2O		H_2O^+			
HCO		HCO^+			
CO_2		CO_2^+			
CH_4					
C_2H_2					
C_2H_4					
		H_3O^+			
		OHH_3O^+			

H_2 just under 10^7 cm^{-3}, and O^2 ~ 10^6 cm^{-3}. Free electrons and H_3O^+ reach their peak of a few 10^6 cm^{-3} within a few tenths of a second. CO_2^+, H_2O^+ and OH^+ are produced very quickly, but desctuctive mechanisms also set in early so that they remain at a low abundance plateau for 10^3 to 10^4 sec. Other ionic species are produced at relatively late times, *e.g.*, O^+ has not yet attained its peak after 3 x 10^5 sec. The steady state is not reached in this time interval. Interchanging the initial abundance of H_2O and CO_2 does not alter the results significantly.

Although the total particle density decreases with distance according to the inverse square law, most of the neutral species (other than H_2O and CO_2) and H_3O^+ (after their initial build-up) continue to be produced such that their net density decreases only at a rate proportional to about r^{-1}.

More reactions involving heavier molecules and all reactions involving nitrogen must still be added to the program. Inclusion of optical depth will decrease chemical reactivity, but catalytic reactions with dust grains and cosmic ray ionization will increase it. Radiative decay from excited states can be added to predict some emission spectra. Fluid dynamics, and solar wind interactions can be coupled to the program at a later time.

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DISCUSSION

DONN: This is an ambitious program and I hope it can be carried through. Several probably important refinements need to be considered. The reactive fragments are produced with energies in excess of thermal energy. A temperature of 200° K may not be relevant. Also, at low pressures species are in the lowest energy states not Boltzmann distribution, the basis for measured rate constants. These rate constants depend upon specific vibrational levels for neutral reactions. This effect may be important for cometary reactions.

HUEBNER: An attempt will be made to include the effects of excess energy on the velocity. Since most of the measured rate constants are obtained at 300° K the problem of vibrationally excited states will not be as severe as is the case when they are applied to interstellar clouds. A more severe problem, namely lack of rate constant data, may be encountered for the electronically excited metastable states, e.g., the triplet states of CO which are the result of dissociative recombination of CO_2^+.

WHIPPLE: Will you add solar energy by absorptions on dust and gas to increase the temperature and velocity of the gas with distance from the nucleus?

HUEBNER: Yes, this is planned.

DELSEMME: Are you going to introduce nitrogen compounds into your model?

HUEBNER: Yes, this will be done next.

OPAL: An electron density of $10^6/cm^3$ *implies a critical frequency in the Megahertz range, so the ionosphere may be detectable with high-frequency radar. Is there any data available on this?*

HUEBNER: Not that I am aware of. The density of 10^6 cm^{-3} *is a preliminary result; addition of more reactions can change this.*

SEKANINA: Is the temperature of 200° K an assumption? CO_2 *should vaporize at lower temperatures than* H_2O.

HUEBNER: Typical temperatures are between 150° and 250° K at 1 AU heliocentric distance depending on composition of the nucleus. For about equal amounts of H_2O *and* CO_2, *200° K is a reasonable assumption since* H_2O *grains will be dragged by the vaporizing* CO_2.

COSMOVICI: What about reactions between neutrals and grain reactions? Are the conditions (ρ,T) *similar to the interstellar medium where the same molecules are observed?*

HUEBNER: Reactions (and the inverse reactions) between neutrals are included. Reactions on grain surfaces have as yet not been included, but I am making preparations to include them. The density of the coma near the nucleus is 10^8 *to* 10^{10} *times higher than in dense interstellar clouds, but similar at about* 10^5 *km from the nucleus. The temperature in the coma is higher than in interstellar clouds where it is less than 100° K.*