Cometary Atmospheres:
Modeling the Spatial Distribution of Observed Neutral Radicals

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16. Abstract

An algorithm for the random walk problem of multiple elastic collisions between newly formed non-thermal neutral cometary radicals and the outflowing cometary molecules has been incorporated into the Monte Carlo particle-trajectory model. Preliminary model analysis has shown that the effects of collision on the observed spatial distribution of cometary radicals becomes important for the larger bright comets, especially at smaller values of the heliocentric distance. The model and early results are discussed herein.

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Program of Research in the Third Quarter

During this past quarter, research activities have concentrated on development of the algorithm for including collisions in the Monte Carlo particle-trajectory model.

Multiple Collisions in Cometary Atmospheres

Models of neutral cometary comae have generally dealt with the two extreme cases: one where the densities are high enough so that all neutral species are thermalized and are characterized by a bulk radial flow away from the nucleus, and the other where the densities are so low that essentially no collisions occur. A characteristic distance from the nucleus separating these two regions has been defined where the mean free path for a collision is equal to the distance from the nucleus. Whipple and Huebner (1976), for example, express this collision radius as

$$r_c = \frac{Q\sigma}{4\pi v}$$

where Q = molecular production rate

σ = cross-section for elastic scattering $\sim 10^{-15}$ cm^2

v = molecular outflow velocity.

The value of r_c varies from $\sim 10^4$ km for a bright comet like Kohoutek near perihelion, down to $\sim 10^2$ km for a small short period comet like P/Encke at 1 AU.

In reality, though, there is no clear separation between the two zones. In order for a typical radical (CN, C_2, OH) which has been emitted from its parent with some exothermic velocity to be truly thermalized, it needs on the order of 10 collisions with outflowing water molecules. On the other hand, many radicals produced outside of r_c will be subjected to at least 1 to 5 collisions, thus questioning the true applicability of a free flow model. What we truly have, then, is a large regime on the order of 0.2 r_c to 5 r_c where partial thermalization will occur.

The true random walk nature of the elastic scattering problem is modeled in a straightforward manner in the Monte Carlo particle-trajectory model (MCPTM). Kitamura et al. (1983) have included collisions in a Monte Carlo

model essentially based on our original model (Combi and Delsemme 1980a). Since they followed the correct procedure, we have adopted a similar algorithm. There is one problem with their procedure which involves the expression they assume for the density of outflowing molecules with which the modeled neutral radicals are colliding. They assume a Haser-like description for the density which is

$$n_{H_2O}(r) = \frac{Q}{4\pi v} \frac{1}{r^2} \exp(-r/v\tau_{H_2O})$$

where Q, v are as above

r = distance from the nucleus

τ_{H_2O} = photochemical lifetime for H_2O.

Strictly speaking, this is the correct density distribution for H_2O molecules, but as the H_2O molecules dissociate, they produce OH and H, which still provide targets with which radicals collide. Since the effective cross-sectional area for the fragments is larger than the parent H_2O but their outflow velocity is, on the average, larger, a better approximation would be to simply drop the exponential term in the density expression. This yields

$$n_{H_2O}(r) = \frac{Q}{4\pi v r^2} .$$

For the simple case of no radiation pressure, this yields a closed form algebraic expression for the collision length of an arbitrarily moving neutral species, in place of the integral found by Kitamura et al.

The random walk algorithm begins with the production of a neutral radical by its parent with a given velocity vector. From this location and velocity vector, a collision length is given by assumed values for the collision cross section, the molecular (H_2O) production rate, and a random number. The neutral is then displaced this distance, scattered elastically off a moving water molecule and continued on for another collision. The trajectory proceeds this way until the observation time snap-shot.

Preliminary model runs have been performed for the case of CN produced by the photodissociation of HCN (Combi and Delsemme 1980b). We have chosen parameters appropriate for the photochemical lifetimes at 1 AU and have neglected radiation presuure, which is of less importance at 1 AU, for the

purpose of simplifying the preliminary analysis. Subsequent models will test both processes simultaneously. The physical parameters of the coma models are listed in Table 1.

Models were run for cases of general molecular production rates from 1×10^{28} s^{-1} to 1×10^{30} s^{-1}. The collision statistics from these model runs are summarized in Table 2. As can be seen, for larger gas production rates, only half of the CN radicals produced are in a true free-flow regime. Furthermore, the effect collisions have on the determination of radical production rates is also evident in these model runs. For the case of the largest gas production rate, if one neglects collisions in the model, an underestimate of 11% to 15% in the determination of radical production rate would be made, depending upon the size of the photometer aperture used. The systematic errors, when reducing data for even smaller heliocentric distances ($r_H \sim 0.5$ AU), should be quite important in bright comets such as P/Halley, since at these distances the collisional effects are compounded by larger gas production rates and smaller radical parent scale lengths.

Program of Research for the Fourth Quarter

Research efforts in the last quarter will concentrate on (1) model analysis of the effect of collisions on the spatial distributions of the neutral radicals, (2) evaluation of newly published brightness profiles of C_2 (Cochran 1985), (3) incorporation of time dependent production rates and lifetimes into the model code, and (4) preliminary model runs for OH, C_2 and C_3.

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Table 1

CN Radical Coma Model Parameters

$r_H = 1$ AU

$\tau(HCN) = 9 \times 10^4$ s

$\tau(CN) = 2.75 \times 10^5$ s

v(parent) = 0.58 km/s

$v_e(CN) = 1.02$ km/s

$\sigma_{scattering} = 1 \times 10^{-15}$ cm^{-2}

Table 2

Collision Statistics for the CN Model at 1 AU

Q_{H_2O} \ n	Fraction of Radicals Undergoing n Collisions				
	0	1–2	3–5	6–10	>10
1×10^{28}	.723	.272	.0042	.0005	.0003
5×10^{28}	.705	.283	.0094	.0023	.0005
1×10^{29}	.681	.296	.0160	.0055	.0009
2×10^{29}	.653	.311	.0247	.0101	.0016
5×10^{29}	.576	.343	.0503	.0252	.0055
1×10^{30}	.503	.355	.0852	.0459	.0147