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Monte-Carlo model for dust/gas interaction in rarefied flows

Valeriy M. Tenishev[*] and Michael R. Combi[†]
Space Physics Research Laboratory, Department of Atmospheric, Oceanic and Space Sciences, University of Michigan, Ann Arbor, MI 48109

I. Introduction

The cometary atmosphere is a unique phenomenon in the solar system. Owing to its negligible gravity, comets produce highly variable extensive dusty atmospheres with a size much larger than the characteristic size of the cometary nucleus. As the comet approaches the sun, the water vapor with some fraction of other gases sublimates, generating a cloud of gas and dust from the surface of cometary nucleus, which consists of the ice and refractory materials (rocky and organic solids and dust). Sublimating gas molecules undergo frequent collisions in the near nucleus region and photochemical processes.

On the basis of the DSMC method a numerical model of cometary comae has been developed. The model includes photolytic processes in the gas phase and interaction of the dust phase with the gas environment.

II. Gas Kinetics of Cometary Comae

Solar radiation is the only source that supplies energy for sublimation of volatiles in cometary comae. There are three major sources of the gas in a coma[7]: the surface of the nucleus (releasing of water vapor), the interior of the porous nucleus (mainly releasing species more volatiles that water) and distributed source (releasing gases from ice and hydrocarbon polycondensates originally trapped and then released and sublimated in the gas).

The simplest models of the cometary gas production assume an optically thin coma and neglect the heat conduction inside the nucleus. The models that are based on the idea of vaporization of volatiles from the surface of the nucleus neglect the differentiated layers within the nucleus and consider it as a homogeneous mixture of volatiles and dust. These models implicitly assume that the outflowing gas instantaneously blows the uppermost dust layer away, so that the surface of the nucleus is covered by ice only. The models assume that the absorbed radiation is balanced by a combination of blackbody reradiation, vaporization of the surface volatiles and maintenance of the thermal structure of the nucleus. It is assumed that the surface does not contain irregularities. In other words, the irregularities are much smaller than the mean free path of the vaporized gas. As the pressure of the cometary atmosphere is much smaller at the nucleus surface then the critical pressure of the transition triple point, the liquid phase is not stable and sublimation of frozen volatiles is responsible for the gas production.

At a typical density of $10^{19}\,m^{-3}$ and water collisional cross section of $10^{-19}\,m^{-2}$, the value of mean free path in the coma is

$$\lambda = \frac{1}{\sqrt{2}n\sigma} < 1m\,, \tag{1}$$

which makes it possible to apply the hydrodynamic approach in the vicinity of the nucleus[1,2] but not for the first few meters from the surface where a so-called Knudsen layer[3,4,5,6] is formed. In the far region, the gas flow is under free molecular conditions and kinetic methods are required.

A. Physical processes in the coma

Several major processes in the gas phase are important in shaping the cometary comae. Intermolecular collisions in the innermost coma, photolytic reactions and radiation cooling are the most important ones in modeling the coma.

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[*] Research Assistant, Department of Atmospheric, Oceanic and Space Sciences. Email vtenishe@umich.edu.

[†] Research Professor, Department of Atmospheric, Oceanic and Space Sciences.

1. *Collisions between neutral constituents of coma*

Collisions between neutral components of a cometary coma are the major mechanism of thermalization of the gas phase within the Knudsen layer. The description of collisional relaxation in cometary comae is possible only on the basis of kinetic theory where the knowledge of collision cross section is required. The values of cross sections for collisions between major neutral components are given in Table II.1.

Table II.1: Cross sections of collision for major components of cometary comae in cm^{-2}

H_2O- H_2O	4.8×10^{-15}	OH-H_2	3.0×10^{-15}	H_2-CO	3.0×10^{-15}
H_2O-OH	3.2×10^{-15}	OH-H	1.5×10^{-15}	H-H	1.2×10^{-15}
H_2O- H_2	3.2×10^{-15}	OH-O	1.5×10^{-15}	H-O	1.2×10^{-15}
H_2O- H	1.8×10^{-15}	OH-CO	3.0×10^{-15}	H-CO	1.5×10^{-15}
H_2O-O	1.8×10^{-15}	H_2-H_2	3.0×10^{-15}	O-O	1.2×10^{-15}
H_2O-CO	3.2×10^{-15}	H_2-H	1.5×10^{-15}	O-CO	1.5×10^{-15}
OH-OH	3.0×10^{-15}	H_2-O	1.5×10^{-15}	CO-CO	3.2×10^{-15}

2. *Photodissociation*

Since the typical size of the collision zone is less than 10^4 km and the lifetimes of many parent species including water are larger than 10^4 s, the daughter species are primarily produced outside of the collision zone[10,11]. At radial distances larger than a few hundred kilometers from the nucleus the gasdynamics is dominated by formation of energetic daughter species[12].

The photodissociation rates and the branching ratios for major components of comeraty comae[13,14,15] are given in Table II.2 and Table II.3. In the case of H_2, the photodissociation reaction $\mathrm{H}_2 + h\nu \rightarrow 2\mathrm{H}$ occurs with the rate of $0.11\times10^{-6}\ \mathrm{s}^{-1}$ and the exothermic velocities of the products of 13 km s^{-1}.

Table II.2: Photochemical branching and exothermic velocities for H_2O vapor.

Wavelength range (Å)	Reaction	Product velocities (km s^{-1})		Branching ratio
1357-1860	$H_2O+h\nu\rightarrow H+OH$	17.5 (H)	1.05 (OH)	0.670
	$H_2O+h\nu\rightarrow H_2+O$	12 (H_2)	1.5 (O)	0.007
1216	$H_2O+h\nu\rightarrow H+OH$	28.7 (H)	1.7 (OH)	0.176
	$H_2O+h\nu\rightarrow H_2+O$	12 (H_2)	1.5 (O)	0.023
	$H_2O+h\nu\rightarrow H+OH^*\rightarrow 2H+O$	<5 (H)	<0.3 (O)	0.027
984-1357	$H_2O+h\nu\rightarrow H+OH$	28.6 (H)	1.5 (OH)	0.03
(excluding	$H_2O+h\nu\rightarrow H_2+O$	12 (H_2)	1.5 (O)	0.004
1216)	$H_2O+h\nu\rightarrow H+OH^*\rightarrow 2H+O$	5 (H)	<0.3 (O)	0.004
<984	$H_2O+h\nu\rightarrow$ionization products			0.059

Table II.3: Photochemical branching and exothermic velocities for OH.

Wavelength (Å)	OH predissociation state	Exothermic velocities (km s^{-1}) H	O	Photodissociation rate (10^{-6} s^{-1})
2160	$A^2\Sigma^+$ (ν´=2)	8	0.5	3.0-6.1
2450	$A^2\Sigma^+$ (ν´=2)	11	0.7	0.5
1400-1800	$1^2\Sigma^-$	22-26	1.4-1.6	1.4
1216	$1^2\Delta$	26.3	1.6	0.3
1216	$B^2\Sigma^+$	17.1	1.1	0.05
1216	$2^2\Pi$-$3^2\ \Pi$	26.4	1.6	0.05
<1200	$D^2\Sigma^-$	22	1.4	<0.01

3. *Photoionization*

Ion creation is a relatively slow process in comparison with the time most species spend in the inner coma. Outside of the collision zone, neutral atoms and molecules of cometary origin move along ballistic trajectories and become ionized with characteristic ionization lifetime of $10^5 - 10^7$ s. The photoionization rates are given in Table II.4. Freshly born ions are accelerated by the motional electric field of the high-speed disturbed solar wind flow.

Table II.4: Photoionization rates of major components of cometary comae.

Component	Photoionization rate (s^{-1})
O	1.1×10^{-6}
H	6.7×10^{-7}
CO	1.4×10^{-6}

4. *Radiative cooling*

Water plays the dominant role in the thermodynamic balance of cometary atmospheres. Its rotational transitions may allow radiative cooling or heating, which could be important in controlling of H_2O outflow velocities and temperatures in the intermediate and outer coma of active comets[12,16,17].

Emission of rotational lines is an efficient way to cool the coma. Based on GEISA spectroscopic data, the cooling rate has been proposed[38] in the form

$$Q_{rad}\left(\mathrm{H_2O}\right) = \begin{cases} -4.4\times10^{-22} T_{\mathrm{H_2O}}^{3.35} n_{\mathrm{H_2O}} \exp\left(-\tau_{IR}\right), T_{\mathrm{H_2O}} < 52\mathrm{K} \\ -2.0\times10^{-20} T_{\mathrm{H_2O}}^{2.47} n_{\mathrm{H_2O}} \exp\left(-\tau_{IR}\right), T_{\mathrm{H_2O}} \geq 52\mathrm{K} \end{cases}, \tag{2}$$

where τ_{IR} is the infrared optical depth

$$\tau_{IR} = 0.4 \frac{n_s \sigma^a R_n^2}{r}. \tag{3}$$

Here, n_s is the number density of absorbing gas at the surface of the nucleus and σ^a is the mean infrared absorption cross section[18].

III. Dust Model in Cometary Comae

The mantle that is formed on the surface of sublimating ice can reach a thickness from millimeters to centimeters before it quenches further sublimation. The pressure build up under the mantle can lead to its disruption and eruption of particles at speeds up to several meters per second[19].

Since cometary dust can be observed from the Earth only by scattered light, the knowledge about its size is dominated by those particles that provide most of the scattering cross section. The sizes of these particles are typically in the range of $1-10\mu m$. Based on observations, a distribution of the particle sizes has been proposed[20,21,22] in the form

$$n_d = g_0 \left(1 - \frac{a_0}{a}\right)^m \left(\frac{a_0}{a}\right)^n, \tag{4}$$

where a_0 is the smallest size of the grain and g_0 is the normalization parameter.

It has been traditional[23] to assume that the value of the density of the dust particles is in the range of $1-3\,\mathrm{g\,cm^{-3}}$. It is possible that the dust grains are porous aggregates and, therefore, have density that decrease with increasing its size. The density of the dust grains has been suggested[24] in the form

$$\rho(a) = \rho_0 - \rho_1 \frac{a}{a + a_1}, \tag{5}$$

where the values of the constants are $\rho_0 = 2.2\,\mathrm{g/cm^3}$, $\rho_1 = 1.4\,\mathrm{g/cm^3}$ and $a_1 = 2\mu\mathrm{m}$.

5. *Distributed source*

Sublimation of water ice and other ices and ejection of the dust particles entrained by the gas flow gradually erode the surface of the active region[25]. Dust particles entrained by the gas into the coma will heat up by sunlight. As the result, the organic component (hydrocarbon polycondensates) can be vaporized depending on heliocentric distance and particle size. Hydrocarbon polycondensates and ice constitute the distributed source[26] in the cometary coma. A large amount of observational evidence of existence of distributed sources is available[23,27,28,29]. For example, a distributed source of water has been detected around comet Hale-Bopp by its infrared spectral signatures.

Spectroscopic observations[27] of comet P/Halley show that while the distribution of water density varies as r^{-2}, which is consistent with the simple radial expansion from the nucleus, the distribution of CO requires an additional source that would reach the maximum value of production rate at a distance of 10^4 km above the surface.

6. *Outflowing*

In the model of the dust particle acceleration within the coma, it has been assumed that (1) the characteristic size of the dust grains is considerably smaller than the local value of the mean free path; (2) all molecules hitting the grain are scattered by it. The extension of the dust-gas interaction region has been estimated to be of the order of few tens of the nucleus radii[30]. Within the region, the solar gravity and radiation pressure can be neglected. Therefore, the equation of motion[31] of the dust grains is

$$\frac{4}{3}\pi a^3 \rho_d \frac{d\nu_d}{dt} = \pi a^2 \frac{C_D}{2} \rho_g \left(\nu_g - \nu_d\right)^2 - \frac{4}{3}\pi a^3 \rho_d m_N \frac{G}{R^2}, \tag{6}$$

where C_D is the drag coefficient. In the simplest case, the momentum exchange through elastic collisions[32] between the dust and the gas particles is assumed, which is equivalent to $C_D = 2$.

A more realistic model that takes into account the energy exchange between the dust grains and the ambient gas has been proposed by Probstein (1969). The energy balance for a dust grain is described by the balance equation

$$\frac{4}{3}\pi a^3 \rho_d c_d \frac{dT_d}{dt} = 4\pi a^2 q_{gd} + \pi a^2 \alpha_d \frac{F_\odot}{r^2} - 4\pi a^2 \varepsilon \sigma_0 T_d^4, \tag{7}$$

where T_d is the temperature of the dust grain, q_{gd} is the heat transfer rate per unit area, c_d is the specific heat of the dust, α_d and ε are the dust absorption in visible light and infrared emissivity, respectively, σ_0 is the Stefan-Boltzmann constant and $F_\odot$ is the solar radiative energy flux at 1 AU. The influence of the initial velocity of the dust grain on the gas flow in the innermost coma has been studied in [33]. Dusty gas hydrodynamic models have been considered in [34,37,21,2,22]. Application of the test particle technique to the problem of dust expansion into the coma has been studied [31,36].

7. *Tail formation*

Beyond the gravitational sphere of influence, the main forces that act on a dust particle are the solar pressure and the solar gravity. These forces are responsible for formation of the cometary tail. The total force acting on a dust grain can be approximated in the form

$$F = F_{grav} - F_{rad} = \left(1-\beta\right)\frac{4\pi}{3} a^3 \rho_d G \frac{M_\odot}{r^2}. \tag{8}$$

The radiation pressure constant, β, is the ratio of the radiation pressure force and the solar gravity force

$$\beta = \frac{F_{rad}}{F_{grav}} = \frac{3}{4}\frac{F_\odot r_0^2}{cGM_\odot}\frac{\eta_{pr}}{\rho_d a} = 5.78\times 10^{-4}\frac{\eta_{pr}}{\rho_d a}\left[\frac{\mathrm{kg}}{\mathrm{m}^2}\right], \tag{9}$$

where η_{pr} is the radiation pressure efficiency, c is the speed of light and $r_0 = 1.5\times10^{11}\,\mathrm{m} = 1\mathrm{AU}$. The constant β does not depend on the distance from the Sun but only on the properties of the dust grains. Assuming that the dust particles are composed from a dark dielectric material, the radiation pressure efficiency has been calculated[35] as a function of its size.

Radiation pressure is ineffective for large particles. For the dust grains of sub-micrometer size, the solar pressure may exceed the solar gravity and is responsible for the dust separation within the cometary tail. Within this approximation, dust particles move along parabolic trajectories. A more realistic structure for the cometary tail can be reproduced by taking into account motion of the comet along its orbit.

$$\frac{d\mathbf{R}}{dt} = \mathbf{v}\,, \tag{10}$$

$$\begin{gathered}\frac{4}{3}\pi a^3\rho_d\frac{d\mathbf{v}_d}{dt} = \pi a^2\frac{C_D}{2}\rho_g\left|\mathbf{v}_g-\mathbf{v}_d\right|\left(\mathbf{v}_g-\mathbf{v}_d\right) - \frac{4}{3}\pi a^3\rho_d m_N\frac{G}{R^2}\frac{\mathbf{R}}{R} + \\ \left(1-\beta\right)\frac{4\pi}{3}a^3\rho_d G\frac{M_\odot}{r^2}\frac{\mathbf{r}}{r}\end{gathered}\,. \tag{11}$$

IV. Results and Discussions

B. Neutral Coma

Comet 67P/Churyumov-Gerasimenko is the target comet for the European Space Agency (and NASA) orbiter/lander mission that was launched in March 2004. The study of its dusty-gas environment between now and encounter in 2014 is of practical importance. The coma has been considered at a set of heliocentric distances. Axis-symmetrical boundary conditions have been assumed on the spherical nucleus. Six species (H_2O, CO, OH, H_2, O, H) were considered in this work. A hard sphere collision was assumed for intermolecular collisions. For water-water collisions the viscosity equivalent cross section has been used. For other collision pairs, collision cross sections based on relevant atomic data were used. It was assumed that only two species (H_2O and CO) sublimates from the surface of the nucleus. All daughter species are produced in photo-dissociation reactions. Photo-ionization processes are taken into account. The gas environment is considered beginning from the surface of the nucleus up to 10^6 km. Some of the obtained results are presented in Figure IV.1-Figure IV.4

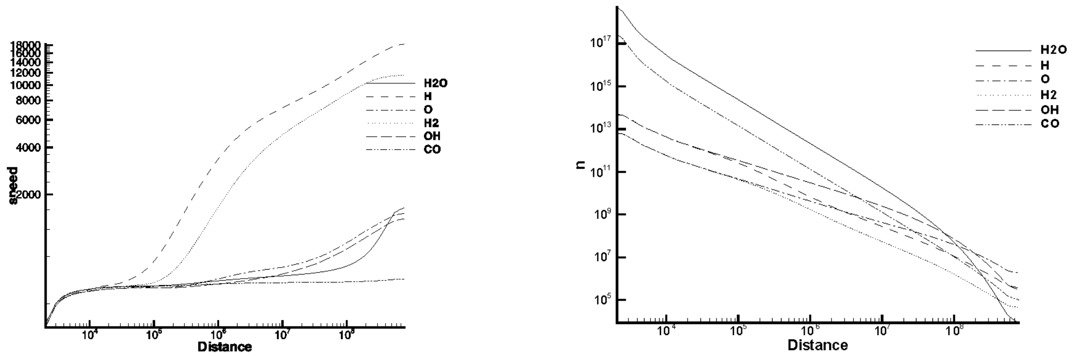

Figure IV.1 Radial speed and the density number distribution for comet Churyumov-Gerasimenko at heliocentric distance of 1.29 AU and zenith angle of 45°

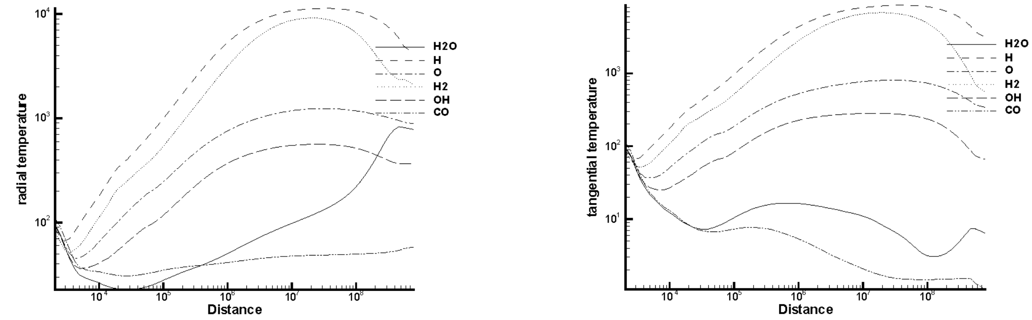

Figure IV.2 Distribution of radial and tangential temperatures distribution for comet Churyumov-Gerasimenko at heliocentric distance of 1.29 AU and zenith angle of 45^o

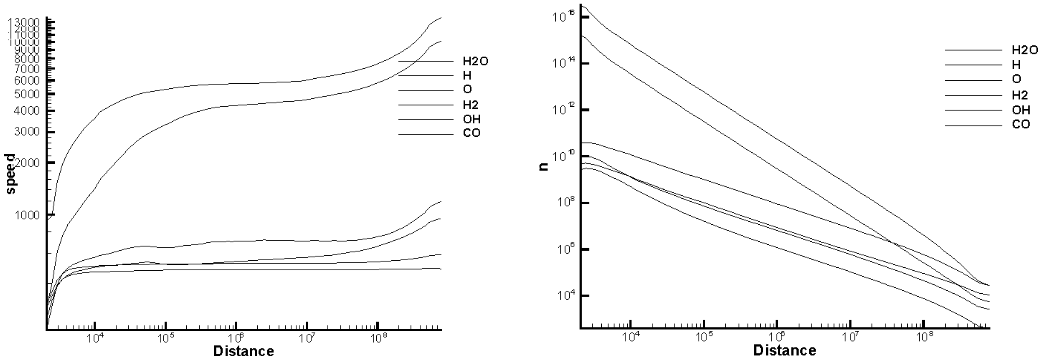

Figure IV.3 Radial speed and the density number distribution for comet Churyumov-Gerasimenko at heliocentric distance of 3.25 AU and zenith angle of 45^o

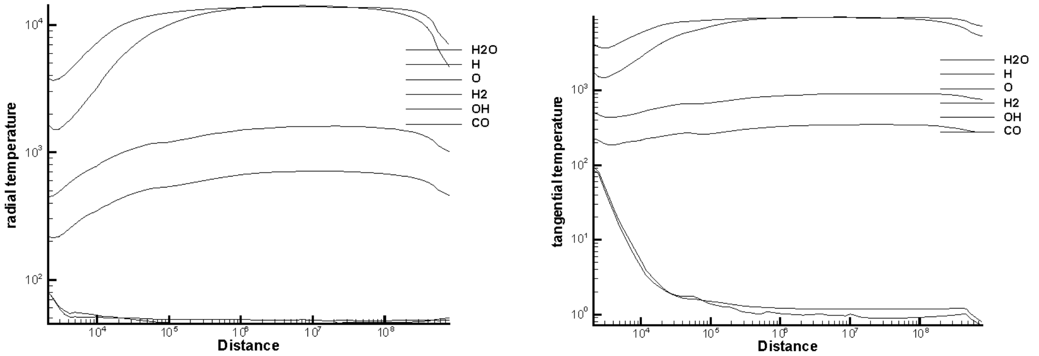

Figure IV.4 Distribution of radial and tangential temperatures distribution for comet Churyumov-Gerasimenko at heliocentric distance of 3.25 AU and zenith angle of 45^o

A strong dependence of temperature and velocity fields on the heliocentric distance of the comet has been found. Due to collisions between water and hot secondary species in the near nucleus region, an enhancement in the tail of water distribution function occurs. The enhancement does not heat water component in the collision region significantly. By distances of $10^5 - 10^6$ km, the slowest water molecules have been preferentially removed from the distribution by dissociation. This effect explains rising of temperature and bulk velocity of water component at small heliocentric distances as it is shown in Figure IV.1-Figure IV.2.

C. Dust-Gas interaction

We have considered a dusty-gas coma in a 1D spherically symmetrical geometry. In this case, a nucleus radius $R = 5.3km$ and gas production rate of 3.5×10^{28} molecules/s correspond to parameters of comet Borrelly at heliocentric distance of 1.36 AU. Comet Borrelly was the target of NASA's Deep Space 1 mission in 2001. It was assumed that only H_2O molecules sublimate from the surface. The dust/gas mass ratio is 0.4. Some obtained results are shown Figure IV.5.

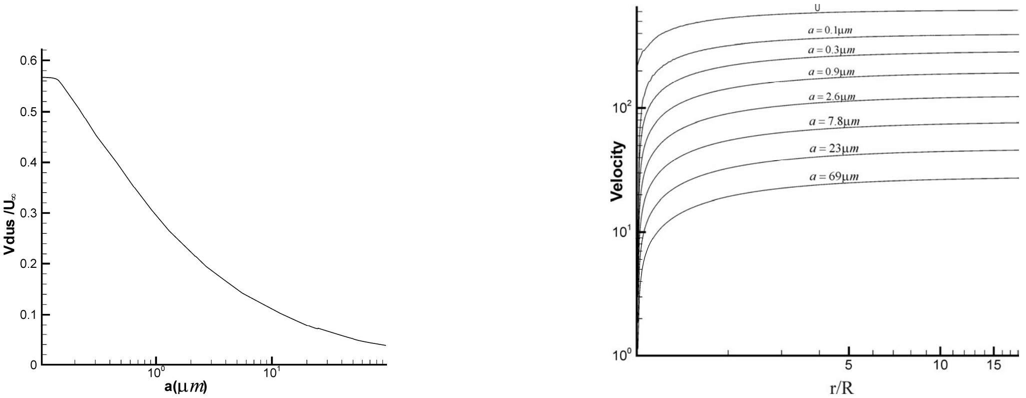

Figure IV.5 Dust particles terminal velocity profile as the function of its radius; Radial mean velocity (m/s) profiles for dust particles of a given size and the gas phase in the cometary coma as a function of a distance from the nucleus

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