Kinetic simulation of neutral/ionized gas and electrically charged dust in the coma of comet 67P/Churyumov-Gerasimenko

Valeriy Tenishev, Martin Rubin and Michael R. Combi

University of Michigan, 2455 Hayward St., Ann Arbor, MI 48109, USA

Abstract.

The cometary coma is a unique phenomenon in the solar system being a planetary atmosphere influenced by little or no gravity. As a comet approaches the sun, the water vapor with some fraction of other gases sublimate, generating a cloud of gas, ice and other refractory materials (rocky and organic dust) ejected from the surface of the nucleus. Sublimating gas molecules undergo frequent collisions and photochemical processes in the near-nucleus region. Owing to its negligible gravity, comets produce a large and highly variable extensive dusty coma with a size much larger than the characteristic size of the cometary nucleus.

The Rosetta spacecraft is *en route* to comet 67P/Churyumov-Gerasimenko for a rendezvous, landing, and extensive orbital phase beginning in 2014. Both, interpretation of measurements and safety consideration of the spacecraft require modeling of the comet's dusty gas environment.

In this work we present results of a numerical study of multispecies gaseous and electrically charged dust environment of comet Chyuryumov-Gerasimenko. Both, gas and dust phases of the coma are simulated kinetically. Photolytic reactions are taken into account. Parameters of the ambient plasma as well as the distribution of electric/magnetic fields are obtained from an MHD simulation [1] of the coma connected to the solar wind. Trajectories of ions and electrically charged dust grains are simulated by accounting for the Lorentz force and the nucleus gravity.

INTRODUCTION

The main scientific objectives of the *Rosetta* mission are the global characterization of the nucleus, the determination of the surface composition and the study of the development of cometary activity. The spacecraft will reach the comet at the beginning of October 2014, when the comet will be at a heliocentric distance of 3.3 AU in the pre-perihelion portion of its orbit and accompany the comet along its way to and through the perihelion. In addition, the *Rosetta* mission includes the Philae probe [2] that will land on the nucleus to perform a detailed investigation of its physical and compositional properties.

In most cases of practical interest and, especially for comet Churyumov-Gerasimenko during most of the *Rosetta* mission, study of cometary comae involves rarefied gas flows under strong nonequilibrium conditions that can be described only with the Boltzmann equation.

The numerical solution of kinetic equations is a challenging problem in modern computational physics. It is convenient to classify all kinetic methods according to the character of approximation related to the velocity space. Examples are a piecewise-constant interpolation or an expansion over a set of basis functions, as in the case of direct integration methods, or an approximation of the distribution function by a set of delta functions in velocity space, as done in direct simulation methods.

One of the most important features of direct simulation methods, which are based on the Monte Carlo methodology, is that they do not require the formulation of integro-differential equations that describes the evolution of the distribution function and, as a result, can be used to solve the Boltzmann equation with a collision integral accounting for elastic and inelastic collisions. Nowadays the Direct Simulation Monte Carlo (DSMC) method is the *de facto* standard numerical method for rarefied gas dynamics. Examples of application of the method for simulating of gas flows in a cometary coma are described in [3, 4, 5, 6].

MODEL OF COMETARY COMAE

A cometary coma is a complex mutually interconnected system consisting of neutral and ionized gas, cometary dust and plasma of solar wind. Due to a negligible gravity of the cometary nucleus, a coma has a characteristic size that by many orders of magnitude exceeds that of the nucleus.

A combination of a large number of physical processes defines a time variable state of a coma. The most important processes occurring in a coma includes momentum exchange [3], photolytic reactions [7], charge exchange, impact ionization, and radiational cooling [8]. A detailed description of model used in this work can be found in [5].

Containing mostly water ice, cometary nucleus gas and dust production is determined by its energy balance that is highly dependent on the comet heliocentric distance. Similarly, the local production [9] of a comet strongly depends on the location on the nucleus surface and may be significantly different on the day- and night-side of the nucleus.

Depending on a heliocentric distance, volatile gases released into the coma can be thermalized through collisions. The size of the zone where momentum exchange between gas molecules is important is usually limited by an inner coma. A traditional definition of the collision zone [7] is a sphere with a radius R_{coll}, where the local value of the mean free path is equal to the distance to the center of the nucleus. Even though this definition is highly oversimplified, it gives some measure of the characteristic size of the area where a hydrodynamic approach remains somewhat valid. The typical size of the collision sphere is $\sim 10^4$ m for bright comets with a gas production rate of the order of $\sim 10^{29}$ s^{-1}. Outside of the collision zone, a coma has to be modeled with a kinetic method. Some recent developments in coupling of DSMC and CFD approaches are presented in [10]. Associated with the coupling, the breakdown parameter is described in [11].

DYNAMICS OF DUST GRAINS IN COMETARY COMAE

A significant improvement in understanding properties of cometary dust has been achieved with the Giotto, Vega, Deep Space 1, Startdust and Deep Impact missions to different comets, where it was found that dust particles are made from carbonaceous and silicate materials [12] ranging from nanometers to millimeters in size. There is a wide list of publications that discuss physical properties of sublimating dust particles based on those observations. Some properties of such particles are discussed in [13].

Among all processes occurring in the dust phase of a coma [14] the most important are the momentum exchange with the surrounding gas, charging by plasma and absorption of solar UV radiation. It is generally recognized that because of photolitic processes and interaction with the plasma environment, dust particles in cometary tails are electrostatically charged. The most important contribution to the charging process [15] comes from ambient electrons and ions and the UV radiation induced photoemission. The electrostatic fragmentation and interaction with the interplanetary magnetic field are the two primary consequences of the dust grain charging.

It is possible that dust grains are porous aggregates [16] and therefore have a density that depends [17] on size. But in this work we limit our model by considering only spherical dusty grains with a constant density of $\rho = 1$ g cm^{-3} and a power law [18] size distribution $f(a) \sim a^s$, where a is a radius of a grain and $s = -4$ is the power index, respectively.

Neutral grains in a coma

Neglecting collisions between dust grains as well as the influence of solar radiation pressure, electromagnetic forces and solar gravity, one can obtain [19] the following equation of motion for an individual grain

$$\frac{4}{3}\pi a^3 \rho_g \frac{d\mathbf{v}_g}{dt} = \pi a^2 \frac{C_d}{2} \rho (\mathbf{v} - \mathbf{v}_g)|\mathbf{v} - \mathbf{v}_g| - \frac{4}{3}\pi a^3 \rho_g \frac{GM_n}{r^2}\frac{\mathbf{r}}{r}, \tag{1}$$

where G is the gravitational constant, M_n is the mass of the comet nucleus, $\mathbf{r}$ is the position of a dust grain in respect to the nucleus, C_d is a drag coefficient, $\mathbf{v}$ is the bulk velocity of a gas in the coma, $\mathbf{v}_g$ is the velocity of a spherical dust grain with a radius a, ρ and ρ_g are the mass density of the surrounding gas and dust grains, respectively. This approximation of the equation of motion was used in this study because the dust grain's motion is considered only within a close proximity from the nucleus where it is dominated by the interaction with the gas phase of the coma and the gravity of the nucleus. Assuming a full accomodation on the surface of a grain, the drag coefficient in a free molecular approximation [19] is

$$C_d = \frac{2}{3}\frac{\sqrt{\pi}}{\omega}\sqrt{\frac{T_g}{T}} + \frac{2\omega^2+1}{\sqrt{\pi}\omega^3}e^{-\omega^2} + \frac{4\omega^4+4\omega^2-1}{2\omega^4}\mathrm{erf}(\omega), \tag{2}$$

where $\omega = |\mathbf{v}-\mathbf{v}_g|(2kT/m)^{-1/2}$. Here, m is the mass of a gas molecule, T and T_g are temperatures of the coma and the dust grain, respectively. For typical conditions in a coma, the drag coefficient can be approximated by a constant $C_d = 2$, which was also done in this work.

In the far region of a coma, the trajectory of a dust grain is determined by the combination of solar radiation pressure and solar gravity. Since we simulate the dust phase of a coma only at cometo-centric distances important for the *Rosetta* mission (within ~ 200 km), they are neglected here. An example of study of dust motion outside of acceleration region is presented in [20].

Charging of dust grains in a coma

Exposed to surrounding plasma and solar UV radiation, dust grains gain an electric charge via electron and ion bombardment, and production of secondary photoelectrons. All of these processes depend on plasma properties (density, composition, energy distribution) as well as properties of dust grains (size, velocity, composition, surface roughness). Theoretical aspects of a large scale simulation of dust flow across the solar system that involves effect of charging of the grains is considered in [21].

The dynamics of grain charging is determined by the sum of electric currents to/from the surface of a grain $\dot{Q} = \sum_k J_k$. As a dust grain collects charges it changes the electrostatic potential distribution in its environment. If a grain initially collects more electrons than ions, the developing negative potential well around it will enhance the ion flux and lower the electron flux. The electrostatic charge on the grain that balances these fluxes is the equilibrium charge.

In the case of a negative surface potential of a dust grain, ϕ, the electron and ion collective currents [22] are

$$J_e = J_{e0}\exp(\chi), \tag{3}$$

$$J_i = \frac{J_{i0}}{2}\left[\left(M^2+\frac{1}{2}-\chi\right)\frac{\pi}{M}\mathrm{erf}(M)+\exp(-M^2)\right], \tag{4}$$

where $\chi = e\phi/kT$, $J_{0i,e} = 4\pi a^2 n_{i,e}(kT/2\pi m_{i,e})^{1/2}$. For an isolated dust grain the surface potential ϕ is related to its net charge via $\phi = Q/a$. In this formulation, it is implicitly assumed that both the electron and ion temperatures are equal to an equilibrium plasma temperature T.

Motion of electrically charged dust grains is affected by the Lorentz force $\mathbf{F}_L = Q(\mathbf{E}+\mathbf{v}\times\mathbf{B})$, where Q and $\mathbf{v}$ are the grain electric charge and velocity, and $\mathbf{E}$ and $\mathbf{B}$ are vectors of electric and magnetic fields, respectively. The force $\mathbf{F}_L$ should be added to the right hand side of the dust grain's equation of motion (Eq. 1). The spatial distribution of the field vectors and plasma flow used in this work is described in [1].

Considering this work as a first step in incorporating dust charging into our model of cometary comae, we have neglected production of secondary electrons. An analysis of photoelectron production by cometary dust can be found in [23].

RESULTS AND DISCUSSION

In this work we study the coma of comet 67P/Churyumov-Gerasimenko at a heliocentric distance of $r_h = 1.29$ AU, which is directly relevant to the *Rosetta* mission. This is a part of a larger effort, organized in connection with a number of Science Working Teams of the *Rosetta* mission. The larger effort also involves a study of the plasma and dust environment, as already mentioned in [1]. While the information presented herein will certainly be useful for various aspects of the *Rosetta* mission planning, the results will also be important for interpretation of the wide range of ground-based and in situ observations of the comet that will both precede and accompany the mission. In particular, the gas velocities and temperatures predicted as well as the extent of the aspherical nature of the coma will be useful in setting model parameters for the interpretation of *in situ* and ground-based observations that have and will be made for this comet during the next decade.

The study was performed with our DSMC model of a multispecies coma coupled through momentum exchange and photolytic processes. The coma was assumed to be axisymmetric, with an axis of symmetry along the solar direction, and consisting of H_2O, OH, O, H_2, H, and CO. Simulations were performed in the region starting from the surface of the nucleus and extending up to 10^6 km. A realistic thermophysical model was used to simulate outgassing from the surface of the nucleus. The detailed description of the numerical model can be found in [5, 24, 25].

Distribution of neutral gas in a coma

The main difficulty in the numerical kinetic simulation of cometary comae is the dramatic variation of the involved characteristic temporal and spatial scales. The lowest limit of spatial scales is determined by the local value of the mean free path that at the subsolar point of the nucleus of comet Churyumov-Gerasimenko varies from approximately 0.5 m at a heliocentric distance of r_h=1.29 AU to about 400 m at a heliocentric distance of r_h=3.25 AU. Assuming a characteristic value for the parent gas molecule velocity in the vicinity of the nucleus to be about 700 m s^{-1}, the lowest limit of the time scale varies starting from 10^{-3} s at a heliocentric distance of 1.29 AU and up to about 1 s at a heliocentric distance of 3.25 AU. In the outer coma, the characteristic time scale is determined by rates of photolytic reactions and can be estimated to be of the order of $10^5 - 10^6$ s at a heliocentric distance of 1 AU.

The general structure of the water flow in the innermost coma is given in the left panel of Fig. 1 for the case of heliocentric distance of 1.29 AU. The gas flux from the surface is produced according to the thermophysical model [9] and is concentrated on the day side at the subsolar point. Momentum exchange with highly energetic daughter species (such as H_2 and H) heats heavy components of the coma and leads to a perturbation of the tail of the water velocity distribution in the collisional transition region of the coma. The further selective photodissociation [26] causes the perturbation to be a dominant component of the distribution, which explains an increase of kinetic temperature and bulk velocity of water in the outer coma.

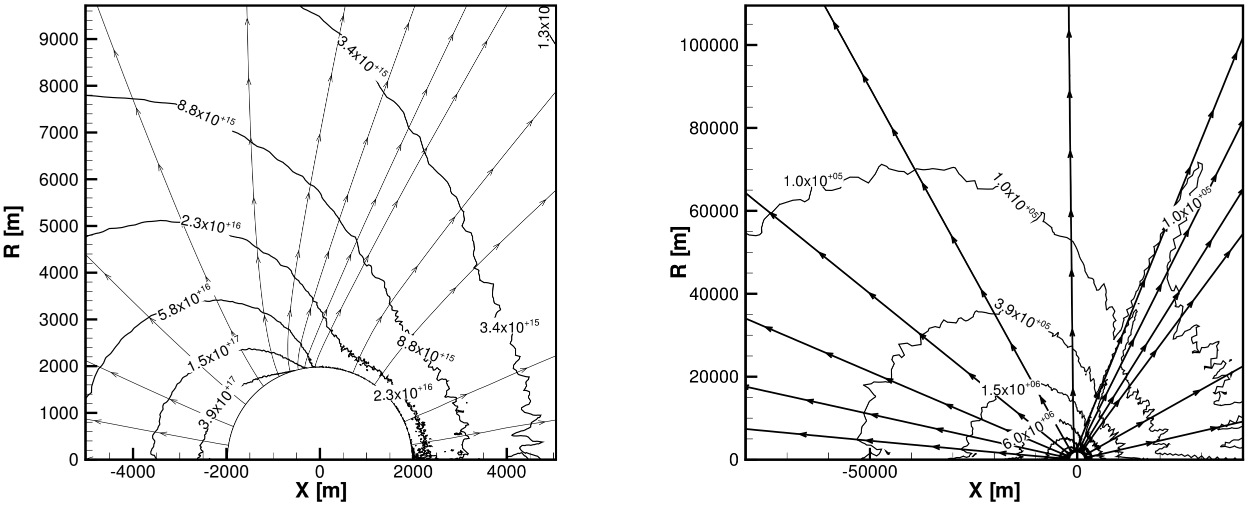

FIGURE 1. On left: Water number density (in m^{-3}) in the near nucleus region at a heliocentric distance of $r_h = 1.29$ AU. The deflection of streamlines that is seen in the figure is due to a sharp variation of sublimated gas flux occurring with a change of the subsolar angle. **On right:** Distribution of dust number density (in m^{-3}) in a vicinity of the nucleus at a heliocentric distance of $r_h = 1.29$ AU. On the day-side of the coma, the density profile follows that of the gas. The most noticeable feature on the night-side of the coma is the density spike [27]. The stream lines illustrate the trajectory of motion of dust grains. Here the X-axis is in the solar direction with the beginning at the center of the nucleus. The R-axis gives the distance of a point from the axis of symmetry.

The region of applicability of a hydrodynamic approach can be determined by studying the distribution of the Knudsen number, which can be defined in the form

$$Kn = \frac{\lambda}{\rho} \left| \nabla \rho \right| , \tag{5}$$

where ρ is the density of the water flow. As a criterion of the validity of a hydrodynamic approach, an upper limit of the Knudsen number $Kn = 0.05$ [28] can be used. From the results obtained during our simulation, it follows that even in the case of a heliocentric distance of 1.29 AU, in the near nucleus region a hydrodynamic approach is valid only within the first tens of kilometers on the dayside of the nucleus above the Knudsen layer.

Electrically neutral dust in the innermost coma

A number of approaches have been used lately for numerical simulation of dust in a coma. All of them can be split into two major classes by their representation of the dust phase. A number of dusty gas hydrodynamic models have been considered in [27, 19]. Application of the test particle technique to the problem of dust expansion into a coma has been studied in [29]. An example of a simulation of the dusty coma of comet Churyumov-Gerasimenko is presented in [6]. An example of application of a Monte Carlo model for simulating a cometary tail formation is presented in [30].

The dust density profile obtained with our model for the case of a heliocentric distance of 1.29 AU is presented in the right panel of Fig. 1. The dust grains are acted upon by the drag force and gravity of the nucleus. The local production rate of dust grains is taken to be proportional to that of water. As a result, both water and dust have the same qualitative pattern of their density profile on the day-side of the coma. The most noticeable feature related to the dust phase is the density spike [27] on the night-side of the coma, which is produced by a combined variation of the local dust production rate and the drag force.

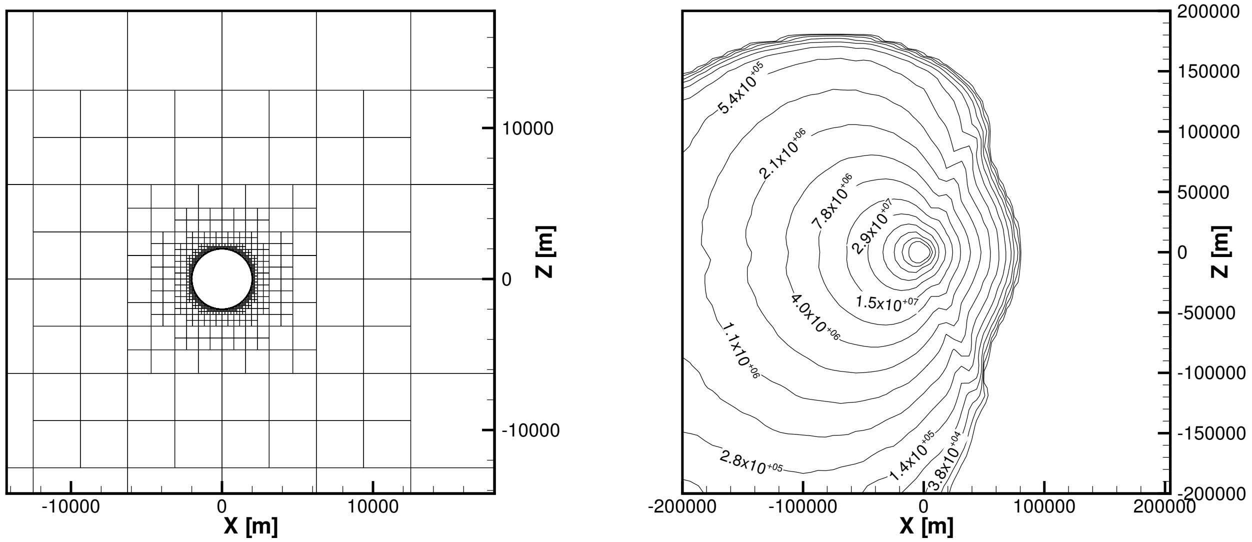

FIGURE 2. **On left**: An example of a 2D cut of a 3D block based adaptive mesh used for simulating the distribution of electrically charged dust grains in the coma of comet 67P/Churyumov-Gerasimenko at a heliocentric distance of $r_h = 1.29$ AU. **On right:** The cut of the number density (in m^{-3}) distribution of electrically charged dust grains in a plane that contains both the vector of bulk velocity of ambient plasma and the vector of the electric field [1]. It can be seen that the dust density has the signature of the dust spike analogous to that in Fig. 1.

Effect of charging processes on the dust distribution

Extending our model of neutral dust, we have added charging of dusty grains described by Eq 3 - 4. For a correct numerical integration a grains' trajectory, it is important to resolve the structure of gas and dust flows in the innermost vicinity of the nucleus, where the variation of the drag force is strongest throughout the computational domain. At the same time, we are interested in determining the distribution of dust within a domain whose characteristic size is larger than that of the nucleus. From the computational point of view, performing a simulation on a mesh with a constant spatial resolution is prohibitively expensive. For this reason, we have preformed the simulation using a block-based mesh that can change its resolution in areas where it is needed. An example of such mesh is presented in the left panel of Fig. 2. In order to capture the geometry of the nucleus, we have implemented a cut-cell approach.

The effect of charging on the structure of dust flow is presented in the right panel of Fig. 2 that shows the density profile of dust within 200 km from the nucleus for the case of a heliocentric distance of 1.29 AU. In the plot, the flow of ambient plasma is aligned along the x-axis and the magnetic field is within the xy-plane. As a result, the electric field is aligned along the z-axis. It can be seen that the presence of an electric field deflects the motion of the bulk dust flow. For this reason, charging of dust grains should be taken into account when modeling the dust phase of a coma. The Lorentz force is obtained using a pre-calculated [1] distribution of the plasma flow and electric/magnetic fields in the coma. Simulation of a grain's motion is performed in fully 3D.

ACKNOWLEDGMENTS

This work was supported by JPL subcontract 1266313 under NASA grant NMO710889, NASA Planetary Atmospheres program grant NNX09AB59G, grant AST-0707283 from the NSF Planetary Astronomy program.

REFERENCES

1. K. C. Hansen, T. Bagdonat, U. Motschmann, C. Alexander, M. R. Combi, T. E. Cravens, T. I. Gombosi, Y.-D. Jia, and I. P. Robertson, *Space Science Reviews* **128**, 133–166 (2006).
2. M. Hechler, *Advances in Space Research* **19**, 127–136 (1997).
3. M. Combi, *Icarus* **123**, 207–226 (1996).
4. J. Crifo, G. A. Loukianov, A. V. Rodionov, and V. V. Zakharov, *Icarus* **176**, 192–219 (2005).
5. V. Tenishev, M. Combi, and B. Davidsson, *Astrophysical Journal* **685**, 659–677 (2008).
6. V. Zakharov, A. Rodionov, G. Lukianov, and J. Crifo, *Icarus* **201**, 358–380 (2009).
7. M. R. Combi, and W. H. Smyth, *Astrophysical Journal* **327**, 1026–1059 (1988).
8. D. Bockelée-Morvan, and J. Crovisier, "The role of water in the thermal balance of the coma," in *Proceedings of the International Symposium on the Diversity and Similarity of Comets*, 1987, pp. 235–240.
9. B. J. R. Davidsson, and P. J. Gutiérrez, *Icarus* **180**, 224–242 (2006).
10. J. M. Burt, and I. D. Boyd, *AIAA Journal* **47**, 1507 (2009).
11. G. Abbate, C. R. Kleijn, and B. J. Thijsse, *AIAA Journal* **47**, 1741 (2009).
12. J. Agarwal, M. Müller, and E. Grün, *Space Science Reviews* **128**, 79–131 (2007).
13. H. I. M. Lichtenegger, and N. I. Komle, *Icarus* **90**, 319–325 (1991).
14. A. Levasseur-Regourd, M. Zolensky, and J. Lasue, *Planetary and Space Science* **56**, 1719–1724 (2008).
15. N. Borisov, and U. Mall, *Planetary and Space Science* **54**, 572–580 (2006).
16. L. Kolokolova, and H. Kimura, *Earth, Moon and Planets* **62**, 17–21 (2010).
17. N. Biver, D. Bockelée-Morvan, P. Colom, J. Crovisier, J. K. Davies, W. R. F. Dent, D. Despois, E. Gerard, E. Lellouch, H. Rauer, R. Moreno, and G. Paubert, *Science* **275**, 1915–1918 (1997).
18. E. Grün, J. Benkhoff, H. Fechtig, P. Hesselbarth, J. Klinger, H. Kochan, H. Kohl, D. Krankowsky, P. Lammerzahl, W. Seboldt, T. Spohn, and K. Thiel, *Advances in Space Research* **9**, 133–137 (1989).
19. T. I. Gombosi, A. F. Nagy, and T. E. Cravens, *Reviews of Geophysics* **24**, 667–700 (1986).
20. T. Bonev, "Dust particles of comet Schwassmann-Wachmann 3 during its return in 2006," in *Exploring the Solar System and the Universe*, 2008, vol. 1043 of *AIP Conference Proceedings*, pp. 163–166.
21. M. Landgraf, M. Müller, and E. Grün, *Planetary and Space Science* **47**, 1029–1050 (1999).
22. M. Horányi, *Annual review of astronomy and astrophysics* **34**, 383–418 (1996).
23. A. Juhász, and K. Szegö, *Journal of Geophysical Research* **103**, 12015–12022 (1998).
24. V. Tenishev, *AIAA-2002-3299* (2002).
25. V. Tenishev, and M. Combi, *AIAA-2003-3776* (2003).
26. M. R. Combi, B. J. Bos, and W. H. Smyth, *Astrophysical Journal* **408**, 668–677 (1993).
27. Y. Kitamura, *Icarus* **66**, 241–257 (1986).
28. P. Chen, and I. Boyd, *AIAA-2003-3783* (2003).
29. Y. V. Skorov, and H. Rickman, *Planetary and Space Science* **47**, 935–949 (1999).
30. S. V. Kharchuk, P. P. Korsun, and H. Mikuz, *Kinematics and Physics of Celestial Bodies* **25**, 189–193 (2009).