Modelling the interaction of multicomponent plasma with a CubeSat 1U microsatellite by the molecular dynamics method

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Abstract. The results of modeling the interaction of a multicomponent thermal cosmic plasma consisting of oxygen ions, hydrogen and electrons with a charged CubeSat 1U microsatellite are considered. For the simulation was used method of molecular dynamics. The characteristic features of the spatial distribution of hydrogen and oxygen ions are considered. Near a positively charged spacecraft, there is a region of negative charge, which eliminate a satellite charge. Behind the satellite is the region of the "ion shadow" in which the concentration of ions is close to zero. The spatial features of the "ion shadow" depend on the type of ion, the temperature of the plasma, the velocity and charge of the satellite relative to the plasma. The process of formation of an "ion shadow" for a number of parameters is considered.

1. Introduction
The rapid evolution of micro- and nanosatellites in recent years has led to the fact that small spacecraft have become a serious tool for research, not only near-Earth, but also interplanetary space. The purpose of such devices is extremely wide: from remote sensing of the Earth to providing radio communications and data transmission. The CubeSat standard, proposed by a group of scientists from the California Polytechnic State University, San Luis Obispo, and the Stanford University Space Systems Laboratory, made it possible to unify the designs of microsatellites and became the de facto standard for their creation [1].

The use of microsatellites for real scientific research imposes certain conditions on their design features. There is a need to minimize the currents on the surface of the microsatellite, but under real conditions, the presence of electric potential on the surface cannot be avoided. At the same time, the need to study the effect of the microsatellite electric charge on the surrounding plasma becomes obvious. Despite the fact that the study of the spatial distribution of thermal low-energy plasma around the apparatus is necessary primarily for analyzing the mass spectrometric measurements of this plasma, and such measurements are currently not available on microsatellites, data on the spatial distribution of the charge will be useful, for example, to calculate radio transmission parameters.

There are several approaches for modeling the interaction of thermal plasma and satellite. The most efficiently Particle in Cell method used. This method is used in the most successful models of the last decade - NASCAP [2], SPIS [3] and MUSCAT [4]. A review and comparison of these models, used to calculate plasma density and the electric field for different condition, are given in [5], [6]. All model calculations show presence ion-depleted wake behind moving satellite. In this work this ion-depleted wake we will calls “ion shadow”.
The need for a detailed study of the spatial distribution of the electric field around the satellites, including microsatellites, is obvious. The distortions introduced by the satellite field are significant. They can strongly affect the results of calculations of the moments of the distribution function of plasma particles [7], [8].

The choice of molecular dynamics method for our study is due to a number of reasons. First of all, the method allows us to analyze the trajectories of individual particles, which is important when analyzing mass spectrometric measurements. The complex shape of the satellite with various rods, antennas and its other components makes the spatial distribution of the electric field very difficult. This is especially important near mass spectrometers, as this can strongly distort the measurements of ion fluxes for different directions (see, for example, [9]). Such distortions may affect the results of measurement processing. They introduce an error not only in determining the angle of arrival of ions, and therefore in the components of the plasma velocity, but also in the magnitudes of the moments of the distribution function.

In addition, the chosen approach makes it easy to change both the shape of the spacecraft and the distribution function of the surrounding plasma. The solutions of the Laplace equation for any complex internal boundary are well studied. For a particular spacecraft, these calculations must be performed once. The ability to modify the particle velocity distribution functions can also be attributed to the advantages of this method.

2. Description of the model

The classical molecular dynamics method (MMD) is currently widely used to model physical, chemical, and biological systems. The founders of this method are considered Alder and Wainwright [10], and since then, MMD has been widely used. (A review of the use of MMD in physics and chemistry is given in [11]). In classical MMD, quantum and relativistic effects are neglected, and particles move in accordance with the laws of classical mechanics.

In this article, instead of the previously considered model with a microsatellite in the shape of a sphere [12], the cubic shape of the satellite (CubeSat 1U format) was considered. The shape of the satellite is important for modeling the detailed spatial distribution of the electric field. However, the large-scale features of the spatial distribution of ions and electrons (such as the ion shadow) remain generally unchanged. In addition, in this article, processes are simulated in a multi-component thermal plasma consisting of electrons and ions of hydrogen and oxygen. Such a composition of thermal plasma is characteristic of the heights of the upper ionosphere and magnetosphere.

Let us consider the 3D simulation of a charged microsatellite and a thermal Maxwellian plasma by MMD in more detail. The plasma consists of protons, oxygen ions and electrons. The force of Lorentz acts on every particle in the process of its motion:

\[ ma = qE + q(v \times B), \]  

where \( m \) is the mass of the ion or electron, \( q \), \( a \), \( v \) is its charge, acceleration and velocity, respectively, \( E \) is the electric field strength, \( B \) is the magnetic field.

The electric field strength at any point in the simulation area is calculated according to the Coulomb law. For its calculation, all the electrons and ions that are in the computational domain are used. The electric field from the satellite is also taken into account.

\[ E = \sum_{i=1}^{n} \frac{q_i}{4\pi \varepsilon_0 r_i^2} \frac{r_i}{r_i} + E_{sat} \]  

Thus, for each particle one can find the value and direction of force in the right side of the equation (1) to obtain the positions and velocities of the particles in the new time level. The spatial distribution of the satellite’s electric field potential is found from the solution of the Laplace equation. From the found values, the components of the electric field strength are determined.

The particles at the initial time of simulation are evenly distributed in space and have a Maxwell velocity distribution.
\[ F(v) = \left( \frac{m}{2\pi kT} \right)^{3/2} \exp \left( -\frac{mv^2}{2kT} \right), \]

where \( v \) - velocity of the particle, \( m \) - its mass, \( k \) - Boltzmann constant, \( T \) - temperature.

The number of particles \( N \) in the speed range \([v, v + dv]\) for the density \( n \) is calculated as

\[ N = \int_v^{v+dv} 4\pi n v^2 F(v) dv \]  

We briefly consider the geometry of this model and the parameters of the thermal plasma used for numerical calculations. The simulation area is a cube with an edge of 1 meter. At its center is the CubeSat 1U microsatellite with an edge of 10 cm. At the initial moment of time, it is surrounded by a quasi-neutral thermal Maxwellian plasma. Plasma consists of electrons with a concentration of \( Ne = 20 \text{ cm}^{-3} \), hydrogen ions and oxygen ions. The concentration of each of the ion components is the same \( N(H^+)=N(O^+) = 10 \text{ cm}^{-3} \).

Thus, the total number of particles in the simulation area is approximately \( 4 \times 10^7 \). Maxwellian temperature for electrons and ions was equal. Its value for various model calculations was 2,500 K and 5,000 K. The relative speed of the microsatellite and plasma was 5 km/s and 10 km/s. The satellite velocity (in the plasma coordinate system) is directed along the X axis to the negative half-plane (in all figures from right to left).

In our calculations, it is believed that the potential of the microsatellite remains fixed. This means that the currents arising due to the incidence of ions and electrons on the surface of the satellite and the photoelectron emission are mutually equals. The calculation of such currents values is certainly possible when specifying the materials of the satellite and the conditions of its illumination, but it was not the purpose of this simulation.

All plasma particles move in accordance with the laws of classical mechanics under the influence of the Coulomb and Lorentz forces. In the calculations below, the Earth’s magnetic field is not taken into account, so only Coulomb interaction is taken into account. At the initial instant of time, the entire model space is filled with plasma particles (electrons, oxygen ions and hydrogen ions), which are uniformly distributed with velocities corresponding to the Maxwell distribution. During each time step, some particles go beyond the model region, while other particles (mainly electrons) fall on the satellite surface. In accordance with the condition of constant electric potential on the satellite’s surface, the number of electrons incident on its surface should be equal to the number of injected photoelectrons (provided that ions are reflected from the surface).

In this model, photoelectrons have the same Maxwellian distribution as the incident electrons. The magnitude of the error of this approximation will be estimated in future work, but according to preliminary estimates, it will not have any serious effect on the results obtained. At each time step, ions and electrons are introduced from all lateral faces of the simulation region in accordance with the unperturbed Maxwell distribution taking into account the speed of the satellite and plasma instead of those that left the simulation region as a result of their motion.

3. Numerical simulation results

Consider the results of calculations of the spatial distribution of oxygen and hydrogen ions in the most informative XOZ plane. This plane includes the satellite’s velocity vector relative to the plasma. In the figures, the speed is directed along the axis OX from right to left. All the figures below correspond to the time of \( 10^{-4} \) seconds from the beginning of the numerical simulation.

The choice of the time step value is determined by the values of the average thermal velocities of the electrons and the features of the model geometry. The average thermal electron velocity for temperatures of several thousand degrees is about 500 km/s. The time step used in the model was 10^{-8} s and corresponds to the characteristic spatial dimensions of the order of 5 mm. As a result of modeling, we tried to obtain a quasi-stationary spatial plasma distribution. The paper presents the results obtained after \( 10^{-4} \) s from the initial distribution, which corresponds to \( 10^4 \) time steps and
approximately corresponds to the value of the plasma frequency. The Debye radius for the selected plasma concentration was 0.7-1.0 meters for temperatures of 2,500K and 5,000K, respectively.

3.1. Spatial distributions of oxygen ions
Consider the results of numerical simulations for oxygen ions. The following parameters were used for calculations: the temperature of all plasma components 2,500 K and 5,000 K, the satellite velocity relative to the plasma 5 km / s and 10 km / s. The satellite potential for all calculations was 5 Volts. The spatial picture for oxygen ions in the XOZ plane is presented after $10^4$ time steps, which corresponds to $10^{-4}$ seconds after the start of modeling.

Figures 1 and 2 show the spatial distributions of oxygen ions in the plane containing the vector of the relative velocity of the satellite and the plasma for various plasma parameters and the relative velocity of the plasma and the satellite.

![Figure 1](image1.png)

**Figure 1.** The spatial distribution of oxygen ions in the XOZ plane for a relative satellite velocity and plasma of 5 km / sec and an ion temperature of $T = 2,500$ K (left) and $T = 5,000$ K (right).

For all variants of numerical calculations, the ion shadow is clearly observed. Its spatial dimensions are determined by the temperature of the plasma and the relative velocity of the plasma and satellite. The transverse dimensions of the shadow range from 0.5 meters to 1 meter, while the longitudinal dimensions exceed the modeling area and are likely to reach one meter or more. Naturally, the longitudinal dimensions of the shadow are greater, the greater the relative velocity of the satellite and the plasma. Obviously, the size and shape of the ion shadow also depends on the positive charge of the satellite. Such calculations were carried out and showed that an increase in the satellite potential leads to an increase in both the longitudinal and transverse sizes of the ion shadow.

Directly in front of the satellite is an area with increased concentration. This region is more explicit at lower plasma temperatures and higher relative velocities of the satellite and plasma. Note that for a speed of 5 km / s there is a region of very low concentration in front of the satellite, which means that mass spectrometric measurements of oxygen ions under such conditions are very difficult. The angular distribution of ion fluxes, which can be measured by mass spectrometers, will be strongly distorted for the considered conditions. Measurements in the direction opposite to the relative velocity of the satellite and the plasma cannot be performed for any conditions.
3.2. Spatial distributions of hydrogen ions

A different spatial picture is observed for light ions, which include hydrogen ions. Figures 3 and 4 show the spatial distribution of hydrogen ions for the same conditions as shown in Figures 1 and 2 for oxygen ions. For a quasi stationary situation, a clear boundary of the ion shadow is practically not determined. Moreover, the difference in the spatial distributions of hydrogen ions for a temperature of 2,500K and 5,000K is difficult to distinguish. For a relative satellite and plasma velocity of 5 km / s, the region of reduced ion concentration is almost symmetrical. Its shape is close to spherical with a radius of about 20 cm.

Figure 2. The same as in Figure 1 for the relative velocity of the satellite and plasma 10 km / sec.

Figure 3. The spatial distribution of hydrogen ions in the XOZ plane for a relative satellite velocity and plasma of 5 km / sec and an ionic temperature of $T = 2,500$ K (left) and $T = 5,000$ K (right).
For a relative speed of 10 km / s (Figure 4), the spatial distribution of hydrogen ions is slightly asymmetric, but even in this case there is no ion shadow behind the satellite. Instead of the ion shadow, a region of depleted hydrogen ion density around the satellite is observed.

![Image](https://via.placeholder.com/150)

**Figure 4.** The same as in Figure 3 but for a relative speed of 10 km / s.

The simulation results are fundamentally different from previous calculations, in which a single-ion plasma consisting only of hydrogen ions and electrons was considered. In this case, the ion shadow was pronounced. The formation of such a hydrogen ion shadow can be seen in Figure 6. Subsequently, as the formation of the oxygen ion shadow and, as a result, the formation of a cloud of negative charge behind the satellite, the boundary of the hydrogen ion shadow is “blurred”.

Note that in any of the cases considered above, correct mass spectrometric measurements of hydrogen ions are impossible.

### 3.3. Formation of spatial ion and electron distributions near the microsatellite

Consider the process of formation of spatial ion distributions around a satellite. For this, for definiteness, we will consider only one case, namely: the temperature of ions and electrons $T = 2,500$ K, the relative velocity of the satellite and plasma $V = 10$ km / s.

The formation of the ion shadow, for which oxygen ions are responsible, is shown in Figure 5. The simulation data corresponds to 1,000, 2,500, and 5,000 time steps. Since the time step was $10^{-5}$ s, the results presented correspond to time intervals of $10^{-5}$ s, $2.5 \times 10^{-5}$ s, and $5 \times 10^{-5}$ s. On the whole, the presented figures fully correspond to the ideas about the formation of the ion shadow behind the satellite. In the process of its formation behind the satellite, in front of the spacecraft, on the contrary, an area of increased concentration is formed.

The ion shadow forms very quickly. Its main spatial features appear during $5 \times 10^{-5}$ s. This time corresponds to several plasma oscillations. The plasma frequency for an electron concentration of $20 \text{ cm}^{-3}$ is $f_{pe} = 4 \times 10^7$ Hz.

The spatial distribution of hydrogen ions is formed differently (Figure 6). Due to the smaller mass and higher thermal velocity, hydrogen ions much faster than oxygen ions compensate for the positive charge of the satellite, but later (due to the spatial redistribution of heavier oxygen ions) their distribution becomes more equilibrium, which can be observed in Figures 4 and 6. In the process of formation, the region of depleted concentration of hydrogen ions first has clear boundaries, and its shape is asymmetric. Behind the satellite, this area is significantly larger than the area in front of it.
Then, as the oxygen ion shadow forms, the boundaries of the region of depleted hydrogen ion concentration become blurred, and it itself becomes more and more symmetrical.

Note that the picture of the spatial distribution for the single-ion situation and the two-ion case differs significantly.

![Figure 5. The formation of the spatial structure of oxygen ions. Figures correspond to $10^{-5}$ (left), $2.5 \times 10^{-5}$ (central) and $5 \times 10^{-5}$ seconds (right) from the start of the numerical experiment.](image)

![Figure 6. The formation of the spatial structure of hydrogen ions. Figures correspond to $10^{-5}$ (left), $2.5 \times 10^{-5}$ (central) and $5 \times 10^{-5}$ seconds (right) from the start of the numerical experiment.](image)

The formation of the spatial distribution of electrons is shown in Figure 7. Due to their low mass and significantly higher thermal velocities, the initial spatially uniform distribution varies over several tens of time steps. First, there is an increase in the electron concentration around the positively charged satellite, which is clearly visible on the left side of Figure 7. The spatial distribution of electrons is shown after 100 time steps, which corresponds to an interval of $10^{-6}$ s from the equilibrium state. After 200 time steps (the middle part of Figure 7), the electron concentration near the satellite begins to decrease. Finally, after 300 time steps (right side of Figure 7) the spatial distribution of electron concentration becomes homogeneous.

Such a simulation result seems unnatural only at first glance. An explanation of the features of the formation of the spatial distribution of electrons is quite simple. To compensate for the satellite’s positive space charge, a negative space charge around it is needed, which is immediately provided by electrons whose thermal velocity is much higher than ion velocities. In this case, the electrons incident on the surface of the satellite are immediately injected back in the form of photoelectrons. This is necessary to maintain a constant electric potential of the satellite, in accordance with the simulation conditions. Over time, the spatial distribution of ions forms a region of low concentration around and behind the satellite. In this case, even an unperturbed spatially uniform distribution of electrons provides the necessary screening of the satellite’s positive charge.
Figure 7. The formation of the spatial structure of electrons. The figures correspond to $10^{-6}$ (left picture), $2 \times 10^{-6}$ (central) and $3 \times 10^{-6}$ seconds (right) from the start of the numerical experiment.

4. Conclusion

Thus, the presented model made it possible to study the spatial distribution of ions and electrons for a multi-component plasma near a charged microsatellite of the CubSat 1U format. It has been shown that the ion shadow is formed mainly by heavier oxygen ions when their concentration is sufficiently high. The spatial dimensions of such an ion shadow are approximately 0.5 m across and more than a meter along the direction of the relative velocity of the plasma and the satellite and is located behind the satellite. Lighter hydrogen ions participate in the formation of the ion shadow only at the initial stage. Subsequently, an almost symmetric region of the depleted concentration of hydrogen ions forms around the satellite. The spatial distribution of electrons differs from equilibrium only at the beginning of the shadow formation process and subsequently becomes spatially equilibrium.

The ionic composition of the plasma can significantly change the processes of formation of ion shadow. So in a one-component hydrogen plasma, an ion shadow is formed by hydrogen ions, and in an oxygen-hydrogen plasma is formed by oxygen ions.

A numerical model based on the molecular dynamics method quite satisfactorily describes the processes of interaction of a charged microsatellite and thermal plasma.

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