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THE NEAR-NUCLEUS ATMOSPHERE OF COMET 67P/CHURYUMOV – GERASIMENKO AT THE MOMENT OF ITS RENDEZVOUS WITH THE ROSETTA SPACE PROBE

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Abstract. The multicomponent atmosphere of a comet with a complex-shaped nucleus has been simulated. The geometry and integral parameters of the gas production of the nucleus correspond to the conditions of comet 67P/Churyumov – Gerasimenko at the moment of its rendezvous with the Rosetta probe. The simulation was performed using both gas-dynamic methods, which involve numerical solution of the Euler/Navier – Stokes equations, and the kinetic approach based on the solution of the Boltzmann equation. The flow structure in the vicinity to the nucleus was analyzed, the applicability of gas-dynamic methods for prediction of a rarefied atmosphere was assessed, and the importance of considering translational-rotational nonequilibrium for interpreting observational data was analyzed.

Keywords: near-nucleus atmosphere of comet, comet 67P/Churyumov-Gerasimenko, rarefied flow, numerical simulation

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ОКОЛОЯДЕРНАЯ АТМОСФЕРА КОМЕТЫ 67P/ЧУРЮМОВА–ГЕРАСИМЕНКО В МОМЕНТ ВСТРЕЧИ С ЗОНДОМ РОЗЕТТА

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Аннотация. Проведено моделирование многокомпонентной атмосферы кометы с ядром сложной формы. Геометрия и интегральные параметры газопроизводительности ядра соответствуют условиям кометы 67P/Чурюмова – Герасименко в момент встречи с зондом «Розетта». Для моделирования применялись как газодинамические методы, предполагающие численное решение систем уравнений Эйлера и Навье–Стокса, так и кинетический подход на базе решения уравнения Больцмана. Проанализирована структура течения в окрестности ядра, выполнена оценка возможности применения газодинамических методов для расчета разреженной атмосферы, проведен анализ необходимости учета поступательно-вращательной неравновесности для интерпретации известных результатов наблюдений.

Ключевые слова: околоядерная атмосфера кометы, комета 67P/Чурюмова – Герасименко, разреженное течение, численное моделирование

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Introduction

Comets are small bodies of the Solar System with a high content of primordial ice; their composition could have remained unchanged since their formation in the protoplanetary disk. As the comet is exposed to solar radiation, the nucleus heats up, the ice sublimates, and the sublimation products leave the nucleus, flowing into outer space and forming a cometary atmosphere. Studies of the composition and structure of cometary nuclei provide important information about the evolution of the Solar System and the processes of planet formation [1, 2].

Since direct exploration of the cometary nucleus is not possible, data on its structure and composition must be inferred from the dynamics, structure, and composition of its near-nucleus atmosphere (coma). Such information is accumulated through observations of comets both from large distances using telescopes located on the Earth's surface or in near-Earth orbits, and from relatively small distances (for example, using space probes).

A physical model is required to derive the physical properties of the nucleus from measurements of the coma's composition and parameters. This model must link the processes occurring within the nucleus and on its surface to those in the near-nucleus atmosphere. A detailed understanding of the coma's structure and the behavior of its components is essential for developing such a model, interpreting observational data, and optimizing observation programs. To this end, this paper considers a possible configuration of the gaseous atmosphere in a comet located at a relatively large distance from the Sun.

Simulation of atmospheric dynamics is a complex computational problem. In general, it is necessary to consider three-dimensional nonstationary processes with a wide range of parameters. Since the gas species produced by the nucleus expand into vacuum, the flow in the cometary atmosphere is characterized by the presence of both non-continuum and non-equilibrium regions. Therefore, such flows should be described by both continuum models (Euler and Navier–Stokes equations) and kinetic models (Boltzmann equation). Furthermore, continuum methods require solving the Knudsen layer problem to establish boundary conditions at the surface of the nucleus. The Knudsen layer is a near-surface region where the initially non-Maxwellian velocity distribution of emitted molecules relaxes to an equilibrium Maxwellian distribution. Kinetic methods, such as the Direct Simulation Monte Carlo (DSMC), make it possible to conduct physically correct simulation of rarefied and non-equilibrium flows, are much more computationally expensive than gas-dynamic methods.

As an example, we selected the 67P/Churyumov–Gerasimenko comet (referred to as 67P for short) as the most thoroughly studied comet in the Rosetta mission of the European Space Agency [3, 4]. The chosen heliocentric distance corresponds to the rendezvous of the Rosetta probe with the comet, when the gas production by the nucleus was still far from its maximum (at perihelion) and the total emissions of different components were comparable.

The objectives of this work are as follows:

(*i*) to determine the flow structure in the vicinity of the nucleus of comet 67P at a heliocentric distance of about 3 AU;

(*ii*) to assess whether the resulting flow can be computed using the Euler and/or Navier–Stokes equations;

(*iii*) to analyze whether translational-rotational non-equilibrium should be included in simulations of cometary atmosphere dynamics.

Problem statement

We consider a computational domain with the nucleus surface as its inner (inflow) boundary and a sphere of 35 km radius circumscribed about the nucleus as its outer (outflow) boundary. The geometry of the nucleus (Fig. 1) corresponds to RMOC Shape 3, one of the first reconstructions for the nucleus of comet 67P. The equivalent radius of this shape is $R_n = 1.7$ km.

It is assumed that the nucleus rotates around the z axis with a period of 12.4 hours. The considered region of the computational domain has a length of 35 km in the radial direction. The characteristic flow velocity in the region is more than 100 m/s, i.e., the transit time for molecules

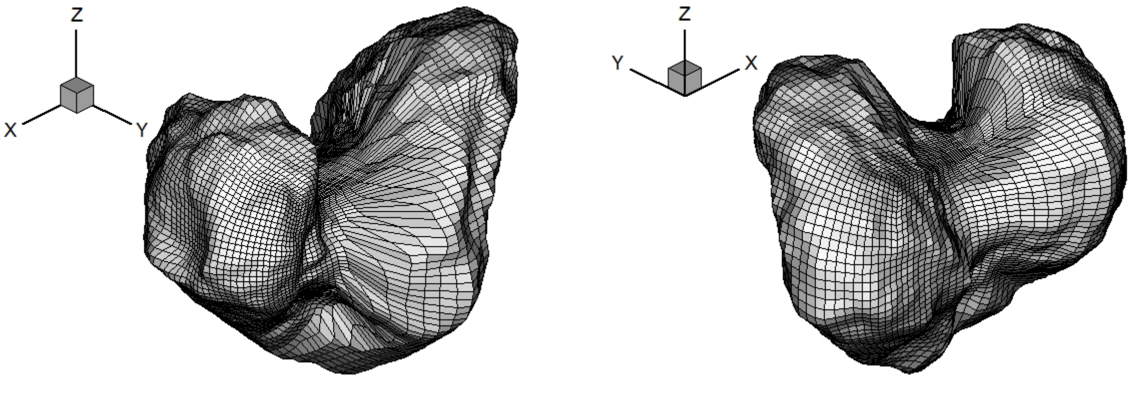

Fig. 1. RMOC shape 3 model of comet 67P/Churyumov–Gerasimenko nucleus (3D views from two angles around the Z axis)

from the surface to the outer boundary of the computational domain is less than 350 s. During this time, the position of the nucleus changes by less than 3°. For this reason, we assumed that the change in the Sun's position over the time required for the flow to settle in the region does not noticeably affect the distribution of surface gas production. Accordingly, steady-state solutions were used to describe the flow in the coma.

The nucleus is assumed to consist of a mixture of water, carbon monoxide and dioxide (H_2O, CO and CO_2) ices, as well as of refractory components. The corresponding ices have different sublimation temperatures. According to [5], H_2O ice is located on the surface, while CO and CO_2 ices lie in the nucleus at some depth. Thus, sublimation of water molecules occurs directly from the surface of the cometary nucleus, while carbon monoxide and dioxide molecules diffuse from the depth of the nucleus.

The H_2O emission model assumes that the cometary surface is covered with a large number of small-sized icy patches with an integral fraction f of the surface area. In this paper, $f = 0.033$ and this fraction is constant over the entire surface of the nucleus.

The solar irradiance per unit area of the illuminated (unshadowed) nucleus surface is given by

$$E_{in} = (1 - A) \cdot c_{sun} \cdot \max[0, \cos(\theta)] / r_h^2, \tag{1}$$

where A is the visual albedo ($A = 0.05$ was taken); c_{sun} is the solar constant, i.e., the solar radiation flux received by a given area one astronomical unit away from the Sun, $r_h = 1$ AU, $c_{sun} = 1360$ W/m^2; θ (rad) is the angle between the local normal to the surface and the direction to the Sun.

The energy balance equation for the icy surface assumes that the incident energy flux is expended on thermal radiation and sublimation of H_2O molecules (heat transfer with the inner layers of the nucleus and with ice-free surface regions is neglected):

$$E_{in} = \varepsilon_n \cdot \sigma_B \cdot T_I^4 + L_s \cdot Z_{0(\mathrm{H2O})}, \tag{2}$$

where T_I (K) is the temperature of ice on the comet's surface; ε_n is the emissivity of the nucleus surface, $\varepsilon_n = 0.9$; σ_B (W/(m^2·K^4)) is the Stefan–Boltzmann constant; $Z_{0(\mathrm{H2O})}$ (kg/(s·m^2)) is the mass flux of water molecules from the unit area of an icy patch on the surface; L_S (J/kg) is the latent heat of ice sublimation.

Water molecules sublimating from the surface of the nucleus have a semi-Maxwellian velocity distribution (i.e., the bulk velocity is assumed to be zero, and the emitted molecules have a positive velocity component normal to the surface). Due to intermolecular collisions, the velocity distribution relaxes (if there are enough collisions) to an equilibrium Maxwellian distribution in the layer above the surface (the Knudsen layer). The gas parameters at the outer boundary of the Knudsen layer should be determined to use continuum methods. Since the nucleus radius is much larger than the thickness of the Knudsen layer, this paper uses an analytical solution for a plane-parallel Knudsen layer obtained by Cercignani [6] from the solution of the Boltzmann equation:

$$Z_{0(\mathrm{H2O})} = \frac{p_s(T_I)}{\sqrt{k_B T_0 / m}} \cdot \sqrt{2} \cdot S \cdot \left\{ \frac{1}{2} - S \sqrt{\frac{T_0}{\pi T_I}} + \left[\left(S^2 + \frac{1}{2} \right) \sqrt{\frac{T_0}{T_I}} - \frac{S\sqrt{\pi}}{2} \right] erfc(S) \exp(S^2) \right\}; \tag{3}$$

$$\sqrt{\frac{T_0}{T_I}} = \sqrt{1 + \left(\frac{S\sqrt{\pi}}{2} \cdot \frac{\gamma - 1}{\gamma + 1} \right)^2} - \frac{S\sqrt{\pi}}{2} \cdot \frac{\gamma - 1}{\gamma + 1}, \tag{4}$$

where k_B (J/K) is the Boltzmann constant; m (kg) is the mass of a water molecule; T_0 (K) is the gas temperature; S is the dimensionless velocity at the outer boundary of the Knudsen layer, $S = u_0 / \sqrt{2 k_B T_0 / m}$ (u_0 (m/s) is the velocity); $p_s(T_\mathrm{I})$ (Pa) is the pressure of saturated water vapor; γ is the adiabatic index.

The flux of water molecules from the surface (comprising both icy patches and ice-free regions) is defined as the product $f \cdot Z_{0(\mathrm{H_2O})}$.

Expressions (3) and (4) depend on the parameter determining the effect of the comet's atmosphere on the flux emitted from the comet's surface. The local Mach number at the surface is used as such a parameter:

$$M_0 = S\sqrt{2/\gamma}\,(M_0 \le 1).$$

The model describing the emission of carbon monoxide and carbon dioxide assumes that ice sublimation occurs within the nucleus and molecules diffuse from the depth through the pores to the surface. Because of the large uncertainty (lack of observational data) in the parameters of the surface layer structure, the simplest model is used in this work, making it possible to qualitatively reproduce the integral characteristics of the observed processes in the nucleus. The emission flux is assumed to consist of two parts (in a certain proportion):

the one evenly distributed over the entire surface,

the one proportional to the incident solar radiation.

The first part is related to the low sublimation temperature of CO and CO_2 (the sublimation temperature of water is much higher). The temperature in the surface layer remains sufficiently high for sublimation of CO, CO_2 throughout the rotation period, even on the night side.

The second part is associated with the variation of the sublimation flux due to the surface heating which is proportional to the incident solar irradiance.

Thus, the flux emitted from a unit surface area is expressed as

$$Z_J = Q_J \left\{ \frac{a_{0,J}}{A_{ext}} + \frac{(1 - a_{0,J})}{A_{\odot}} \max\left[0, \cos(\theta)\right] \right\}, \tag{5}$$

where the subscript J corresponds to CO or CO_2; Q_J (kg/s) is the total flux of component J from the comet's surface (an input parameter of the model); A_{ext}, $A_{\odot}$ (m^2), are the total surface area and the cross-sectional area of the nucleus illuminated by the Sun, respectively; $a_{0,J}$ is the fraction of emission uniformly distributed over the surface ($a_0 = 0.11$ in this paper).

The gas emission models used in this work are the simplest with the minimum number of parameters. However, a number of studies confirmed that these models are capable of reproducing the integral and qualitative variations in gas production for different comets (see, for example, [5, 7–10]). The model parameters were adjusted in [5] to fit the *in situ* measurements of the coma composition and density along the probe trajectory, as well as the variations in the total gas production of the nucleus. These simplest models (neglecting heat conduction within the nucleus) yield satisfactory agreement with the observational data for a certain angle between the rotation axis of the nucleus and the direction towards the Sun, i.e., only for a limited segment of the comet's trajectory and a limited time interval.

The initial surface for solving the Euler and Navier–Stokes equations is the outer boundary of the Knudsen layer, whose thickness is assumed negligible compared to the nucleus radius, so the geometric position of this boundary coincides with the nucleus surface. The emission flux is assumed to be directed normal to the surface. The remaining gas parameters (density, pressure, velocity) can be calculated for simulation by continuum methods based on the values of the emission flux and temperature obtained at the outer boundary of the Knudsen layer, along with the Mach number M_0 (set at the surface).

A free outflow condition was imposed at the outer boundary of the computational domain (a 35 km radius sphere around the nucleus). The radial component of velocity is supersonic, making this boundary condition well-posed.

The continuum description of the flow in this paper is based on solving either the Euler equations or the Navier–Stokes–Fourier equations (for viscous heat-conducting compressible fluid).

A second-order Godunov scheme proposed by Rodionov and described in [11] is used to solve the equations of gas dynamics. This scheme has a distinctive feature: a linear distribution of parameters is used within each cell to obtain second-order spatial accuracy (using Kolgan or van Leer limiter reconstructions). The second-order time accuracy is achieved by using a predictor-corrector procedure. The computations were performed based on the time-marching method, where the steady-state solution is obtained by long-time integration using unsteady solvers.

To solve the Navier–Stokes equations, their right-hand sides (the terms describing viscosity, thermal conductivity, and diffusion of the mixture components) are approximated explicitly using central differences. Unlike the solution of Euler equations, simulation of a highly rarefied coma can be problematic, as dissipative processes (the right-hand sides of the Navier–Stokes equations) begin to dominate over convective processes (advection of mass between cells). In such cases, computations based on the Navier–Stokes equations do not yield a steady-state solution.

The DSMC method [12, 13] is used for kinetic description of the flow. It is a stochastic method for solving the Boltzmann equation. The DSMC method does not require special treatment of the Knudsen layer; the values of the emission flux and temperature for H_2O follow from the solution of Eq. (2), and the respective values for CO and CO_2 follow from Eq. (5). The emission of molecules from the surface is described by a semi-Maxwellian velocity distribution, i.e., the velocities of the emitted molecules follow a Maxwellian distribution with zero mean velocity and have only a positive velocity component normal to the surface.

The Variable Hard Sphere (VHS) model and the no-time-counter (NTC) collision scheme were used for the particles within the DSMC approach [12]. The Larsen–Borgnakke model with the number of collisions necessary to establish translational–rotational equilibrium $\Lambda = 1$ was used to describe the translational-rotational energy transfer. The vibrational degrees of freedom of the molecules were assumed to be relaxed in the given temperature range. A fraction β of the molecular flux returning to the surface ($\beta = f$) condensed, while the remaining fraction $(1 - \beta)$ was reflected diffusely with full energy accommodation.

A detailed description of the parameters (the dependences of viscosity on temperature, collision cross-section, etc.) used in gas-dynamic and kinetic simulations is provided in [14–18].

Computational results and discussion

We consider gas flow in the vicinity of the nucleus of comet 67P, positioned at a heliocentric distance of 3.22 AU. It is assumed that the Sun is in the *XZ* plane and the direction to the Sun is 50° from the *Z* axis (towards the *X* axis).

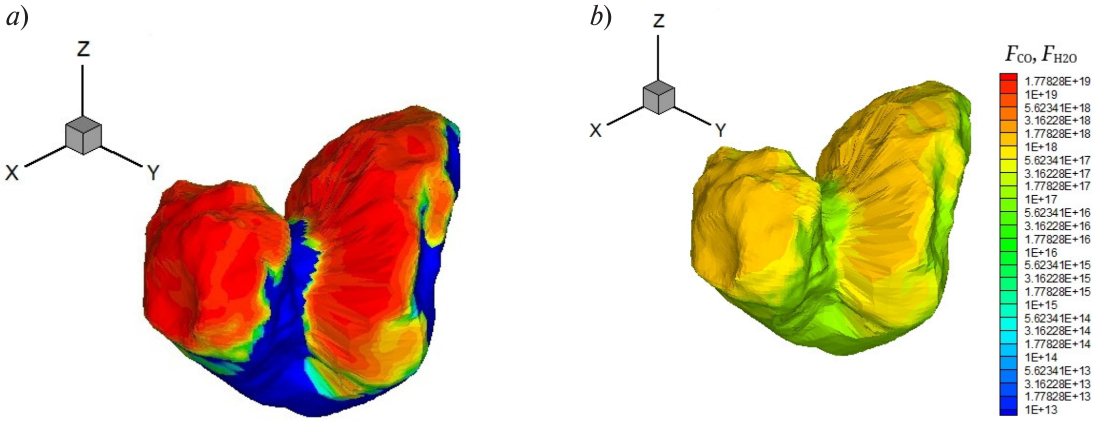

Fig. 2. 3D views of emission flux distributions over nucleus surface (in $m^{-2} \cdot s^{-1}$), calculated for H_2O (*a*) and CO (*b*)

Fig. 2 shows the distribution of gas emission fluxes over the surface of the comet's nucleus. The distributions of CO ($Q_{CO} = 2 \cdot 10^{25}$ s^{-1}) and CO_2 ($Q_{CO_2} = 3 \cdot 10^{24}$ s^{-1}) fluxes for the adopted model of gas production differ by a constant factor $Q_{CO_2}/Q_{CO} = 0.15$. For this reason, Fig. 2 shows only the gas flux distribution for CO. The emission of H_2O is determined by surface sublimation of ice. The intensity of this emission is highly sensitive to temperature, so the fluxes from illuminated and shadowed surfaces differ by orders of magnitude (from 10^{10} to 10^{21} $m^{-2} \cdot s^{-1}$). CO and CO_2 emission fluxes are set independently of the surface temperature as a sum of two components:

the one evenly distributed over the entire surface,

the one depending on the illumination of the surface.

The values of the emission fluxes on illuminated and shadowed surfaces are comparable for these components:

$$5.0 \cdot 10^{16}–1.0 \cdot 10^{18}\ \mathrm{m}^{-2} \cdot \mathrm{s}^{-1} \text{ for CO},$$

$$7.5 \cdot 10^{15}–1.5 \cdot 10^{17}\ \mathrm{m}^{-2} \cdot \mathrm{s}^{-1} \text{ for } CO_2.$$

Fig. 3 shows the density and velocity distributions (with streamlines) in the *XZ* plane, obtained from solving the Euler and Navier–Stokes equations, as well as the DSMC method (for regions up to $3R_n$ and up to $15R_n$).

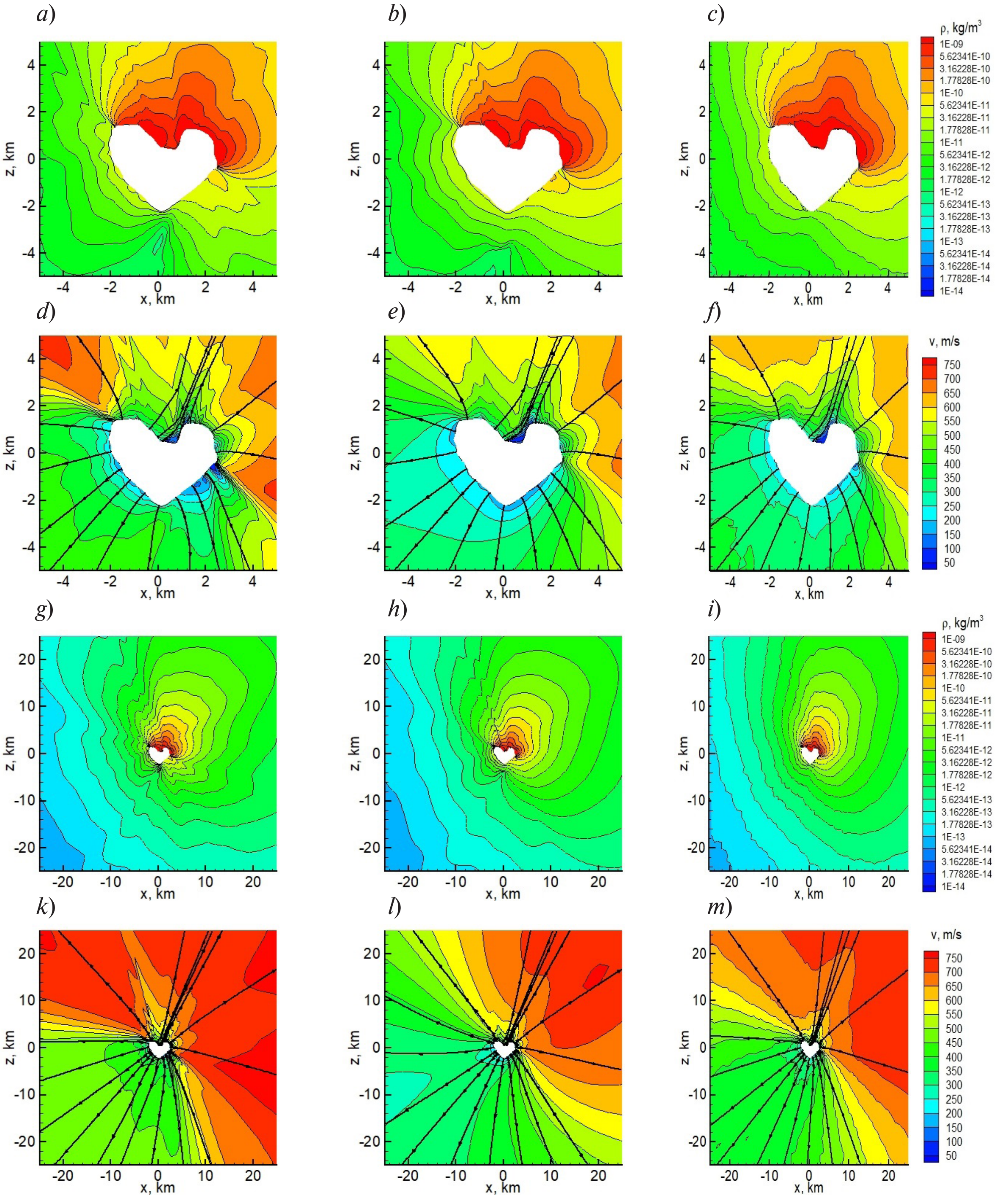

Fig. 3. Isolines of density (kg·m⁻³) (*a–c, g–j*) and velocity (m·s⁻¹) (*d–f, k–m*) of the gas mixture (H_2O, CO, CO_2) flow in the *XZ*-plane, in the vicinity of the comet's nucleus (regions up to $3R_n$ (*a–f*) and up to $15R_n$ (*g–m*)), computed using Euler equations (*a*, *d*, *g*, *k*), Navier–Stokes equations (*b*, *e*, *h*, *l*) and DSMC method (*c*, *f*, *j*, *m*)

A good qualitative agreement between the solutions obtained by different methods (see Fig. 3, *a–f*) is observed in the vicinity of the comet's nucleus (a region smaller than $5R_n$). The solutions obtained by continuum methods assuming flow equilibrium yield more intense expansion and acceleration of the flow. Furthermore, pronounced shock wave structures are obtained in simulation by continuum methods. These structures are either absent in the kinetic simulations, or are strongly diffused due to the insufficient collision frequency of the molecules.

The discrepancies in the solutions become more pronounced with distance away from the nucleus. The qualitative agreement between the Euler solution and the solution obtained by the DSMC method is preserved at large distances away from the nucleus (see Fig. 3, *g–m*). According to the solution of the Navier–Stokes equations, artificial flow deceleration begins at a distance of about $5R_n$. The reason for this is that strong rarefaction of the flow leads to predominance of dissipative processes over convective ones.

Macroscopic flow parameters (density, velocity, etc.) are the averaged values of the corresponding molecular quantities (the average number of molecules per unit volume, their average velocity, etc.) in the flow. Therefore, they can be determined only as long as there is a sufficient number of molecules in the smallest representative volume of the flow. The equations for conservation of mass, momentum and energy in the flow can be derived from continuum and/or kinetic models, but these equations are not closed until the tangential (shear) stresses and heat fluxes are expressed in terms of lower-order macroscopic quantities. This condition imposes a constraint on using continuum equations. The terms of the equations responsible for transport in the Navier–Stokes equations do not reflect the process under consideration if the gradients of macroscopic variables become so large that their characteristic length is commensurate with the mean free path of molecules between their collisions.

The considered heliocentric distance and the corresponding gas production of the comet's nucleus generate a very rarefied flow in the immediate vicinity of the nucleus. Fig. 4,*a* illustrates the distribution of the Knudsen number Kn in the flow field:

$$\mathrm{Kn} = \lambda / L, \tag{6}$$

where λ is the mean free path of the molecules; L is the characteristic length of the flow, determined by the density gradient, $L = \rho/(d\rho/dr)$.

An area with $\mathrm{Kn} < 1$ is found on the day side, up to a distance of about $5R_n$; $\mathrm{Kn} > 1$ on the entire night side of the flow. It is generally assumed that the applicability of gas-dynamic methods based on the Navier–Stokes and Euler equations is limited by the values of the Knudsen number: $\mathrm{Kn} < 1$ [9, 6]. However, it was found in [10, 13, 14] that gas-dynamic methods can give qualitatively correct distributions of density and flow velocity even at $\mathrm{Kn} > 1$.

The equilibrium between the translational and rotational degrees of freedom of the molecules (characterized by the temperature ratio $T_{tr}/T_{rot} > 0.9$) is preserved only on the day side, in a region extending for a few nuclear radii (Fig. 4,*b*), even with the fastest possible translational-rotational energy transfer adopted in the computations ($\Lambda = 1$). Insufficient collision frequency leads to

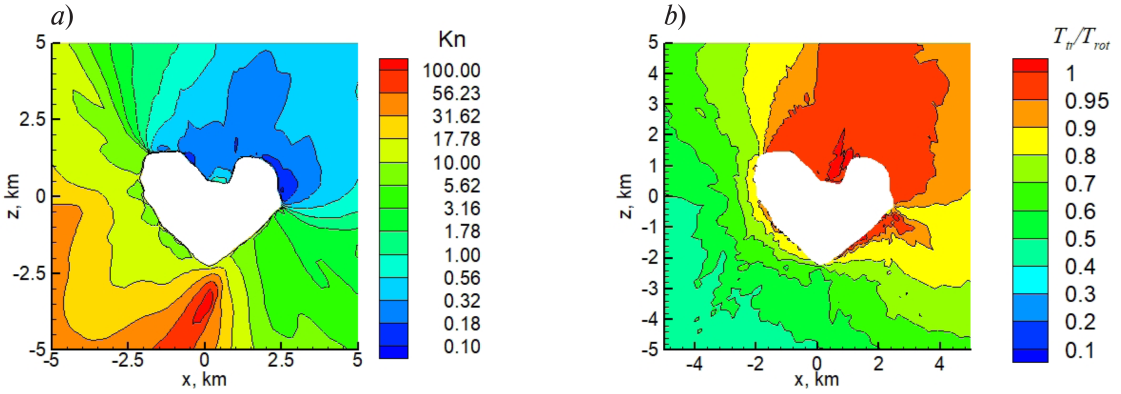

Fig. 4. Isolines of Knudsen number (Kn) (*a*) and the ratio of translational to rotational temperature (T_{tr}/T_{rot}) (*b*) in the *XZ* plane

freezing of internal energy of molecules, reducing the fraction of the gas thermal energy converted into translational motion and, consequently, reducing the flow acceleration rate.

Fig. 5 shows the distribution of the relative concentration of H_2O, CO, CO_2 molecules in the flow (solution by the DSMC method). Due to the significant difference in H_2O, CO and CO_2 emission fluxes from the illuminated surface (see Fig. 2), H_2O dominates in the flow of the gas mixture. Conversely, CO dominates on the night side. The presence of CO and CO_2 emissions on the night side and in the shadowed regions limits the expansion of H_2O from the day side to the night side and prevents the formation of condensation flow onto the unilluminated surface. The relative concentration of CO_2 has a maximum on the night side, but even there it does not exceed 15%. The relative concentrations of H_2O and CO on the day side near the shadowed regions of the surface are comparable (amounting to about 50%). Water (the component with the highest total gas production) gradually starts to dominate in the entire region with distance from the comet's nucleus.

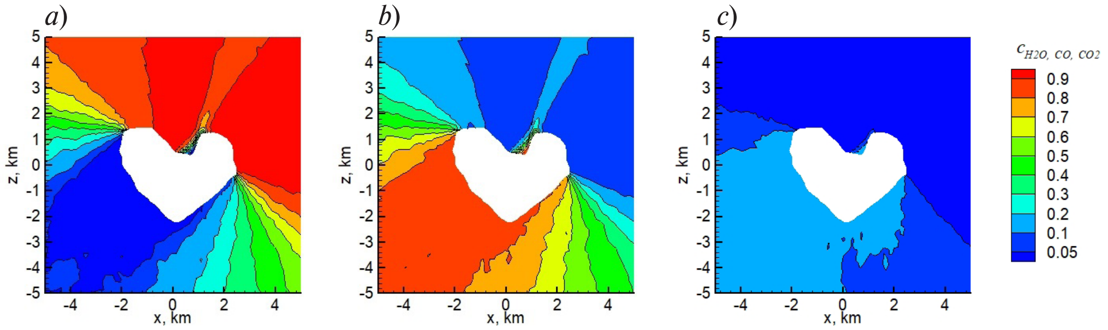

Fig. 5. Isolines of relative concentrations of H_2O (*a*), CO (*b*) and CO_2 (*c*) molecules in the flow obtained by DSMC

Numerical simulations were run on a computing cluster equipped with 2.20 GHz Intel Xeon E5-2650 v4 processors. With Hyper-Threading disabled, the Euler equations required 3 hours of CPU time, the Navier–Stokes equations 5 hours, and the DSMC 48 hours.

Conclusion

Numerical simulation of the flow in the near-nucleus coma of comet 67P/Churyumov–Gerasimenko at the time of its rendezvous with the Rosetta probe was performed using gas-dynamic and kinetic methods. The following conclusions on the processes occurring within the coma can be made based on the simulation results.

Multicomponent emission from the surface of the nucleus with a complex shape produces multidimensional flow with a complex structure and regions of different molecular composition in the immediate vicinity of the comet's nucleus. However, at a distance of about $5R_n$, the flow structure already approaches that of the flow from a point source with variable angular intensity, namely, the gas expands radially with an almost constant (but direction-dependent) velocity.

The density and velocity distributions of the flow, obtained by solving the Euler equations, are qualitatively consistent with the DSMC results. Given the large uncertainty in the surface emission parameters (stemming from the absence of directly measurable data) and the computational expense required for inverting the data from indirect observations (e.g., coma spectrometry), solutions of the Euler equations remain the most efficient tool for interpreting observational data.

The considered heliocentric distance (3.2 AU) and the corresponding gas production of the nucleus result in strong rarefaction and non-equilibrium of the flow in the larger part of the computational domain. Translational-rotational non-equilibrium must be taken into account in the simulation of radiative transfer for modeling the rotational spectra in the submillimeter range. The reason for this is that the rotational temperature determines the energy level populations, while the translational temperature governs the collision frequency and the magnitude of the Doppler shift.

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