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Direct Statistical Simulation of the Near-Surface Layers of the Cometary Atmosphere. I. A Spherical Nucleus

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Abstract—The key to the explanation of the variety of processes associated with the activity of comets lies in a more profound understanding of the events that occur in the near-surface layer of the cometary nucleus and in the inner part of the cometary atmosphere, which is formed under the action of solar radiation. A complete description of the mass- and energy-transfer processes inside and outside the cometary nucleus, which can be presented as a body with a complex morphology and high porosity and which is composed of mineral, organic, and volatile components, is an extremely complicated problem of space physics. The nucleus and the inner part of the coma are closely related to each other as physical subsystems, and physical processes in these regions are in close symbiosis because of the permanent exchange of both energy and mass. The thermophysical model of the circumnuclear coma cannot be confined only to the consideration of the processes in the nucleus—the entire system should be simulated as a whole. A consistent model of the inner part of a cometary atmosphere of this kind has been developed in this paper within the framework of the gas-kinetic approach. Based on direct statistical simulation with weights, we simulated the two-dimensional gas flow from the cometary nucleus. The nucleus was assumed to be spherical. We considered different models of the nucleus morphology that determined the effective gas production: the homogeneous nucleus, the "spotty" nucleus with its active area in the vicinity of the subsolar point, and the "spotty" nucleus with its active area in the form of a spherical segment. For the first time, the boundary conditions at the inner boundary of the simulation domain required for the kinetic modeling of the inner coma were found from a self-consistent model of the heat and mass transfer in a porous cometary nucleus. The model was earlier developed by the authors. The basic new features of the model included taking into account the volumetric character of the radiation absorption in a porous medium, the kinetic simulation of the transport of sublimation products in the pores, and the consideration of the backward fluxes from the coma due to the intermolecular collisions. The kinetic simulation was performed using the SMILE program package. The parallel computer implementation of the model made it possible to calculate the spatial fields of the basic macrocharacteristics of the gas flow. It was demonstrated that the structure of the inner coma is essentially dependent on variations in the effective gas production. In all the cases considered, the main part of the coma is far from thermodynamic equilibrium. This means that the entire structure of the inner cometary atmosphere can be accurately studied only within the framework of the kinetic approach. In a general case, it can result from the interaction of gas flows generated by different active subregions on the nucleus surface. Thus, fine structures are formed and local efficient gas recondensation from the coma occurs in the model for some regimes with "spotty" activity (where considerable variations in gas production take place on small spatial scales).

INTRODUCTION

As our knowledge of comets increases, and, especially, as cosmic expeditions are planned in the near future (such as, for example, Rosetta and Deep Impact IV), more interest is appearing in the theoretical simulation of energy- and mass-transfer processes in the cometary nucleus and in the near-surface layer of the cometary atmosphere—in the inner coma. Earlier laboratory (Grün *et al.*, 1993; Benkhoff *et al.*, 1995; Kossacki *et al.*, 1997) and theoretical (Skorov *et al.*, 2002; Davidsson and Skorov, 2004) studies demonstrated that these regions are closely related to each other and that the processes in the nucleus cannot be understood if the inner cometary atmosphere is not taken into account; vice versa, any meaningful simulation of the coma is impossible without a physical model of the cometary nucleus. In actuality initial and boundary conditions, primarily the effective gas production, are necessary for numerical simulations of the cometary atmosphere (both in the macroscopic gas-dynamic approximation and using the gas-kinetic approach). These can be quantitatively defined only within the framework of a model of heat and mass transfer in the cometary nucleus. In a series of papers (Skorov *et al.*, 1999, 2001; Davidsson and Skorov, 2002a, 2002b), we presented a thermophysical model of a cometary nucleus, which takes into account a number of previously neglected effects. We were the first to demonstrate that the processes of both radiation and mass transfer are volumetric in character. If we take this into account, we should revise the earlier developed models of the cometary

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atmosphere and the theoretical results obtained with these models. The effect of the near-surface layer on the cometary nucleus is not so obvious, and until recently, it was either neglected or taken into account in some very idealized and simplified form in publications devoted to the physics of the cometary nucleus. This situation is to a great extent associated with the considerable computational difficulties that arise when the inner coma is modeled. The first, and so far the only study, in which an attempt at the quantitative analysis of this influence was made and its role was demonstrated, is the study of Davidsson and Skorov (2004).

According to the current theories, the cometary atmosphere is formed during the evaporation (sublimation) of volatile components of the cometary nucleus. The main volatile component of the known comets is water ice. Approaching the Sun, it evaporates due to the solar heating of the nucleus, and this leads to the formation of the developed gaseous coma at negligible heliocentric distances. Even in the most simplified case, in which evaporation is assumed to occur from a perfect smooth plane surface, the distribution function of the evaporated molecules is significantly different from the local-equilibrium Maxwell distribution function (Bird, 1994; Huebner and Markiewicz, 2000). Because of intermolecular collisions, the so-called gas maxwellization, that is, the transfer to the local kinetic equilibrium, takes place. It seems very important to model this process. First, the macroscopic characteristics of a gas (density, momentum, temperature) change by several times during its maxwellization in the near-surface kinetic-non-equilibrium layer (the Knudsen layer). These variations must be taken into account in the development of a macroscopic model of the cometary atmosphere, which, strictly speaking, can be applied only to the domain of the kinetic-equilibrium gas flow. The macroparameters obtained at the outer boundary of the nonequilibrium layer are the inner boundary conditions for the gas-dynamic model. Second, only such a kinetic model can provide the values of the backward fluxes of density, momentum, and energy. These values can be used in the model of heat and mass transfer in the cometary nucleus, as well as in the boundary conditions for the energy balance equation at the surface of the nucleus.

In the case of evaporation from a perfect plane solid surface, the only characteristic determining the solution for the kinetic-non-equilibrium domain is the surface temperature, which can be estimated from the total energy balance at the surface of the nucleus. In a more realistic approximation, it should be taken into account that, according to the analysis of the observation data (Keller, 1990; Marov, 1994; Rickman, 1994), cometary nuclei seem to have noticeable porosity. It can be assumed that pores, cracks, and fractures of quite different sizes are typical of cometary nuclei (Britt *et al.*, 2004). In this case, the simulation of the Knudsen layer becomes even more complicated because information about the effective rate of evaporation from a porous nonisothermal ice layer and about the shape of the distribution function of the evaporated molecules can be obtained only from modeling all the basic transfer processes in the cometary nucleus. Thus, these problems are closely connected, and the solution of each of them becomes even more difficult because the related problems should be considered as well.

The question of whether there is any kinetic-equilibrium coma region that can be modeled using the macroscopic gas-dynamic approach and, if so, then where are its boundaries, cannot be answered without using a kinetic model. Simple quantitative estimates of the gas production of the cometary nucleus and of the molecule free-path length show that one can expect that, even at negligible heliocentric distances (of about 1 AU), there are regions where the gas flow is different from the kinetic-equilibrium flow (Skorov and Rickman, 1999). Large variations of the local gas production, which are associated with both a complex relief of the surface of the cometary nucleus and with a diversity in its chemical composition and structure, can result in deviations of the gas flow from the equilibrium regime. As the Sun becomes farther away, and, accordingly, as the rate of sublimation rapidly falls, the flow becomes more nonequilibrium. Note that, in the Rosetta space project, the probe is to meet a comet at a distance of approximately 3 AU, where the coma is highly rarified. Thus, it becomes an urgent practical task to model with kinetic methods not only the near-surface layer but the entire inner region of the cometary atmosphere.

Very few studies have so far been devoted to the numerical simulation of the Knudsen layer and the kinetic-non-equilibrium inner region of the cometary atmosphere. In this paper, we give a brief review of the models published and the results obtained. We consider the thermophysical model of energy and mass transfer in the near-surface layer of a porous cometary nucleus. The model is used to determine the consistent boundary conditions at the sublimating surface in the kinetic model. We also describe a kinetic model of the inner cometary atmosphere. Within the framework of this numerical model, we calculate the spatial fields of the basic gas-dynamic characteristics, such as density, Mach number, temperature, and velocity. Different structures of the nucleus surface are examined. In conclusion, we discuss and summarize our results and suggest directions for further studies.

KINETIC MODELS OF THE INNER COMA

Crifo was the first to consider (in 1987) the problem of the variation of gas flow parameters within the Knudsen layer as applied to the simulation of cometary atmospheres. It was mentioned (Crifo, 1987) that the boundary conditions for the gas flow can be correctly defined only within the framework of the molecular kinetic theory. Such quantitative estimates, linking the macrocharacteristics of a monoatomic gas at the inner (the phase

boundary) and outer (the distance at which the locally equilibrium molecular velocity distribution is achieved) boundaries of the Knudsen layer were analytically obtained by Anisimov (1968). The method was based on the balance approach and on an assumption of the conservation of the summatory invariants of motion. The nonequilibrium layer was considered to be a flow discontinuity, and the resulting molecule distribution function near the evaporating surface was assumed to be a weighted sum of the semi-Maxwellian distribution function of the evaporated molecules and the local-equilibrium Maxwellian function specified at the outer boundary of the layer. These assumptions are certainly a very strong simplification and are not theoretically based. This technique was extended for a polyatomic gas by Cercignani (1981). Crifo (1987) applied the results of Cercignani to calculate the macroparameters of a gas flow composed of water molecules at the outer boundary of the Knudsen layer of the cometary atmosphere. The analytical expressions obtained by Crifo can be considered only as very approximate. In addition, they contain a free model parameter, the local Mach number at the outer boundary of the layer, whose value cannot be defined within the framework of the approach applied.

Note that only algebraic relations linking the temperature and the pressure at the boundaries of the nonequilibrium layer were obtained in the papers mentioned above. The spatial structure of the layer and the type of variations in the gas-flow characteristics were not considered. This more general problem was solved by a number of researchers using the method of direct statistical simulation (DSMC) suggested by Bird (1994). This method involves a computer simulation of the behavior of a system of a large number of model particles (hundreds of thousands and even millions). However, this number is much smaller than the number of real molecules; therefore, each model particle characterizes the behavior of a considerable number of molecules. The computational domain is divided into cells, whose sizes are small as compared to the typical scales of variations of the flow parameters. These cells are used to select pairs of particles whose collisions are then modeled, and to define the macroparameters (for example, density, temperature, flux of momentum, etc.) of a flow. The basic idea of the method is that the continuos motion and collisions of particles at a time step are replaced by free molecular transfer and collisional relaxation. The time step should be small compared to both the time between the particle collisions and the average time taken by a particle to pass through the space cell. To calculate the probability of collisions and the post-collisional velocities, a model of intermolecular collisions must be specified.

The first study that we know of that presented a computational model of a kinetic-non-equilibrium region of a cometary atmosphere is the study published by Bisikalo *et al.* in 1989. That paper presented a one-dimensional plane-parallel model of the Knudsen layer. The calculations were performed for the stationary flow of a monoatomic gas in the approximation of the solid sphere model. The scheme of intermolecular collisions given in (Shematovich *et al.*, 1982) was applied. The molecular collisional relaxation leading to the maxwellization of the velocity distribution function of the sublimated gas molecules was clearly shown. Both the spatial profiles of the basic characteristics of the gas flow and the relations connecting the macroparameters at the inner and outer boundaries of the study region were obtained. The latter confirmed that variations in density, velocity, and temperature are large within this layer, and that they should be taken into account in standard gas-dynamic models of a cometary atmosphere.

The next step was made in the study of Skorov and Rickman (1998), in which the nonstationary evaporation of one- and two-component gases was considered. Simulations were made with the scheme of intermolecular collisions from Korolev and Yanitskii (1985), which was different from that applied by Bisikalo *et al.* (1989). The results obtained for the nonstationary evaporation of a one-component gas were in fine agreement with Bisikalo *et al.* (1989). In their next study, Skorov and Rickman (1999) considered the case in which the evaporating surface was not perfectly smooth. As an example, they simulated a gas flow from under the porous dust crust that covers the ice surface. The presence of such a dust mantle results in a change of the effective temperature of the escaping molecules and to a difference of their distribution function from the semi-Maxwellian one.

Davidsson and Skorov (2004) were the first to develop a consistent approach to the definition of the boundary conditions at the surface of a nucleus. The authors considered an ordinary one-dimensional plane-parallel model of the Knudsen layer. The water-ice evaporation was simulated using the same computational technique as that applied by Crifo *et al.* (2002). However, while the latter paid more attention to the comparison of the results of kinetic simulation (DSMC) with the results obtained from the solution of the Navier–Stokes equations, Davidsson and Skorov primarily considered the relation between the processes of heat and mass transfer in a porous cometary nucleus and the processes of gas transfer in the Knudsen layer. They performed a series of calculations of the temperature distribution inside the nucleus and the corresponding efficient gas production. Both the volume absorption of the solar radiation and evaporation from the entire near-surface porous nonisothermal ice layer were taken into account. Such computations were made for a large set of model values. The complete information about the velocity distribution function of the outcoming molecules was used as a boundary condition for the kinetic model of the Knudsen layer. As a result of the series of model computations for a wide set of parameters, a practical tool was obtained that allows the backward fluxes of density, momentum, and energy at the surface of the nucleus to be found with sufficient

accuracy without laborious computations. The tables, their descriptions, and auxiliary materials can be found in the file knudsen.tar using the ftp address ftp://astro.estec.esa.nl/pub/bdavidss/Knudsen (login anonymous). (Some aspects of this model will be presented below.)

The aforementioned studies were devoted to the simulation of the near-surface layer, whose thickness is not more than several tens of the molecule free-path length. At the same time, the computer simulation of the entire circumnucleus region of a cometary atmosphere, which, as mentioned above, can be either totally or partially in a kinetic-non-equilibrium state, arises great interest.

Since the early 1990s, the DSMC method has been actively applied for simulations of two- and three-dimensional flows of a rarified gas, for example, near spacecraft (see Ivanov and Gimelshein, 1998). Great interest in DSMC is provoked by the following features of the method: the relative ease of passing from one- to two- and three-dimensional problems, and the possibility of using different models of the interaction of gas particles to take into account the internal degrees of freedom of molecules and chemical reactions without making the algorithm overly complicated. However, in spite of the rich possibilities provided by the DSMC method, it has so far been seldom used for simulations of the rarified atmospheres of small bodies. Combi (1996) was one of the first to apply the DSMC method for the simulation of one- and two-dimensional flows in a cometary atmosphere. In his study (Combi, 1996), he gave a detailed description of the gas-kinetic model that allowed one to calculate nonstationary two-dimensional flows in an inner coma. In one of the variants presented in this study, he modeled the stationary gas jet with its axis of symmetry passing through the subsolar point. He considered evaporation of water ice from the surface of a homogeneous compact spherical nucleus. The applied spatial grid was regular, nonuniform in radius, and uniform in angle: 50 zones in radius and 20 zones in angle; that is, the total number of spatial cells was 1000. It was demonstrated that a substantial mass transfer from the day hemisphere to the night hemisphere occurs in the inner coma, and the gas flow is kinetic-non-equilibrium on the night side even in the direct vicinity of the surface of the nucleus. Since the conditions at the phase boundary (at the surface of the nucleus) were specified in quite an arbitrary way (for example, it was assumed that the gas density at the surface varies proportionally to the squared cosine of the zenith angle and that the temperature is constant and equal to 180 K), the results can be considered only qualitatively and have a methodic character. Because of the specific nature of the realization of the computational model, a satisfactory statistical accuracy of the computations could be achieved only in the coma region over the day hemisphere of the nucleus. Presumably, the model cannot be considered a high-resolution one because too few spatial cells were used. This approximation cannot be used to study a detailed structure of the inner coma. However, the author did not have such a task in mind. A considerable part of this interesting study deals with the simulation of a spherically symmetric coma at distances that are several orders of magnitude larger than the nucleus radius, thus landing out of the scope of the problem considered here.

We should mention the recent paper of Crifo *et al.* (2002), which presents calculations of the inner region of a cometary atmosphere that were performed based both on the solution of the Navier–Stokes equations and on the DSMC method. In this paper, the authors also consider water-ice evaporation from the surface of a homogeneous compact spherical nucleus. The boundary values of temperature and gas flux were defined from the energy balance at the illuminated side of the nucleus. The gas production was assumed to be constant at the night side, and a small free model parameter was introduced to specify it. The heat transfer due to heat conduction was neglected in the energy balance equation. The VHS model was used to describe molecular collisions, and the internal degrees of freedom of water molecules (rotational and vibrational) were taken into account by the Larsen–Borgnakke model (see the section "Model of an inner cometary atmosphere"). The authors applied a regular spatial grid that was nonuniform both in radius and angle: the cell sizes increased in a geometric progression as the distance from the nucleus surface and the axis of symmetry increased. The axis of symmetry defined the direction to the Sun. To model the intermolecular collisions, each cell was divided into 20–25 subcells, each with a size that was less than the free-path length. In the variants presented, the total number of such cells was as large as 500000. The total number of model particles ranged from 10^6 to 10^7. The spatial fields for density, temperature, and the local Knudsen number were obtained for several model parameters. Unfortunately, in Crifo *et al.* (2002) nothing is said about the computation accuracy, and the method used to present the DSMC results and to compare them with the solution of the Navier–Stokes equations makes one doubt the accuracy of these DSMC results and the corresponding quantitative comparisons.

The main purpose of the present study is to perform a two-dimensional calculation for the entire circumnucleus region of a cometary nucleus rather than for the near-surface Knudsen layer, as the authors did in their earlier one-dimensional models. A principal difference is that the boundary conditions that are necessary for the kinetic model are specified using the approaches developed in (Davidsson and Skorov, 2004); that is, the effective local gas production is defined in a thermodynamically consistent way. Before we give a detailed description of this model, let us first consider the thermophysical model of a cometary nucleus that is applied in our calculations.

THE MODEL OF HEAT AND MASS TRANSFER IN A NUCLEUS

The thermophysical model describes the processes of energy and mass transfer in the near-surface layer of a porous-ice cometary nucleus and consists of the main block, where the heat conduction equation is solved, and of three auxiliary blocks, where the following are modeled: (1) the absorption of the solar radiation in a layer; (2) the transport of products of sublimation in the near-surface layer resulting from nucleus heating; and (3) the backward gas flow caused by intermolecular collisions in the inner coma.

In the one-dimensional case (the variables depend only on the distance from the surface to the nucleus depth), the equations of heat conduction in a porous water-ice layer have the form

$$((1-\psi)(\rho_i f_i c_i(T) + \rho_d f_d c_d(T)) + \psi\rho_g c_g)\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(T)\frac{\partial T(x,t)}{\partial x}\right) - c_g\phi_g(p,T)\frac{\partial T(x,t)}{\partial x} - E_{IR}(x,t) - q(p,T)L(T). \quad (1)$$

Here, ψ is the bulk porosity of a medium; ρ_i and ρ_d are the densities of the solid ice and dust, respectively; ρ_g is the gas density; f_i and f_d are the volume fractions of ice and dust in the solid phase; $\phi_g(p, T)$ is the mass flux through the unit area; $q(p, T)$ is the mass of the gas produced in a unit volume per unit time due to sublimation and condensation; $\kappa(T)$ is the effective heat conductivity of the solid phase; $c_i(T)$, $c_d(T)$, and c_g are the heat capacities of the ice, dust, and gas phases, respectively; $L(T)$ is the heat of sublimation; and $E_{IR}(x, t)$ is the additional source of energy due to the volume absorption of radiation. The values of the parameters applied here are the same as in the papers by Davidsson and Skorov (2002b) and Skorov *et al.* (2002). Note that the porous character of the medium is taken into account phenomenologically by introducing into the heat-conductivity formula the so-called Hertz factor h, which characterizes the contact area between particles in a porous medium and takes values from 1 to 0.001 in different calculations (Kossacki *et al.*, 1999):

$$k(T) = h\frac{k_i(T)f_i + k_d(T)f_d}{f_i + f_d}. \quad (2)$$

The volume source of energy is given in the form

$$E_{IR} = K\frac{S_\odot(1-A_{dh})I(t)}{r_h^2}\frac{\partial F(x,t)}{\partial x}, \quad (3)$$

where K is the model parameter, equal either to 0 (the surface energy absorption model, SEAM) or 1 (the layer energy absorption model, LEAM); $S_\odot$ is the solar constant; A_{dh} is the wavelength-averaged albedo; r_h is the heliocentric distance; $I(t)$ is a function of illuminance, which defines the cosine of the angle between the local normal and the direction to the Sun and describes the proper rotation of the cometary nucleus; $F(x, t)$ is the effective flux of energy normalized by the flux at the nucleus surface.

The form of the function F for some model parameters was first derived by Davidsson and Skorov (2002a). They assumed that the nucleus consists of a porous mixture of water ice and silicate and organic dust. The simulation was performed in six stages: (1) materials and composition were chosen for an individual particle, and its refractive indices were calculated; (2) the particle morphology was specified; (3) the optical characteristics (absorption, scattering, and the phase function) were calculated for the isolated particle; (4) the transition was made from the single-particle properties to the volume properties of the porous medium composed of these particles; (5) the radiative transfer equation was solved for the modeled medium; (6) the wave-dependent geometric albedo was calculated for the nucleus along with the profile of the radiation absorption in the layer. The calculations were performed with an application of the Mie theory, the discrete–dipole approximation (Draine, 1988), the theory of Hapke (1993), and the numerical solution of the radiation-transfer equation (Kisselev *et al.*, 1985).

Six different types of forming particles were considered in the simulations, including closely packed clusters of spherical two- and three-layer particles and large (100 μm–1 cm) porous irregular-shaped ice particles. In the last case, it was assumed that the spherical mineral particles covered with an organic mantle compose 23% of the total volume of the particle as internal inclusions. It was demonstrated that radiation can penetrate quite deeply into a porous medium formed by irregular relatively large particles composed of dust and ice and that the widely used assumption of the surface absorption of energy is not true. For a medium of this kind, the radiation absorption obeys the exponential law

$$F(x,t) = e^{-x/(\zeta\cos\gamma)}, \quad (4)$$

where $\gamma(t)$ is the local zenith angle and ζ is the exponential coefficient determined in terms of the computational model of the volume absorption of radiation.

To calculate the temperature distribution within the nucleus and to calculate the mass transfer and the effective gas production, it is necessary to solve the above differential equation with the corresponding boundary conditions. The boundary conditions at a given depth can be specified in different ways: if the simulation domain is quite large compared to the depth of the thermal front propagation, the isothermal condition can be applied; for the rotating nucleus, when the diurnal variations of temperature are examined, it is nature to require that both the spatial and the time derivatives of temperature are equal to zero. The boundary condition at the surface of the nucleus is given by the energy bal-

ance: the flux of the incoming energy is connected with the incoming solar radiance and may be connected with the heat flux due to heat conduction (if the temperature gradient is positive) and to recondensation of molecules from the coma; the loss of energy is due to the heat emission from the surface, to gas sublimation directly from the surface, and, possibly, to the loss of energy due to heat conduction. The corresponding equation can be written down in the form

$$(1-K)\frac{S_\odot(1-A_{\rm dh})I(t)}{r_{\rm h}^2} = \varepsilon\sigma T_{\rm s}^4 + (1-\psi)f_{\rm i}Z(T_{\rm s})L(T_{\rm s}) - \kappa(T_{\rm s})\left.\frac{\partial T}{\partial x}\right|_{x_{\rm s}}, \quad (5)$$

where σ is the Stefan–Boltzmann constant; ε is the coefficient of heat emission; and $Z(T_{\rm s})$ is the rate of sublimation for pure and compact ice, which is given by the Hertz–Knudsen formula

$$Z(T_{\rm s}) = p_{\rm sat}(T)\sqrt{\frac{m_{\rm H_2O}}{2\pi kT_{\rm s}}}, \quad (6)$$

where $m_{\rm H_2O}$ is the mass of a water molecule, k is the Boltzmann constant, $T_{\rm s}$ is the ice temperature, and $p_{\rm sat}(T) = 3.56\times10^{12}{\rm e}^{-6141.667/T}$ is the corresponding pressure of the saturated water vapor. The additional coefficients introduced in Eq. (5) into the relation for the rate of sublimation are due to the fact that we consider porous dusty ice.

The classic Hertz–Knudsen formula given above is often used in studies in which the heat and mass transfer in cometary nuclei are simulated. At the same time, the results of different experiments referred to in Kossacki *et al.* (1997), in which the evaporation of ice was examined, show that the mass flux calculated by this simple formula at conditions close to the cometary-like ones may exceed the experimental values by nearly an order of magnitude. The analysis of the experiments in which the growth of ice crystals was investigated (see Kossacki *et al.*, 1999) leads to the conclusion that only a part of the molecules that have collided with the ice surface are absorbed by the crystal; the rate of both the direct and the reverse processes is a function of the ice temperature. These effects can be taken into account in the first approximation by introducing phenomenological coefficients into the relations for the rates of sublimation (index "s") and condensation (index "c"). The following empirical interpolation formulas, which allow one to interpret the experimental results satisfactorily, were obtained for these coefficients:

$$\alpha_{\rm s} = \left(1-\frac{1}{a_1}\right) + \frac{1}{a_1}\tanh\left[-a_3\tan\left(\pi\frac{T-a_2}{273-a_2} - \pi/2\right)\right], \quad (7)$$

$$a_1 = 2.342, \quad a_2 = 150.5, \quad a_3 = 4.353, \quad (8)$$

$$\alpha_{\rm c} = 1.387 - 4.464\times10^{-3}T. \quad (9)$$

Of course, the presence of impurities and microscopic defects in a crystalline lattice should be taken into account in a more general case. However, these problems are far outside the scope of this paper.

In addition to the temperature dependence of the sublimation and condensation coefficients, the backward flow of molecules condensed on the nucleus surface from the inner coma should be taken into account. If the ratio of the direct flux to the backward flux is characterized by the parameter $a_{\rm c}$, the expression for the term in Eq. (5) describing the loss of energy due to evaporation will finally take the form

$$Q_{\rm eff} = (1-\psi)f_{\rm i}(1-a_{\rm c})\alpha_{\rm s}(T_{\rm s}) \times p_{\rm sat}(T_{\rm s})L(T_{\rm s})\sqrt{\frac{m_{\rm H_2O}}{2\pi kT_{\rm s}}}. \quad (10)$$

In the simplest case, in which evaporation from the perfect compact ice surface is considered, to the first approximation we can use the algebraic relations obtained in Crifo (1987) and Skorov and Rickman (1999) to determine the backward flow of molecules. However, these simple formulas cannot be applied in the model of evaporation of the nonisothermal porous ice layer, as they introduce rather large errors into the calculation results. In this case, we used the results obtained by Davidsson and Skorov (2004). The authors presented a tool that allows one to take into account the presence of a coma in simulations of the energy transfer in the nucleus accurately and nearly without any additional computational cost. The tool consists of two-dimensional interpolation tables that relate the temperature at the nucleus surface and the temperature gradient in the near-surface layer to the relative values of the backward fluxes of mass, momentum, and energy. The tables were obtained as a result of the solution of an adjoint problem of heat and mass transfer in a nucleus and in an inner coma.

Now let us pass on to the last auxiliary block, which describes the transport of the products of evaporation in porous ice. The heat-conduction equation includes the gas flow through a horizontal control surface $\phi_{\rm g}(p, T)$ and the volume source (or sink) of mass $q(p, T)$ due to the sublimation and condensation processes in an elementary layer. We shall note two main approaches used in the physics of comets to calculate these characteristics: the macroscopic approach, in which the transport of water vapor is modeled in the approximation of the dynamics of a continuous medium, and the kinetic approach to the description of this transport process. In the first case, which until recently has been the only one, the heat-conduction equation is supplemented by the continuity equation for a gas, and the necessary boundary condition for the gas density or pressure are added to the boundary conditions for temperature. In our studies (Skorov and Rickman, 1995; Skorov *et al.*, 1999, 2001) we thoroughly analyzed the shortcomings of this approach and demonstrated the considerable dif-

ferences between the solutions obtained with the use of macro- and microscopic approaches. We shall not concentrate on this once more, but shall directly pass to describing possible kinetic methods.

At the temperatures typical of cometary nuclei, one can expect that a Knudsen flow regime occurs in a gas in the near-surface porous layer of a cometary nucleus; that is, intermolecular collisions in pores can be neglected. The methods used to calculate the gas flow and the local mass production are determined by the method applied to describe the porous medium. We used the two types of models in our studies: the capillary model and the disperse model. In the first case, the porous medium is described as a system of cylindrical (straight or broken) unconnected channels of a length Δx and a radius r_p. To specify the mass transfer, often the differential generalized Knudsen-like formula (Steiner, 1990; Kömle and Steiner, 1992)

$$\phi_g = -\frac{8\psi r_p}{3}\frac{\partial I_s}{\partial x}, \quad I_s = \frac{p_{sat}(T)}{\sqrt{2\pi m_{H_2O} kT}}, \tag{11}$$

or the Clausing formula (Skorov and Rickman, 1995)

$$\bar{\phi}_g(p,T) = -\frac{20\Delta x + 8\Delta x^2/r_p}{20 + 19\Delta x/r_p + 3(\Delta x/r_p)^2} \times \frac{\psi}{\xi^2}\sqrt{\frac{m_{H_2O}}{2\pi k}}\frac{\partial(p/\sqrt{T})}{\partial x} \tag{12}$$

are used. We have already considered in detail the problems arising due to the use of these formulas and shall not stop at them here.

The kinetic model describing the gas diffusion in an ice nonisothermal channel was first published in Skorov *et al.* (2001). Based on the Clausing probabilistic formalism, accurate formulas were found there for the calculation of gas flows. The method is based on a simple geometric idea that allowed us to calculate the probability of the passage of the trajectory of a test particle through the control surface. The entire sequence of calculation formulas is quite a long one; thus, we present only the final expressions for the mass flux on an element of the channel wall

$$I_h(X) = I_s(0)P_2(X) + \int_0^{L_c} I_s(\tilde{X})P_3(|\tilde{X} - X|)\mathrm{d}\tilde{X} \tag{13}$$

and for the vertical flow of particles

$$I_v(X) = \pi r_p^2 I_s(0)P_0(X) + 2\pi r_p \int_0^X I_s(\tilde{X})P_2(X - \tilde{X})\mathrm{d}\tilde{X}. \tag{14}$$

Here,

$$P_0(X) = \frac{1}{2r_p^2}(X^2 - X\sqrt{X^2 + 4r_p^2} + 2r_p^2), \quad P_1(X) = -\frac{\mathrm{d}}{\mathrm{d}X}P_0(X), \tag{15}$$

$$P_2(X) = \frac{X}{2r_p}\left(\frac{X}{r_p\sqrt{X/r_p + 4}} - 1\right), \quad P_3(\eta) = -\frac{\mathrm{d}}{\mathrm{d}X}P_2(X). \tag{16}$$

The advantage of the method is its low computational cost: its formulas can easily be incorporated into a general thermal model. The limitation of the method follows from the applied description of a random porous medium by cylindrical capillaries.

In the disperse model, a porous medium is characterized by the bulk porosity ψ; the size (or the size distribution function) of forming particles (for example, spherical); the ice and dust volume fractions f_i and f_d, respectively; and by the given temperature profile $T(x)$. At the first step, the method of random wandering is applied for the given morphology of the medium, and the distribution function F of the free-path lengths of molecules in a layer is precalculated. Then, the following algorithm is realized: (1) a test particle is generated at some depth x in the modeled layer that corresponds to the local sublimation rate; (2) its vector velocity is defined; (3) for the given function F, the position of the point of interaction of the test particle with the solid phase is determined; (4) the type of collision is determined: if the test particle has collided with the ice, condensation or scattering (diffuse or mirror) occurs depending on the coefficient of condensation, which varies with temperature; if the particle has collided with the dust fraction, scattering always takes place; (4) if the test particle has crossed the boundaries of the region or has condensed, it is no longer considered. The process is repeated until the statistical perturbations become small enough. A more detailed description of the model can be found in Davidsson and Skorov (2004). The model seems to be more general and natural in comparison with the capillary one. It can obviously be developed and made more complex, but the implementation of its algorithm needs much computation time because of the statistical approach applied. Thus, it cannot be widely used for computations now.

The thermophysical model presented above allows one to calculate the effective gas production (the number density and the form of the velocity distribution function of outflowing molecules), the gas temperature, and the condensation coefficient as functions of time and cometocentric coordinates. These data are used in the kinetic model of the near-surface area of the cometary atmosphere as the boundary conditions.

MODEL OF AN INNER COMETARY ATMOSPHERE

Now we pass on to the description of the kinetic models of an inner cometary atmosphere. As noted above, the processes of energy and mass transfer in the cometary nucleus should be modeled while taking into account the surrounding cometary atmosphere. Because of intermolecular collisions, the backward mass and energy flows are formed in its near-surface layer. They must be taken into consideration when one specifies the boundary condition that represents the energy balance at the nucleus surface. To calculate these flows, one can deal with a domain whose thickness is only 10–20 free-path lengths. This means that the spatial one-dimensional model of the near-surface layer can give the appropriate results. We shall now start considering this model.

The one-dimensional model of the near-surface Knudsen layer was implemented on the basis of the program code DSMC1.FOR, which was created by Bird (1994). We considered the domain with a height equal to 20 free-path lengths of molecules and a base of 1 m^2. The domain was partitioned into 200 cells, each of which was divided into ten subcells. The time step was chosen so that the average time necessary for a particle to cross a cell was approximately equal to four time steps. The boundary conditions at the lower boundary (that is, at the surface of the nucleus) were specified based on the results of modeling heat and mass transfer in the nucleus. The particles escaping through the outer boundary of the domain were excluded from our consideration; this corresponds to the noncollisional gas expansion into a vacuum. Such an idealized boundary condition has an undoubtedly large effect on macroparameters in the vicinity of the outer boundary but does not result in any considerable change in macrocharacteristics of the backward gas flow at the surface of the nucleus. We continued to calculate the backward flows until the total number of the model particles that had crossed the surface of the sublimating nucleus was10^6–10^8. To describe elastic collisions, we used the model of variable hard spheres (VHS) (Bird, 1994), and the Larsen–Borgnakke model was used to describe the internal degrees of freedom (Borgnakke and Larsen, 1975). The scattering cross section in the VHS model depended on the relative velocity of the colliding molecules, so that, at the macroscopic level, the viscosity of the gas of test particles depends on temperature in a manner analogous to the water-vapor viscosity. The empirical values of the parameters necessary for the model were taken from Weast (1974). The Larsen–Borgnakke model was used to describe the energy redistribution between translational and rotational degrees of freedom. This model is the simplest one and is most frequently used in DSMC models. It is assumed in this model that the energy spectrum of the internal degrees of freedom is continuous and can be described by the Bolzmann distribution. The postcollisional energies are calculated based on this distribution and the energy conservation law. Note that, at temperatures typical of cometary physics, the vibrational degrees of freedom are not excited. A more detailed description of the model and the calculation results are given in the paper by Davidsson and Skorov (2004).

The Knudsen layer calculations are auxiliary in this model; most attention is given to the calculation of the axisymmetric inner coma with a size equal to several radii of the nucleus. The latter were performed using the SMILE program (Ivanov *et al.*, 1998a). This code was developed at the Institute of Theoretical and Applied Mechanics SB RAS in Novosibirsk in order to calculate flows around spacecraft, thruster plumes, and the interaction between the plume and the spacecraft surface. With regard to the advantages of this program, we should first emphasize that the program is based on the following:

(1) the majorant frequency scheme (Ivanov and Rogasinsky, 1991) of the DSMC method, which is derived from the basic kinetic equation and which allows a correct simulation of the frequency of collisions while applying a smaller number of model particles in a cell as compared to the NTC scheme (Bird, 1994);

(2) the realistic models of particle collisions, in which energy exchange between the translational and internal energetic modes and chemical reactions are taken into account (for example, in the code a generalized Larsen–Borgnakke model is developed and implemented for a continuos description of the rotational mode of polyatomic molecules, as well as the model with the temperature-dependent rotational relaxation number);

(3) the effective numerical algorithms that are intended to reduce the computation time.

In the last point, we mean the parallelization of numerical algorithms, the two-level Cartesian grids used to choose the pairs of model particles that will collide and be used to determine macroparameters, the radial weights for the simulation of axisymmetric flows, and the partition of the computational domain into subdomains with different model time steps. The high accuracy of the results obtained by SMILE was multiply confirmed by comparing them with the available experimental data, for example, with the aerodynamic characteristics of the landing capsule of the *Soyuz* spacecraft (Ivanov *et al.*, 1998b) and with the measured density and temperature profiles in thruster plumes (Ivanov *et al.*, 1997).

In the present study, the application of SMILE made it possible to take into account the variable activity of the nucleus (the variable gas production) and the nonsphericity of the sublimating surface. Variations in the nucleus activity are mainly due to the following two factors: variations in the solar energy that falls on an elementary area of the surface, and the local morphology (structure) of the nucleus. The first value is related to the spatial orientation of the area and, for a spherical

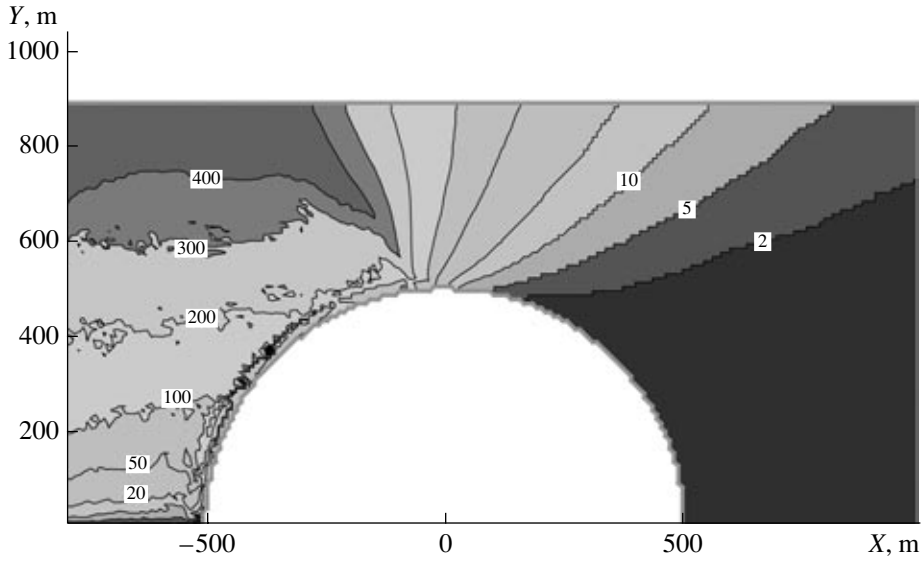

Fig. 1. The field of time steps of model particles divided by the minimal time step.

nucleus, is determined by the cometocentric latitude of the element. The influence of morphology on the gas production is associated, for example, with the material porosity or with the presence of a dust layer that attenuates the gas flow on the nucleus surface. The main difficulty arising in computer simulations is connected with the necessity of modeling the process of sublimation of the cometary nucleus, at the surface of which the gas density changes by several orders. Very large variations in density accordingly result in considerable variations in the molecule free-path length and the intercollisional time within the computation domain. For example, in our calculations the free-path lengths at the subsolar point and at the shadow side of the nucleus differed by four to five orders of magnitude. The traditional numerical algorithm with an invariable time step that is equal to the minimal time between the collisions is not efficient, since the particles in the shadow zone move a very small distance during this step in comparison to the local molecule free-path length. In addition, they practically do not collide for tens or hundreds of time steps.

The numerical algorithm "subdomains with different time times," realized in SMILE, allowed us to use an optimal time step for each collisional cell. The optimal step was determined during the calculations (Fig. 1 shows the field of the time steps divided by the minimal step). This approach is based on the relation $N_{\text{mod}}\Delta t =$ const, where N_{mod} is the number of molecules presented by a single model particle and Δt is the time step. Thus, when the time step is changed, the weight of the particle also varies, thus allowing us to avoid rejecting or "cloning" the particle in the case in which it crosses the boundary between subdomains with different model time steps. However, when the atmosphere around the nucleus is calculated, this leads to a decrease in the number of particles in the shadow zone as compared to that in the approach involving an invariable time step. If we try to ensure the presence of the required number of particles in a collisional cell in the shadow zone by simply increasing the total number of model particles, this results in an excess of particles in the vicinity of the axis of symmetry passing through the subsolar point. To avoid this problem, we modified SMILE so that each collisional cell was characterized not only by its own time step but also by the individual particle weight, which should ensure the required number of particles in the cell. The weight for each cell was found during the calculations (Fig. 2 shows the field of weights related to the minimal one). We used the buffer of delayed particles (Bird, 1994) in order to diminish the effect on the flow parameters of similar particles formed by the "cloning" of a particle that has moved from one cell to another. The "twin" particle is placed in this buffer at a random position, and the particle that was previously in this position is returned to the computation set. Therefore, similar particles were spaced in time by several time steps.

In our calculations with SMILE, we used the model of hard spheres (HS) to describe molecular collisions; the internal rotational energy degrees of water molecules were taken into account either within the framework of the Larsen–Borgnakke model (for the continuos description of the rotational mode) or in the model with the temperature-dependent rotational relaxation number. The molecule interaction with the surface of the cometary nucleus was modeled by the diffuse reflection of particles with parameters corresponding to the local temperature of the nucleus surface. Anywhere from 2 to 52 million model particles were used in different computation versions so that the size of the collisional cells was less than or equal to the local mole-

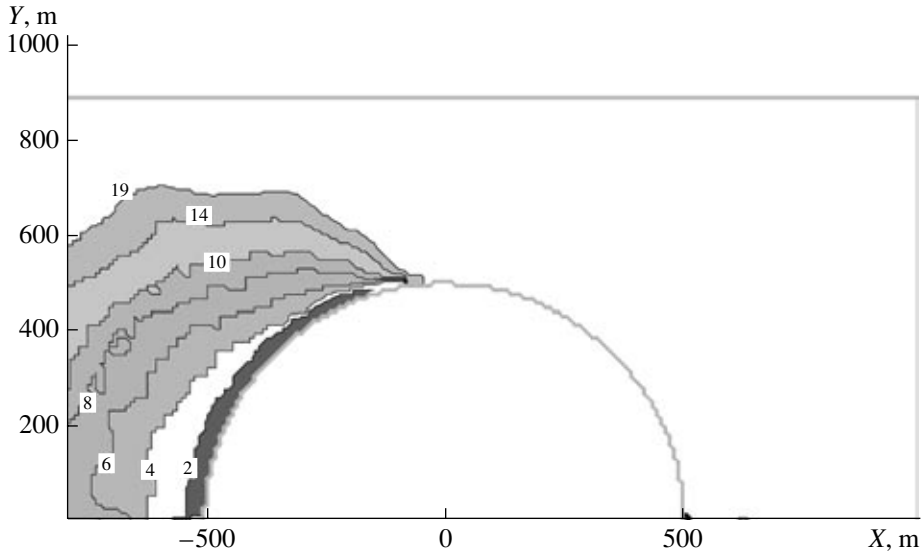

Fig. 2. The field of weights of model particles divided by the minimal weight.

cule free-path length. (Computations show that a reduction in the size of collisional cells from 1.6 to 0.8 free-path lengths has hardly any effect on the backward molecular flows. Thus, for the aforementioned cell sizes, the corresponding differences were less than 0.5% and 2.0% for the particle flow and the heat flux, respectively.)

RESULTS

In this section, we shall present the results of numerical kinetic simulations for nuclei with different types of gas production. The spherical homogeneous and heterogeneous nuclei will be considered. The axis of the proper rotation of the nucleus is directed at the Sun. Of course, both the sphericity assumption and the chosen orientation of the rotation axis are idealizations. In the general case, the shape of the nucleus can be very different from the sphere. At present, we reliably know the shape of only three comets: comet Halley (Keller, 1990), comet Borrelly (Britt *et al.*, 2004), and comet Wild-2 (http://stardust.jpl.nasa.gov). In the first two cases, the cometary nucleus is approximately a spheroid with a 2:1 axis ratio; in the last case, the deviation from the spherical shape is not so large. The axis of rotation may precess, and the period of rotation may vary. Simplifications are used in the present study in order to retain the axial symmetry of the problem and, thus, to reduce the computation time. Note that, although one can solve three-dimensional problems with the application of the program package SMILE, at the present stage it does not seem reasonable to make the model so complicated.

Now let us consider the boundary conditions at the nucleus surface that are required for kinetic simulations. We need to specify the effective gas production (with allowance for backward flows from the coma) and the coefficient of condensation on the ice surface as a function of the local temperature. The selected geometry of the problem allows us to find the complete temperature distribution in the near-surface layer of the cometary nucleus by solving the nonstationary heat-conduction equation for elementary areas with different cometocentric latitudes. Let us consider a nucleus located at a distance of 1 AU. In Fig. 3, one can see the computation results for the versions in which the entire solar energy is either absorbed by the surface (SEAM) or the absorption occurs in the near-surface layer (LEAM), i.e., has a volume character. We assumed that the pore size (the size of the forming particles) is 1 cm, the porosity is 0.7, and the Hertz factor is 0.01. Numerical estimates showed that visible radiation can penetrate rather deeply into a medium with the aforementioned characteristics. In the case of the volume absorption, the temperature reaches its maximum at some depth; that is, the so-called "greenhouse effect" is observed. The zone of effective heating extends, and thus, more energy is transferred deep into the nucleus. At the day side of the nucleus, the net gas production that corresponds to the calculated temperature distributions is several times lower in LEAM than in SEAM. It is interesting to mention that, in the case of the surface absorption of radiation at the day side, the pores and the compact part of the nucleus surface equally contribute, while in the model with the volume absorption, the major part of the released gas is produced by the pores, and the contribution of the surface itself is small.

Let us begin considering the simulation results for the inner coma for the simplest case, in which the nucleus has a spherical shape and a homogeneous structure. The density fields are presented in Fig. 4 for the boundary conditions determined by SEAM (a) and

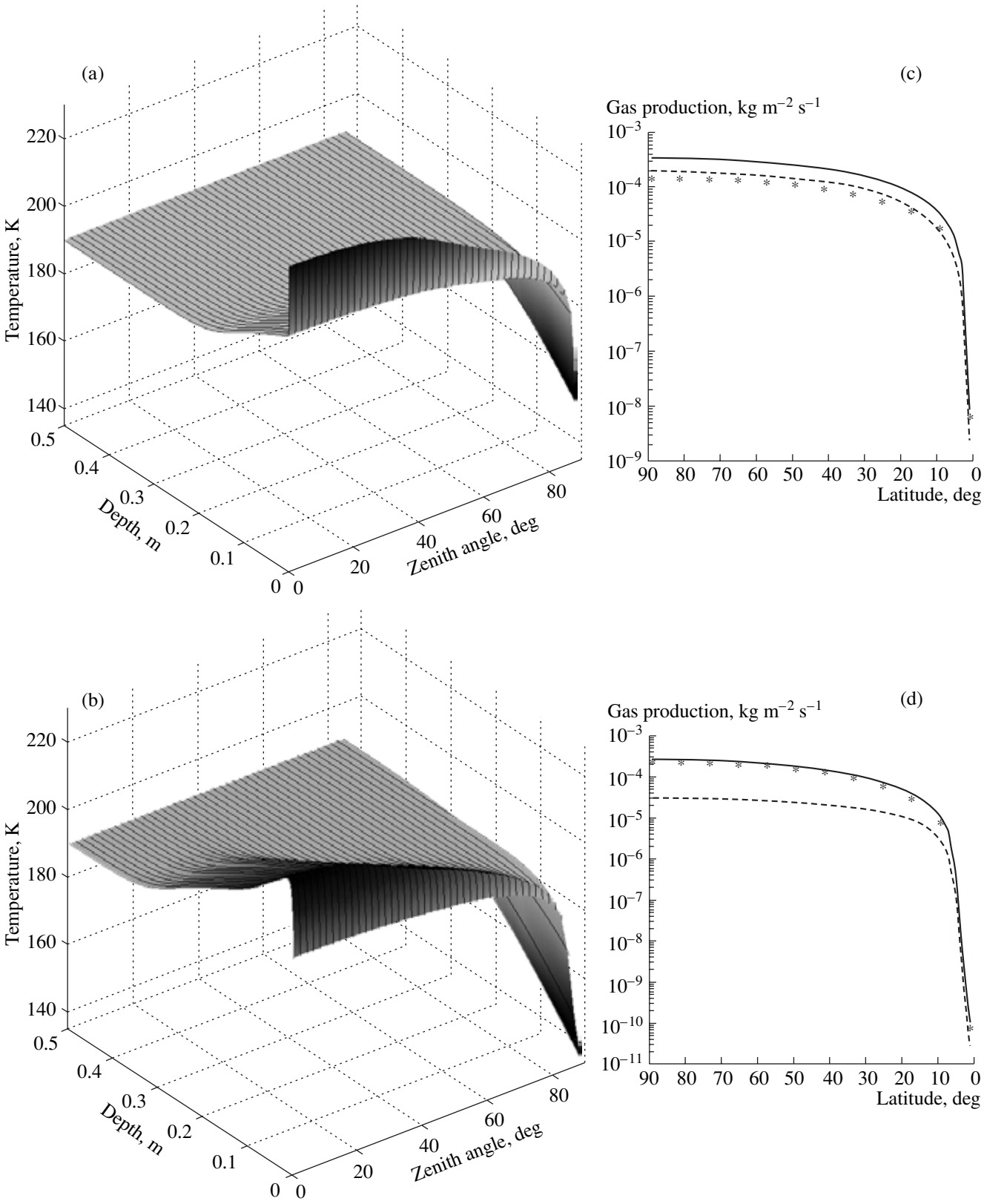

Fig. 3. The distribution of temperature (a, b) and efficient gas production (c, d) over the surface of a spherical nucleus with the Sun-directed axis of rotation obtained (c) by the model with the surface absorption of radiation (SEAM) and (d) by the model with the volume absorption of energy (LEAM). The solid line shows the total gas production, the dash line shows the contribution of the surface, and the stars demonstrate the contribution of the pores (sublimation from the layer). The nucleus is homogeneous, so the entire surface is active. The heliocentric distance is 1 AU.

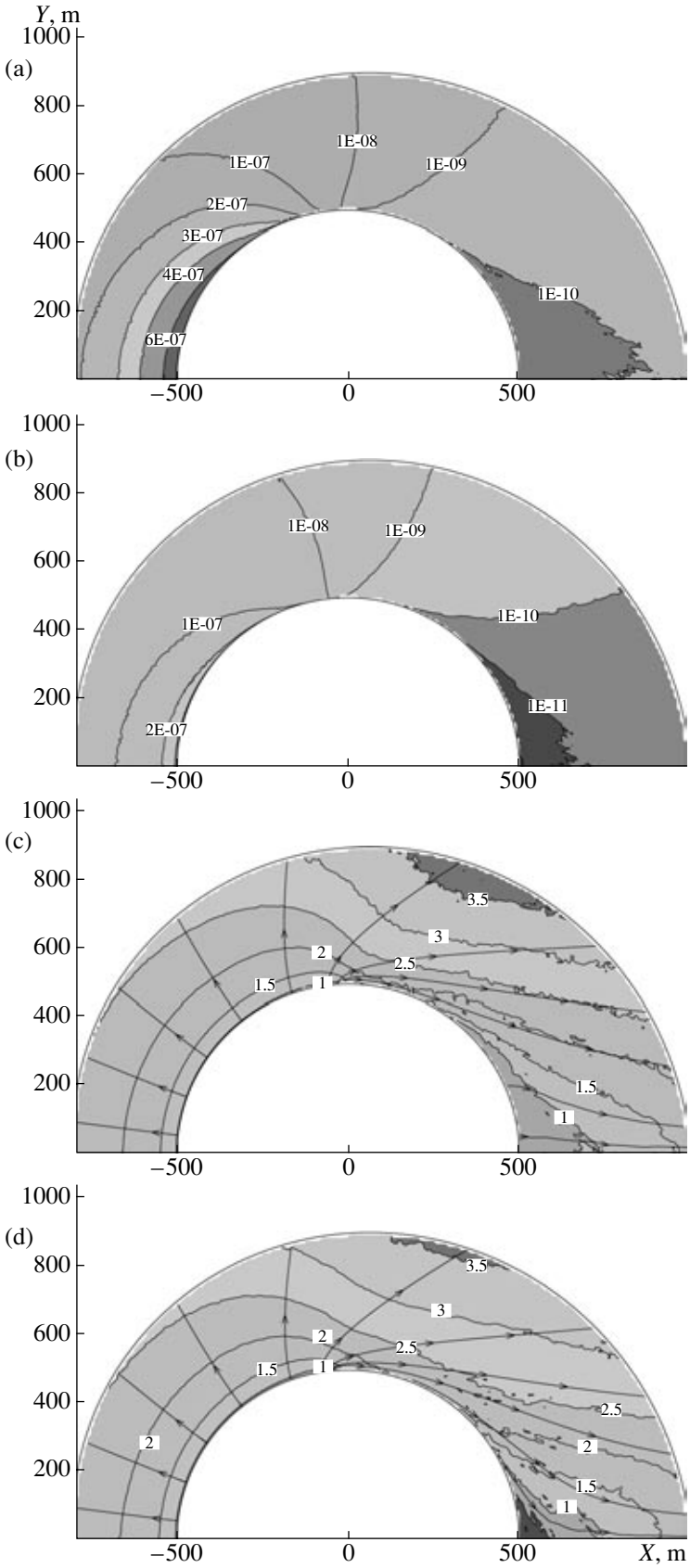

Fig. 4. The density field in the inner coma calculated for the boundary conditions specified using SEAM (a) and LEAM (b). The bottom panels show the distributions of the corresponding Mach numbers and the stream lines of the gas flow for SEAM (c) and LEAM (d). The nucleus is homogeneous, so the entire surface is active.

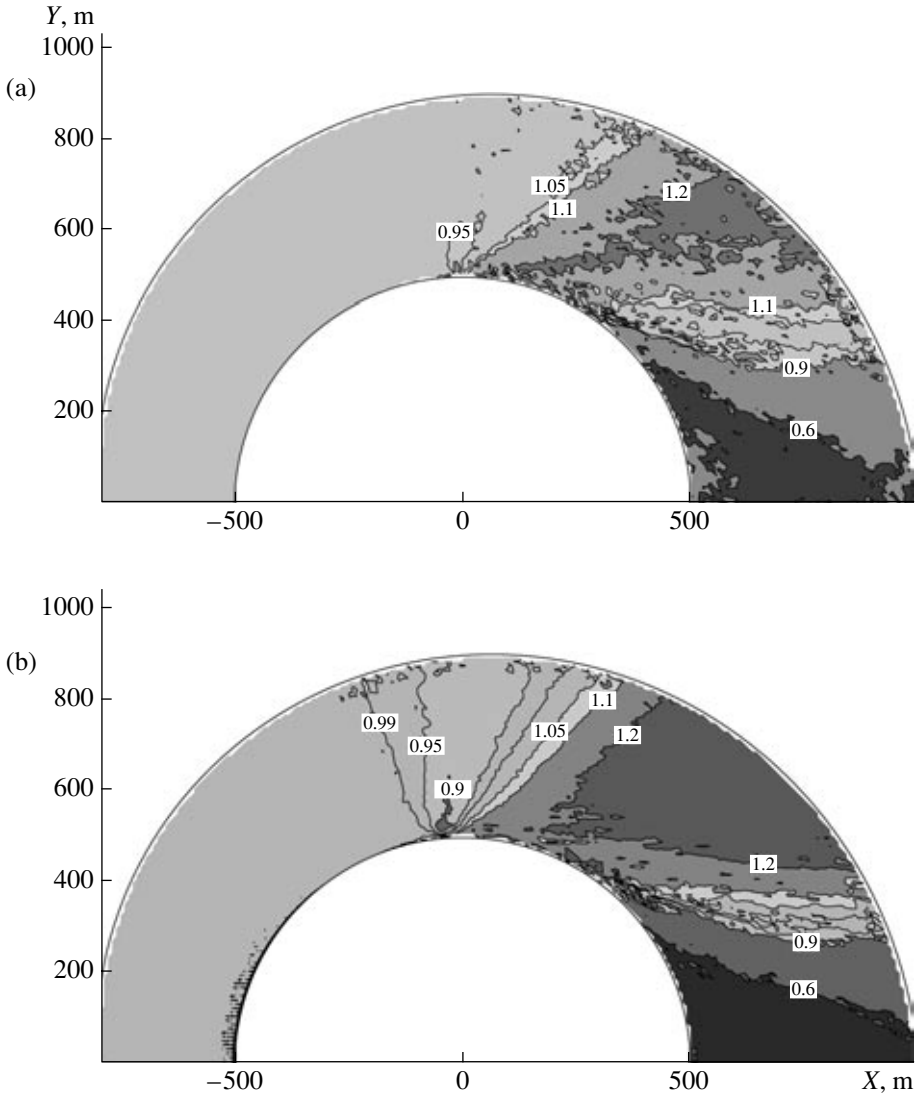

Fig. 5. The fields of temperature, calculated from the components of the molecule velocity, along the *Ox* axis, divided by the mean gas temperature (a) for the SEAM model and (b) for the LEAM model. The nucleus is homogeneous, so the entire surface is active.

LEAM (b). In this case, sublimation occurs from the entire surface (the entire surface is active). As should be expected, the density rapidly falls as the distance from both the nucleus and the axis of symmetry of the problem—the direction to the Sun—increases. In the region with an outer radius of only 1.5 nuclear radii, the density falls almost by a factor of four as the distance from the nucleus along the axis of symmetry increases. There are no qualitative differences between the considered models. At the same time, the quantitative differences are obvious: the inner coma is considerably denser in the model with the volume absorption of energy than in the classic model with the surface energy absorption. However, the typical velocities of the gas flow are nearly similar. One can suggest that the exchange of momentum and energy between the gas and the dust fractions is less intensive in LEAM; this means that, in a slightly dusty coma, all other conditions being equal, it takes dust particles more time to be sped up by the gas flow. The analysis of the distribution of the local Mach number shows that the flow is smooth. The flow is supersonic in almost the entire region, and only near the surface is there always a zone of subsonic flow. This zone is very small at the illuminated part of the nucleus and becomes much larger at its night side. The flow is nearly radial near the axis of symmetry, and there is no substantial tangential mass transfer from the more heated polar region. Closer to the terminator, the deviation from the radial flow becomes more significant. Considering this region, we can speak about strong cometary winds—the gas flows with a considerable velocity component with respect to the surface. It is well known that the degree of the kinetic nonequilibrium of the flow can be qualitatively estimated from the

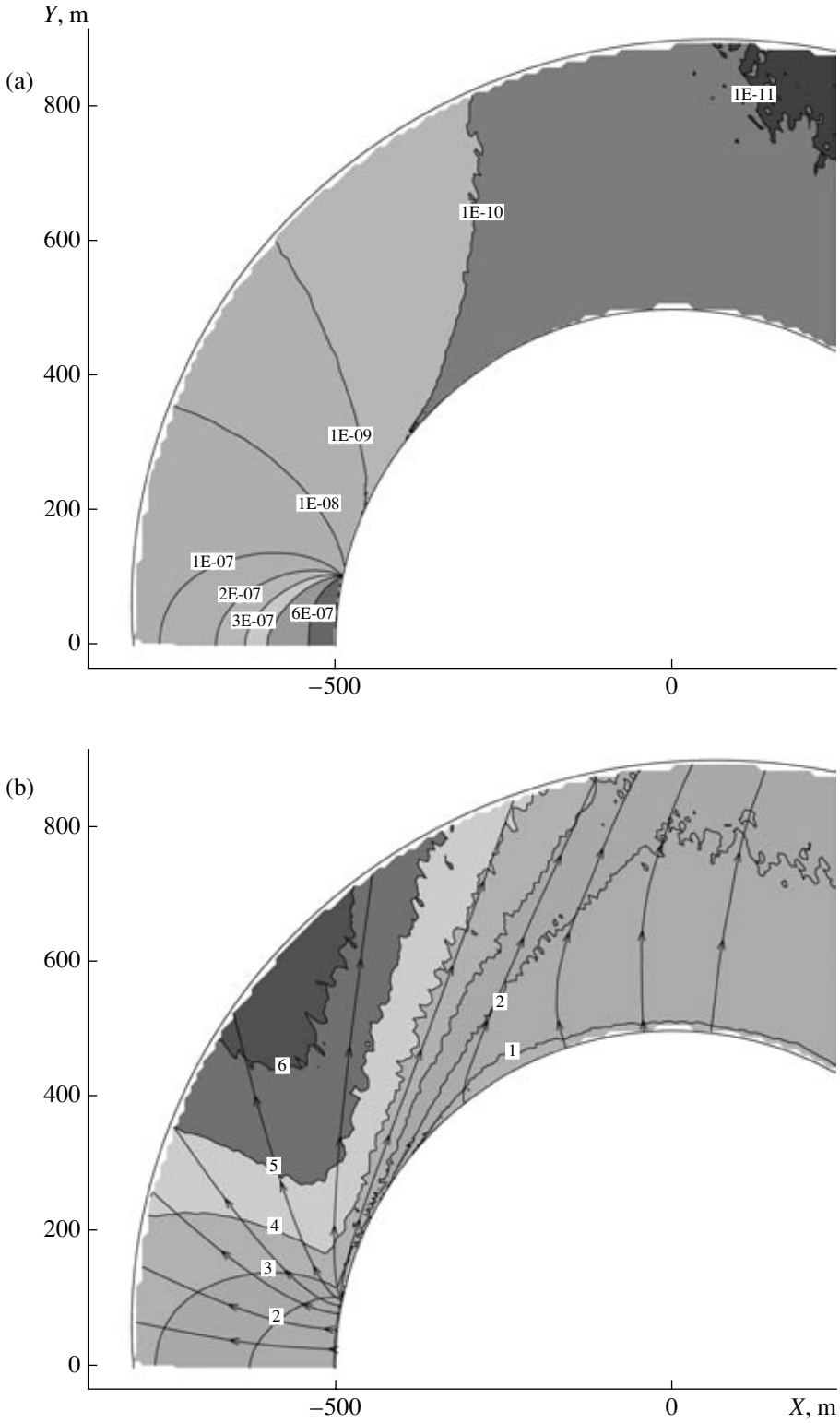

Fig. 6. The distributions of density (a) and the Mach number and the vector flow velocity (b) in the inner coma of the nucleus with an active polar region. The surface energy absorption model is used.

ratio of the gas temperature, calculated from different components of the molecule velocity, to the average gas temperature. In the equilibrium case, this ratio is obviously equal to unity. Simulations have shown that, in the hemisphere that is turned to the Sun, the temperature ratio near the nucleus is approximately unity for

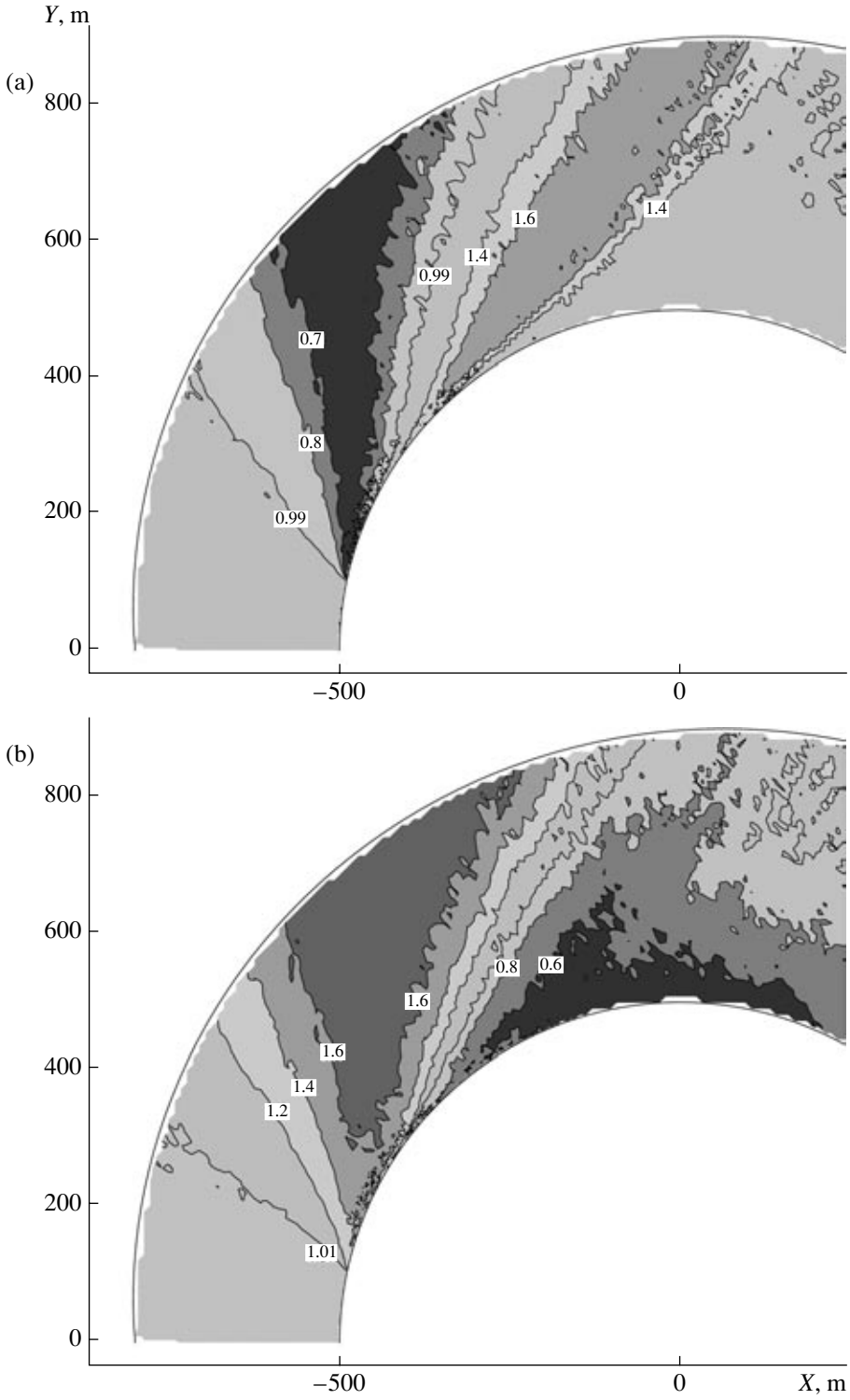

Fig. 7. The fields of the ratios of the axial temperature component T_x (a) and its transversal component T_y (b) to the average temperature. Sublimation occurs only from the polar region. The surface energy absorption model is used.

both SEAM and LEAM. A considerable deviation from equilibrium can be found in the "night" part of the coma, where temperatures calculated by different methods can vary by a factor of two (Fig. 5).

Therefore, we can expect that, under the conditions considered above, both the macroscopic and kinetic approaches can be successfully applied to model the "day" part of the inner coma of a spherical homoge-

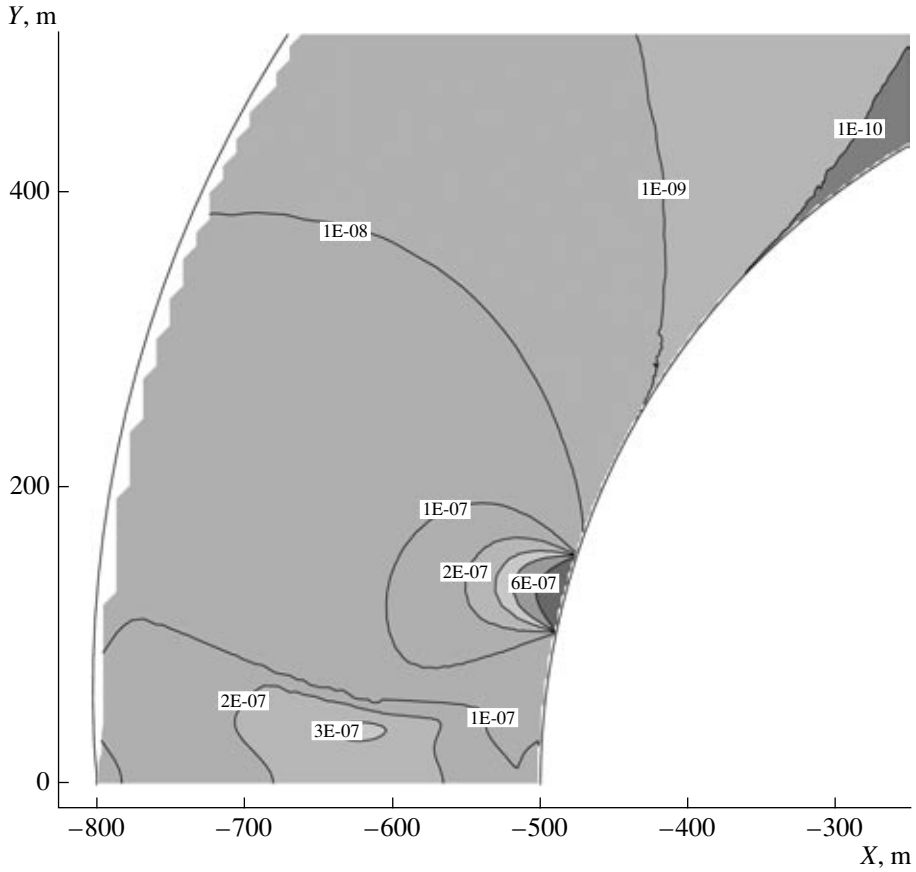

Fig. 8. The density distribution in the inner coma. Sublimation occurs from the "ring" centered at the polar point. The surface energy absorption model is used.

neous nucleus. If the conditions at the inner boundary of the simulation domain are specified correctly (that is, with allowance for the Knudsen layer), the hydrodynamic model should give results that are very close to the results of kinetic simulations. This conclusion agrees with the earlier conclusions of Combi (1996) and Crifo *et al.* (2002), who considered directly the case in which sublimation occurred from the surface of a homogeneous spherical nucleus.

Now let us consider the variants in which the gas production is a nonmonotonic function of the cometocentric latitude. As mentioned above, such nonmonotonicity can be associated with the presence of a dust layer on the surface of the nucleus. In the present study, we modeled two idealized variants of distribution of the gas production: (1) in the first one, we assumed that only the polar region of the nucleus is active and there is no sublimation from the rest of the surface; (2) in the second case, we assumed that a narrow segment of the sphere is active; that is, sublimation occurs only from a "ring" with its center at the subsolar point. Both variants are certainly idealizations but physically reasonable. An additional stimulus for considering such variants was the fact that directly the same gas flow models were used by Keller *et al.* (1994), who applied the hydrodynamic approach to the description of the inner coma. Unfortunately, in their paper (as in all other studies we know to be devoted to the inner coma simulations) the boundary conditions at the nucleus surface were specified in an arbitrary way, thus giving no possibility of making a quantitative comparison of the DSMC results presented below with the published results of hydrodynamic modeling. However, even a qualitative comparison of the structure of the flow is of evident interest.

The density distribution in the inner coma for a nucleus with an active polar region is shown in Fig. 6a. As should be expected, the gas stream is clearly evident in this case. The density rapidly falls as the distance from the axis of symmetry—the direction to the Sun—increases. This fall is most rapid outside the cone bounding the active region. The expansion of the gas stream is such that, at a distance of one radius of the nucleus, the entire "day" hemisphere of the coma is already filled with gas. The field of the flow velocity (Fig. 6b) clearly shows how the mass transfer occurs near the nucleus. Note that there is no significant condensation on the nonactive surface of the nucleus. The field of the Mach number combined with that of the density shows that the flow has a smooth character; the

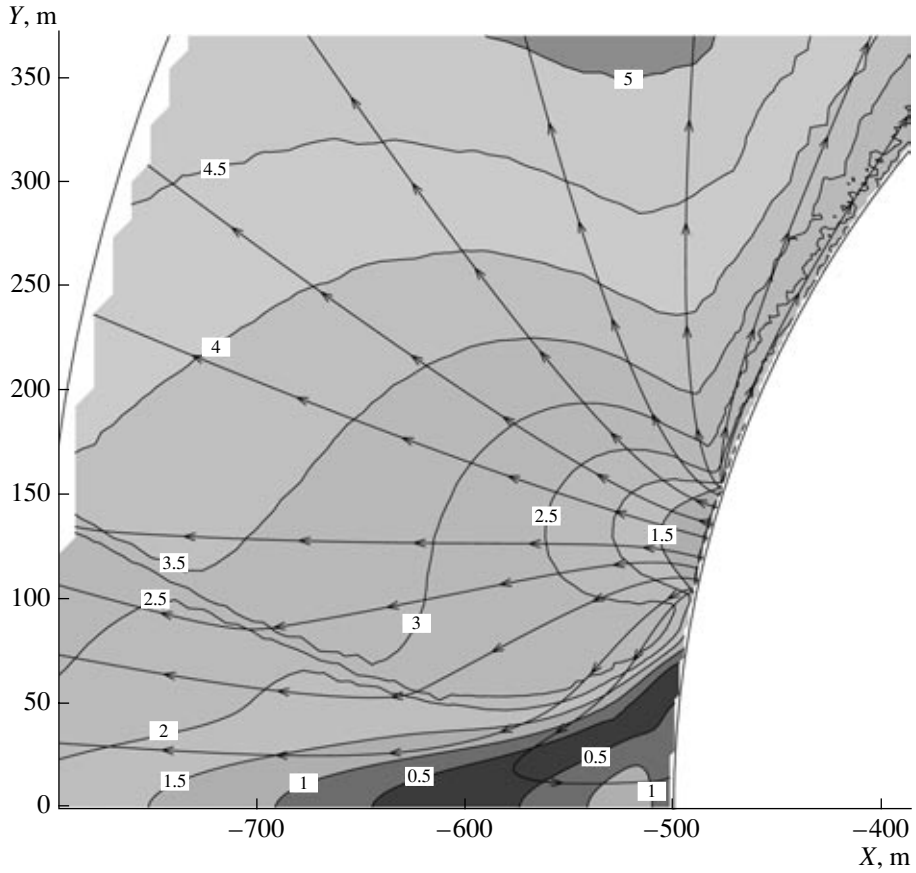

Fig. 9. The distribution of the Mach number and the vector flow velocity in the subpolar region. Sublimation occurs from the "ring" centered at the polar point. The surface energy absorption model is used.

subsonic flow zone still exists near the nucleus, and the flow becomes supersonic as the distance from the surface increases. However, in contrast to the previously considered variant, in which the entire surface of the nucleus was active, in this case the size of the zone of the subsonic flow considerably increases as we pass from the subsolar point to the midnight one. The degree of the nonequlibrium of the gas flow (and, consequently, the degree to which the macroscopic equilibrium description can be applied) is characterized from a kinetic point of view by the fields of the ratios of the transverse (T_y) and axial (T_x) temperature components to the average temperature (Fig. 7a and b). In the case of a homogeneously structured nucleus, this ratio was close to unity almost over the entire "day" hemisphere of the simulation domain, but now the pattern is quite different. Considerable deviation from equilibrium can be observed for the whole simulation domain outside the cone bounding the active region. The character of the variations of different temperature components is also different. A comparison of the fields of translational and rotational temperatures leads us to the same conclusion about the highly nonequilibrium character of the flow. It can be concluded that, strictly speaking, the hydrodynamic approach can be applied only in a small vicinity of the axis of symmetry of the flow.

Now let us move on to the model in which sublimation occurs from the "ring" centered at the subsolar point. In this case, the active region is surrounded by nonactive ones, and the structure of the gas flow accordingly becomes more complex. The density field is shown in Fig. 8. It can be clearly seen that, in addition to the high-density area that corresponds to the active ring zone itself, a secondary central high-density zone arises in the coma as a result of the gas stream extension in the direction of the axis of symmetry of the model. The zone is at some distance from the surface; this distance obviously depends on the size of the central nonactive zone. This size mainly determines the relative density excess over the pole as well. The density variations with distance have a nonmonotonic character in the vicinity of the axial line—we may speak about a density maximum that is displaced from the nucleus surface.

Let us consider the distribution of the Mach number (Fig. 9). For the first time, the flow is discontinuous. Comparing the field of the Mach number with the field of the gas flow velocity, we see in the inner coma not only the already familiar acceleration and transition from the subsonic to supersonic regime, but also the

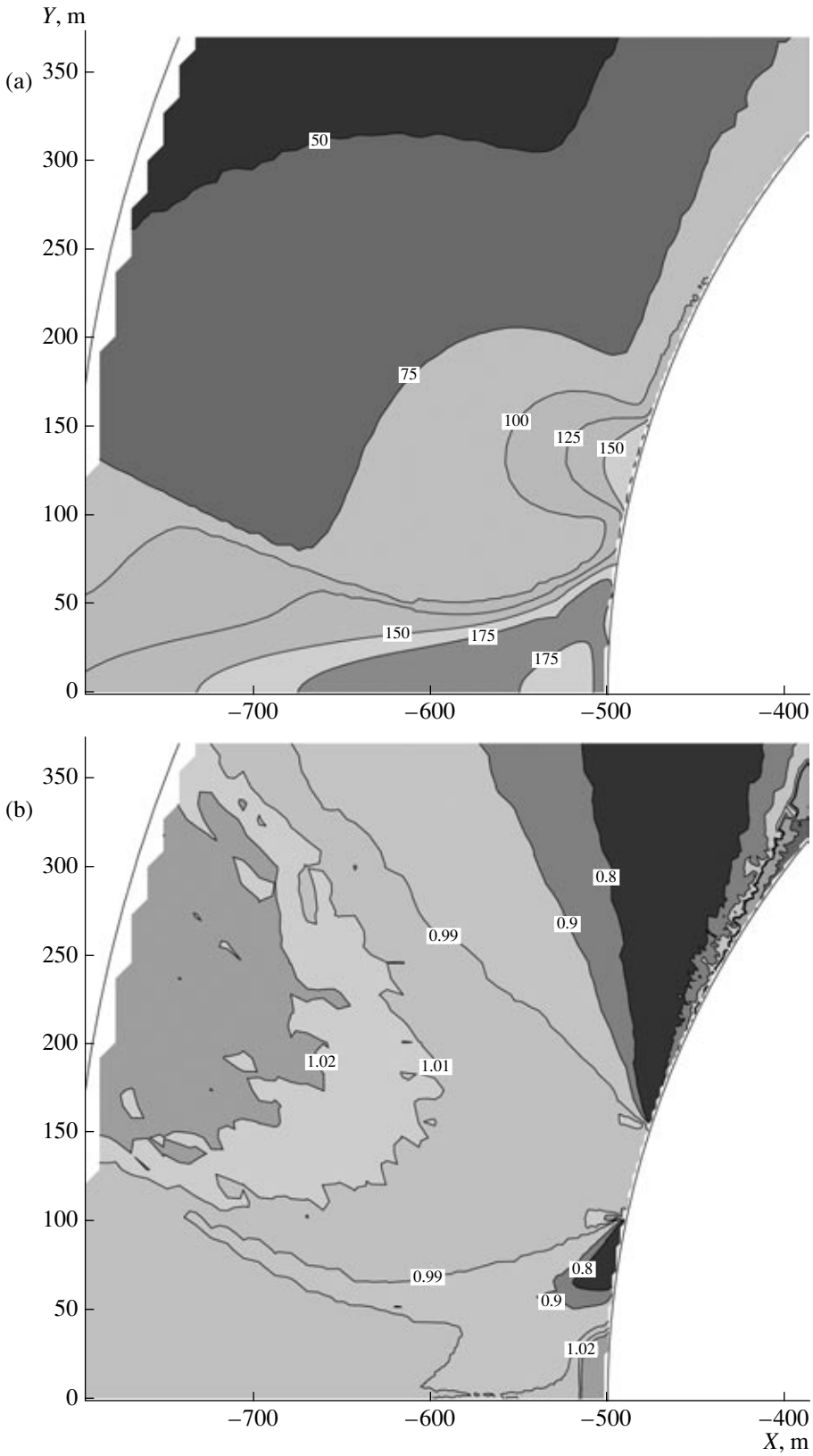

Fig. 10. The field of the rotational temperature component (a) and the field of the ratio of the axial temperature component T_x (b) to the average temperature in the subpolar region. Sublimation occurs from the "ring" centered at the polar point. The surface energy absorption model is used.

inverse transition from the supersonic to the subsonic one. Figure 9 also shows the vector field of the average gas flow velocity. It is clearly seen how the mass transfer from the active region to the central nonactive region occurs. It is interesting to note that the velocity of the gas flow is directed to the surface in the subdomain over the pole. This can cause the condensation associated with macroscopic transport instead of intermolecular collisions. The interaction of gas streams generated in different elements of the active region leads to the formation of shock waves in the vicinity of the surface. In these regions, the gas flow slows down and the density increases. Inside the central region of the subsonic flow, we can see a subregion in which the gas moves very slowly and the Mach number is approximately 0.10–0.15. The maximal values of both translational and rotational temperatures are observed in this region. These temperature maximums are clearly seen in Fig. 10. Analyzing the degree of equilibrium of the flow, we see that the flow can be assumed to be nearly equilibrium only within the cone containing the active region, as was the case in the model with the active polar region. It is interesting to note that the coma region near the axis of symmetry is also in a state that is close to kinetic equilibrium. The ratios of different temperature components to the average temperature are very close to unity. The values of translational and rotational temperatures are close as well. This is probably caused by effective intermolecular collisions that are maxwellizing the gas: the mass-averaged particle velocity is small in this subregion, and, as a result, the particles have time for collisional maxwellization.

The exception is a small region near the inner boundary of the active ring near the nucleus surface, which is characterized by an extremely low gas density. Here, the frequency of molecular collisions is insufficient to reach a kinetically equilibrium state.

CONCLUSIONS

This paper is devoted to the numerical modeling of the inner region of the cometary atmosphere formed due to water-ice sublimation. We used the kinetic approach (the DSMC method) in our calculations. This allowed us to model efficiently both the day (where the flow may be close to the kinetic equilibrium) and the night (where the flow is kinetically highly nonequilibrium) regions of the coma. Auxiliary one-dimensional calculations for the Knudsen layer were performed in order to specify the boundary conditions at the surface of the nucleus. Models with different types of sublimation were considered for spherical nuclei (both homogeneous and heterogeneous) with the axis of rotation directed to the Sun.

In the case of the homogeneous nucleus, the entire surface of which is active, the characteristics of the gas flow obtained by kinetic and hydrodynamic models are similar. In both cases, a well-pronounced stream is generated near the axis of symmetry of the problem. The gas density rapidly falls as the distance from the axis of symmetry and from the surface of the nucleus increases. The analysis of the results of kinetic simulations confirmed the assumption that, at negligible heliocentric distances (this distance was assumed to be equal to 1 AU in our calculations), for active comets the flow is nearly equilibrium near the nucleus in the whole day hemisphere, and the equilibrium macroscopic approach can be applied to describe the gas.

The situation becomes more complicated in the cases in which the gas production of the nucleus varies considerably on small scales. If active evaporation occurs from the limited region surrounded by the nonactive medium, the hydrodynamic approach can be applied only to the conical domain containing this active region of the nucleus. The DSMC results for the density distribution and the field of the vector velocity qualitatively agree with the results published by Keller *et al.* (1994) and Knollenberg *et al.* (1996), who used the macroscopic hydrodynamic approach. Outside this cone (especially near the terminator and in the whole night hemisphere), the flow is essentially nonequilibrium. Here, the kinetic approach is the only possible numerical method that can be used to model the coma structure. In the case in which evaporation occurs from a spherical segment (from a "ring" with a nonactive center), the results of the hydrodynamic simulation of the density distribution and the vector velocity field are also in qualitative agreement with the results of kinetic simulations. It is interesting to note that the macroscopic model allows us to simulate in general quite a complex flow structure inside the active zone. In the figures presented in (Keller *et al.*, 1994) one can see the high-density region that departed from the nucleus surface in the vicinity of the axial line, as well as the macroscopic backward gas flow inside the active ring.

Thus, we can conclude that, in the cases in which the flow is close to the kinetically equilibrium one, there is a qualitative agreement between the results of the micro- and macrosimulations. At the same time, the kinetic approach always provides more complete and reliable information about the flow. A basic advantage of this approach is that it provides a possibility for a consistent simulation of the mass transfer in the cometary nucleus and of the coma surrounding the nucleus. In the general case, this cannot be performed within the framework of the hydrodynamic approach. In the hydrodynamic approach, in addition to the problem of specifying the correct boundary conditions, we always face the problem of the applicability of this method to the simulation of the inner cometary atmosphere, that is, of the reliability of the results obtained by this method. As was shown above, the region where the macroscopic approach can be applied depends on the morphology of the nucleus, as well as on the type and degree of its activity. Consequently, further modifications of the computing program and considerations of the models describing the inner coma around a nonspherical nucleus with variable gas production is of

inevitable interest. This problem will be considered by the authors in their next study.

When speaking of the advantages of the kinetic method, we should mention the basic unresolved problem that arises during its application: this approach can be applied only for a purely gaseous coma. In our models we neglected the effect of dust particles, the number of which in the cometary atmosphere is large. Based on observational data, we can suggest that the characteristics of the dispersed dust fraction in the inner coma may be considerably different from the corresponding gas characteristics. This must result in intense interphase exchanges of mass, momentum, and energy. It is of the highest priority to take this complex of unresolved problems into account.

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