Simulation of gas-dispersed flow particles’ interaction with a solid body

I A Amelyushkin\textsuperscript{1} and A L Stasenko\textsuperscript{1,2}

\textsuperscript{1}Central Aerohydrodynamic Institute named after Prof. N.E. Zhukovsky, Zhukovsky, Russia
\textsuperscript{2}Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Russia

amelyushkin_ivan@mail.ru

Abstract. Mathematical models and numerical algorithms for the interaction of particles of an aerosol stream with a relief surface of a solid are developed as applied to the problem of aircraft icing. The developed technique allows to study the interaction of particles with a solid at various speeds and particles’ sizes the spreading coefficient characterizing the hydrophobic properties of the surface.

1. Introduction
Modeling the control of the interaction of a flow with a streamlined surface is of great interest in various fields of science and technology. One of the urgent physical problems of aviation is the problem of icing of an aircraft in droplet-crystalline clouds. Investigations carried out for almost a century [1–3] were based, as a rule, on experimental data and phenomenological description of the process in the framework of continuum mechanics. However, to successfully solve the problem, it is necessary to develop mathematical models and numerical algorithms that take into account the physical processes that accompany icing at a fundamental level. In this regard, the most important aspect is the interaction of an individual particle with a rough body [4].

The main difficulties in modeling such phenomena are related to the fact that a mathematical description of the collision process requires information on such macrocharacteristics of a substance as viscosity, thermal conductivity, yield strength, elastic modulus, and a number of others, which are usually measured under static conditions and are not always suitable for descriptions of fast-flowing shock interactions. In this regard, it is natural to consider these phenomena at a higher level of detail. Note that the real surface of an aircraft is almost always rough. So, in aviation technology, the average surface roughness is of the order of $h \sim 1 \mu m$.

In [5], the results of calculations by the molecular dynamics method of droplet behavior on a relief body, whose surface has hydrophobic properties, are presented. According to this study, short-wave (molecular) roughness is not very important. For rough hydrophobic surfaces, there is no hysteresis of the contact angle of the droplet due to intense thermal fluctuations that occur near the solid-liquid boundary at the molecular level. In [6], the results of molecular-dynamic modeling of the boundary layer of a single-component fluid on a wavy surface are presented using a simplified calculation using the well-known Langevin thermostat and artificial friction coefficient. The interaction of solid microparticles with a rough surface was previously studied theoretically and experimentally in [7, 8].
The aim of this work is to create algorithms that allow calculating the interaction of a heterogeneous flow with nanostructured surfaces of solids from various materials, wetting processes, and particle motion on the surface in an air stream. The specifics of the problems considered is the need to describe the flow of hydrothermodynamics and mass transfer of an air-drop-crystalline stream with a nanorelief surface of a solid in a shear flow of a carrier gas.

Note that a real gas does not only consist of molecules, but also contains their agglomerates — clusters, and their concentration and the number of 2, 3, ..., N molecules that compose them increase with decreasing temperature. This applies in particular to water vapor in a pre-condensation state; their clusters, flowing together with the carrier air, structural elements of the aircraft, can participate in the "preparation" of the latter for icing.

2. Mathematical model and numerical method

In the approach under consideration, the intermolecular interaction parameters play an important role, which can be obtained both on the basis of both quantum-mechanical calculations and the equation of state of a real gas, for example, Van der Waals:

\[(P - \rho a / V\mu) (1 - b \rho / \mu) = \rho R_o T / \mu,\]

where

\[a = -2\pi N^2 d \int_0^\infty U(r)r^2 dr = \pi N^2 \frac{10\sqrt{2}}{9} \sigma^6_0 = N_{\lambda} \sigma^6_0 / 3 \rho e, \quad b = N_{\lambda} \frac{2}{3} \pi d^3, \quad \sigma_0 = \frac{d}{\sqrt{2} \sqrt{2\pi N_{\lambda}}}.\]

In a more general case, the spherically symmetric potential has the form

\[U(r) = A \left( \left( \frac{\sigma}{r} \right)^6 - \left( \frac{\sigma}{r} \right)^q \right),\]

(1)

Tables 1 and 2 give the parameters of the equation of state of the van der Waals gas and the associated parameters of the pairwise interaction of substances A, p, q and χ; \(\sigma_0 = \sigma_{H_2O} \approx 2.6\ \text{Å}\) — the characteristic distance at which the pair interaction potential vanishes, \(\mu\) is the molar mass, \(R_0\) is the universal gas constant, \(N_{\lambda}\) is the Avogadro constant, \(d\) is the "diameter" of the molecule.

| Gas   | Van der Waals gas parameters \(a, \text{Pa}\cdot\text{m}^6/\text{mol}^2\) | LD potential parameters | LD potential parameters \(\sigma_0, \text{Å}\) | ε / \(k_b\), K |
|-------|-------------------------------------------------|--------------------------|-----------------|-----------------|
| \(N_2\) | 0.1408                                        | 2.80                      | 260             |
| \(O_2\) | 0.1378                                        | 2.61                      | 313             |
| \(H_2O\) | 0.5536                                        | 2.58                      | 1310            |
| Air   | 0.141                                        | –                        | –               |

Note that the approach used in this work allows one to circumvent the difficulties of taking into account the unpaired nature of the interaction of molecules, as well as the angular dependence of intermolecular forces, for the determination of which, strictly speaking, quantum chemistry methods for solving the Schrödinger equation for a multi-electron system of atoms are needed. This approach allows one to calculate both the continuous and free molecular modes of interaction between particles and droplets with a solid, taking into account a number of physical phenomena: phase transitions, the dependence of the surface tension coefficient on the curvature of the interface, the processes of fragmentation, coagulation and heat transfer with a relief body, whose atoms are in thermal
movement. Moreover, the reliability of the results obtained in this work is justified by comparison with theoretical and experimental estimates of researchers described in [7]. The numerical algorithms and software developed in this paper allow the use of various interaction potentials of molecules and schemes for integrating equations of motion.

Note that in the considered model, the asymmetry of the interaction potential of water molecules with each other and with a solid is not taken into account. Such an assumption is reasonable for the study of hydrodynamic processes accompanying the interaction of particles and droplets of an aerosol stream with a solid.

Table 2. Parameters of potentials (expression (1)).

| Interacting elements       | $A/\epsilon_0$ | $\xi$ | $\chi$ | $p$ | $q$ |
|---------------------------|----------------|-------|--------|-----|-----|
| H$_2$O--H$_2$O            | 1              | 1     | 1      | 12  | 6   |
| H$_2$O--Al                | AK             | 1.19  | 1      | 12  | 6   |
| H$_2$O--H$_2$O(w)         | 2.53           | 1     | 5/33   | 9   | 3   |
| H$_2$O--Al(w)             | 2.99 AK        | 1.19  | 5/33   | 9   | 3   |
| H$_2$O(w)--Al(w)          | 13AK$\cdot$S, nm$^2$ | 1.19  | 5/132  | 8   | 2   |

In the present work, under the assumption of the potential nature of the interaction between atoms or molecules, various schemes for integrating the equations of molecular dynamics were tested in present study.

It is assumed that the particle colliding with the surface of the solid is accelerated by the air flowing around it, which is a mixture of nitrogen (79%) and oxygen (21%) with Van der Waals gas parameters, which were calculated according to the Lorentz–Berthelot mixing rule:

$$a = \left( \sum \alpha_j \mu_j \right)^2 \left( \sum \frac{\alpha_j}{\mu_j} \right)^2 \left( \sqrt{\alpha_j} \right)$$

$$b = \sum \alpha_j \mu_j \cdot \sum \frac{\alpha_j}{\mu_j} b_j$$

$$R = R_0 \sum \frac{\alpha_j}{\mu_j}.$$  

The substance of the wall is described by the parameter introduced earlier [3]

$$AK=\epsilon_{w-m}/\epsilon_{m-m} \approx 0.5 \left( 1 + \cos \theta_0 \right)$$  \hspace{1cm} (2)

It is so called spreading coefficient, which can be considered as the ratio of the energy $\epsilon_{w-m}$ of the interaction (A means adhesion) between the flow molecule (index m) and the atom or molecule of the surface (index w) to the characteristic energy $\epsilon_{m-m}$ of the interaction of the flow molecules with each other (K means cohesion). This parameter characterizes the properties of a solid material that determine the rate of adherence of a liquid to it. Interactions of molecules belonging to all three phase states of substances are considered: the carrying gas, an incident particle, liquid or solid, and the surface of a streamlined body.

In this work, we constructed a model for the interaction of flow molecules with solid atoms in thermal motion, depending on the temperature and physical properties of the substance, determined by the Debye temperature and molar mass of atoms, as well as the unit cell size of the solid crystal lattice.

Using the expressions for the interaction potential, the vibrational amplitudes of the atoms of the lattice of the solid body $\Delta a$, the thermal conductivity and the specific heat of substances, we obtained the values of the coefficients of the interaction of water molecules with a solid under the assumption that the characteristic surface relief sizes $\lambda$, $h$ (figure 1a) significantly exceed the size of the molecules. Based on the law of change in momentum, the expression for the speed of the reflected molecules (upper index $r$ – reflected) from the surface of the particle’s body depending on their initial (upper index $i$ – incident) speed can be obtained in the following form:
\[ V' = V'(1 - \mu_{r} / \mu) + \left( \frac{2}{\sqrt{3}} \right) \mu_{t} / \mu (n + 2 \tau) \Delta a \sin \omega t \]

Here \( n \) and \( \tau \) are the unit vectors of the normal and the tangent. For the interaction of water with an aluminum surface, we have

\[ V' = -0.2V' + 0.693(n + 2 \tau) \Delta a \sin \omega t, \quad \omega_{0} = \sqrt{\frac{3R_{T} / \mu_{r}}{\Delta a / \sqrt{2}}}, \]

where \( \omega_{0} \) is the cyclic vibrational frequency of atoms in the crystal lattice of a streamlined body.

Note that the second term in the numerator of the expression for \( V' \) contains one degree of freedom of oscillations along the normal and two degrees of freedom along the tangent to the surface, which describe the contribution of the vibrations of the atoms of the crystal lattice of the relief body (figure 1b) along the directions of surface vibrations. The amplitude of oscillations of the atoms of the surface \( \Delta a \) depending on the temperature \( T \) is determined by the well-known expression from solid state physics:

\[ \Delta a^{2}(T) = \frac{9h^{2}}{4\sigma_{s}k_{B}\theta_{D}} \left( 1 + 4 \left( \frac{T}{\theta_{D}} \right)^{2} \int_{0}^{\theta_{D}} \frac{\theta}{e^{\theta} - 1} d\theta \right). \]

Here \( \theta_{D} \) is the Debye temperature of the solid material, \( k_{B}, h \) are the Boltzmann and Planck constants, respectively. The advantage of such a model is the possibility of taking into account the thermal vibrations of atoms and a more approximate to reality (compared with traditional models) description of the interaction of flow molecules with a solid. Its disadvantages include large computational costs when calculating flows in a large computational domain. So, for example, when modeling two layers of the surface of a streamlined body (aluminum) with a size of 100–100 nm², about \( 10^{5} \) atoms interaction with flow and particle’s molecules re required to be taken in account. With an increase in roughness, this figure increases significantly.

**Figure 1.** a) a diagram of the interaction of particles with a relief body at the bottom of the boundary layer of a real gas; b) the scheme of interaction of molecules of the flux \( m_{i} \) with atoms of the solid body \( m_{A} \). Angles \( \alpha', \alpha' \) are between the particle velocity vector and the normal to the average surface of the body.

The lower boundary of the computational domain (Fig. 1a) is the rough surface of the streamlined body, the interaction with which is described by mathematical models defined below. In this area, water and air molecules interact with atoms of a solid body, taking into account their physical
properties and temperature. The thermal velocities of all gas molecules and particles are determined in accordance with the Maxwell velocity distribution.

In the case of a flat surface, assuming that the interaction of a water molecule with an atom is described by the Lennard–Jones potential with parameters $\varepsilon_w = AK_\text{water}$ (index $w \equiv \text{wall}$), solid body was divided into many flat layers of thickness $dy$ parallel to the surface of the solid. The interaction potential between the molecule and the body surface is given in the form

$$U(h) = \frac{8}{15} \frac{\rho_w}{m} \pi \varepsilon_w \sigma_w^3 \left( \frac{5}{33} \left( \frac{\sigma_w}{h} \right)^9 - \left( \frac{\sigma_w}{h} \right)^3 \right).$$

Based on quantum chemical estimates, $\sigma_w \approx \xi \sigma_0$ (table 2). To estimate the energy density of the interaction of particles, the size of which is significantly larger than the size of the molecule, we use the model of two flat surfaces – a solid body and the "foot" of the particle. Note that the expression for the surface density of the interaction forces $P$ between the plate of a given material and the flat surface of the water has the following form

$$P = -\frac{1}{S} \frac{\rho}{m_w \partial h} \frac{\partial}{\partial y} (U(h)) = B \left( \frac{5}{33} \left( \frac{\xi \sigma_0}{h} \right)^9 - \left( \frac{\xi \sigma_0}{h} \right)^3 \right),$$

$$B = \frac{8}{15} \frac{\rho_w}{m} \pi \xi^3 \rho \sigma_0^3 \varepsilon_w A K_{\text{water}} \sigma_o^3.$$

From the last relations, the equilibrium distance between two surfaces is determined in the absence of external forces: $h_e = \xi \sigma_0 (5/33)^{1/6}$. Here $\xi$ is a dimensionless quantity equal to the ratio of the characteristic length of the interaction of the molecules of the streamlined body with the water molecule to the length of the interaction of the water molecules with each other. For aluminum, $\xi \approx 1.19$. It is clear that the smaller the particle, the sooner it is slowed down in the boundary layer on the streamlined body, but the greater the role in its dynamics is played by thermal fluctuations (Brownian motion). If for a water molecule the average speed of thermal motion is about 600 m/s, then for the considered clusters its values are approximately 25, 20 and 10 m/s. Thus, despite the rapid relaxation of small particles near the surface of a solid, the total speed of their collision with a solid can reach tens of meters per second. The developed algorithms can be used both for a drop and for an ice crystal, while expressing the strength of elasticity through the total strength of the intermolecular interaction. The question of the phase state of the particles under consideration is nontrivial. Even M. Faraday suggested (1842) the existence of liquid layers on the surface of an ice crystal below the freezing temperature. In a recent work [12], the existence of such layers was confirmed in the temperature range from $-90$ to $-1^\circ$ C. The situation is similar to the absence of a sharp boundary between the liquid and vapor. However, since the sizes of the considered clusters are of the order of the thickness of the transitional interfacial layers, in the present work such molecular formations are called simply particles.

3. Conclusion and discussion
Mathematical models, numerical algorithms, and programs for calculating the interaction of particles of a dispersed stream and gas phase molecules of this stream, a carrier particle, with a nanostructured solid surface with specified physical and geometric properties are developed. These models allow us to formulate the boundary conditions on the streamlined surface, optimize the interaction of the flow with the body, calculate the modes of collision of particles and drops with a solid, simulate wetting and movement of drops on the surface, and can also serve as the basis for solving problems of modeling and control of near-wall turbulent flows.
The molecular dynamics method used is an intermediate between the methods of quantum chemistry, and the continuum approach. When analyzing unsteady processes (in particular, shock processes), it avoids the need to use macroscopic physical and mechanical characteristics of substances obtained under quasistatic conditions. The simplifying assumption accepted in the present work on the spherical symmetry of atomic-molecular potentials is justified by the scale of the phenomenon under study (the characteristic particle size significantly exceeds the intermolecular interaction distance). Note that in the gas flow region with nanoparticles, which is difficult to access for experiments, this method allows one to obtain information about the “preparatory” period of icing of the aircraft.

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