Dynamics of Molecules in a Supercooled Water Nanoparticle during the Ice Accretion on the Aircraft Surface

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Introduction

The process of ice accretion on a body surface is being under investigation almost during the whole aviation history, but up today the physics of this process needs more deep understanding. It concerns especially an initial touch of a droplet to the solid body surface.
As the characteristic scale (either spatial or temporal) of fluids is getting smaller, investigations with experimental apparatus become difficult. Conventional theoretical/numerical approaches can also be problematic when continuum mechanics and kinetic theory of fluid are no longer assumed a priori.
Theoretical approaches (e.g., the well-known Laplace equation for mechanical balance) sometimes lead to incredible conclusions and unsettled problems, while experimental investigation of nanoscale particles require extremely sophisticated techniques.
Another approach for nanoscale fluid phenomena is used in this work. Interaction of water nanoparticles in the air with solid surface of the body is investigated via molecular dynamics simulation techniques. In comparison with the similar investigations (e.g. [1–3]) in this paper more elaborated model which takes into account some essential physical effects and some addition parameters were controlled during the water particle impingement (on the aircraft surface) investigation via molecular dynamic technique.
The principal idea of this work is to adequately ascribe certain macroscopic characteristics of a water nanoparticle. No doubt, these characteristics may significantly differ from those indicated in physical reference books for bulk materials.

Molecular dynamics simulation

Throughout the simulation works in this paper, a molecular dynamics (MD) technique was adopted and based on the classical Newtonian mechanics. Assuming a potential interaction among particles (atoms or molecules), the equations of motion are numerically integrated to trace the particle motions. In the first part of this work monatomic model with the well-known symmetrical Lennard-Jones (LJ) two-body interaction, for the particle diameter, being appropriately chosen, various time- and volume averaged fluid properties can be investigated. When necessary, more elaborated interaction models (e.g., more complex molecular potential, a rigid rotor with partial charges on interaction sites for water [4-5]) could be utilized. In the second part of this work a new model of water molecules interaction is proposed. A system of 12 (N–1) equations describes self organization and the behavior of water molecule in a presence of other molecules. A preliminary numerical experiment showed an appearance of organized structures – water clusters from a water molecular chaos [6].
Potential energy of pair interaction $U(r)$ can be represented as a sum of orientation, induction, dipole interaction energy and also a repulsion interaction energy:

$$U_{\text{or}}(r) = -\frac{p_e^4}{24\pi^2\varepsilon_0^2 kT}\frac{1}{r^6}; \qquad U_{\text{ind}}(r) = -\frac{\alpha p_e^2}{8\pi^2\varepsilon_0^2}\frac{1}{r^6}; \qquad U_{\text{disp}}(r) = -\frac{e^4 h\nu_0}{32\pi^2\varepsilon_0^2 a^2}\frac{1}{r^6}; \qquad U_{\text{rep}}(r) \sim \frac{1}{r^{12}};$$

$$U(r) = U_{\text{or}}(r) + U_{\text{ind}}(r) + U_{\text{disp}}(r) + U_{\text{rep}}(r).$$

Here $\nu_0 = \frac{1}{2\pi}\sqrt{\frac{a}{m}}$ – atom-oscillator frequency, a – coefficient of proportionality, α – is molecular polarizability, ε_0, k and h – electrical, Boltzmann and Plank constants respectively, T – is a particle temperature, p_e – dipole momentum, r – is a distance between centers of inertia of two molecules.

A system of molecular dynamic equations of $i^{\text{-th}}$ water molecule is as follows:

$$m_0 \frac{\mathrm{d}\boldsymbol{V}^i}{\mathrm{d}t} = \sum_{j=1}^{N_{\mathrm{H_2O}}} \left\{ -\nabla U^{ij}_{\mathrm{H_2O}} \right\} + \sum_{k=1}^{N_{\mathrm{Air}}} \left\{ -\nabla U^{ik}_{\mathrm{H_2O\text{-}Air}} \right\} + \sum_{m=1}^{N_{\mathrm{Wall}}} \left\{ -\nabla U^{im}_{\mathrm{H_2O\text{-}Wall}} \right\} + m_0 \boldsymbol{g} + \boldsymbol{F}_{\mathrm{dis}}$$

The first, the second and the third components of equation are forces which act on i^{th} molecules from other water molecules, from air molecules and from molecules of the surface respectively. Via integration along the aircraft surface and into its depth, a new potential of the molecule – surface interaction is proposed and used in order to investigate impinged water particles and droplets behavior. The last component F_{dis} describes the energy dissipation of the molecule which could exist. It wasn't taken in account in this work. The last but one component is a force of gravity.

The wall temperature was defined via thermal quantum oscillation of the atoms of the aircraft's surface aluminum crystal lattice. It was possible to estimate characteristic frequencies and amplitudes of atoms of nanostructured hydrophobic material for the aircraft surface.

Simulation conditions

A liquid particle consisting of 50 ÷ 15000 molecules was generated and equilibratedt at various temperatures close to the temperature of flying vehicle in an aerosol flow. The system is a cubic region; symmetrical boundary conditions for molecules were set for all horizontal and top directions. The characteristic size of a cubic region is by one-two orders higher than the characteristic size of nanoparticle. On the bottom of a cubic cell a wall boundary condition was set.

Maxwell velocity distribution function was used for molecules velocities in order to define a drop temperature. Onto the bottom wall, the water nanoparticle was impinged at various angles with various mass centre initial speeds V_{imp} of nanoparticle from a fixed position. During the simulation water molecular radial distribution of velocity distribution function, density, temperature and pressure were controlled. The temperature was controlled as an average thermal kinetic energy of molecules in a reference frame connected with the inertial center of nanoparticle. Calculating the speed of the inertial center of a nanoparticle, it was assumed that a molecule belongs to a particle if this molecule situated in the area, where drop density more than 10 kg/m^3. An original numerical algorithm of pressure calculation is proposed and used in this simulation. Of cource, these parameters should depend on the dimension of molecular cluster – nanoparticle. For example, the well-known Tolman's formula [7] for $\sigma(r)$ may be regarded as an attempt to reveal such a dependence.

Various combinations of impinging speed, impinging angles, temperature and intensity of wall interaction are examined. There could be two relevant factors [2] in choosing V_{imp}. One is the Reynolds number $\mathrm{Re} = \rho V_{\mathrm{imp}} a_d / \mu_{\mathrm{H_2O}}$ which indicates the effect of viscosity. The other is the Weber number defined as $\mathrm{We} = \rho V_{\mathrm{imp}}^2 a_d / \sigma$, which shows how the effective surface tension affects the system. Fluids with the same Re and We are expected to show a similar behavior. However, in the case of nanoscale droplet impingement, the surface tension has a much more relevant effect, so one can choose V_{imp} which gives similar We to the real systems.

Droplet impingement

Ice accretion is a problem in aerospace science and industry. However its applications have been expand to various areas, such as inkjet printing technology, fabrication of electronic devices and biomaterials [2]. Although the technology to generate and impinge pico-liter (~10 nm in diameter) droplets with sufficient precision is well established, it is highly required to manage the behaviors of submicro- or nano- droplets and to control precisely the geometry after the impingement [2].

Numerical simulations are usually carried out with continuum hydrodynamics schemes, gas kinetic theory equation and sophisticated quantum-mechanical calculations. Well known methods of quantum chemistry cause enormous computer power to calculate a molecular configuration of a nanoparticle – a big molecular cluster. Here is a review of our recent progress in studies of droplet impingement process by MD simulation, in which the influence of governing parameters on droplet dynamics, such as wettability, impingement speed, droplet size, water, air and surface temperature, energy of surface interaction were investigated. During the impingement limiting wetting angles in addition to above described physical parameters were estimated and controlled.

In case of hydrophilic surface, the nanoparticle starts to spread after the collision, and reaches a final state, in which the shape of nanoparticle depends on the impinging speed. The initial behavior of deformation on a hydrophobic surface looks similar, but later the liquid nanoparticle bounces back.

Various quantities were defined in order to examine the water nanoparticle behavior during the impingement, such as droplet height, contact area, contact angles, direction of the liquid flux inside the liquid nanoparticle – the droplet (fig. 1). As the impingement speed V_{imp} increases, the droplet becomes more flatten, covers larger area, and leads to

more evaporation. These facts indicate that an optimum V_{imp} exists when one could apply the droplet impingement technique to thin film fabrication. On fig. 1 and fig. 2 one can see the droplet impingement on the aircraft surface.

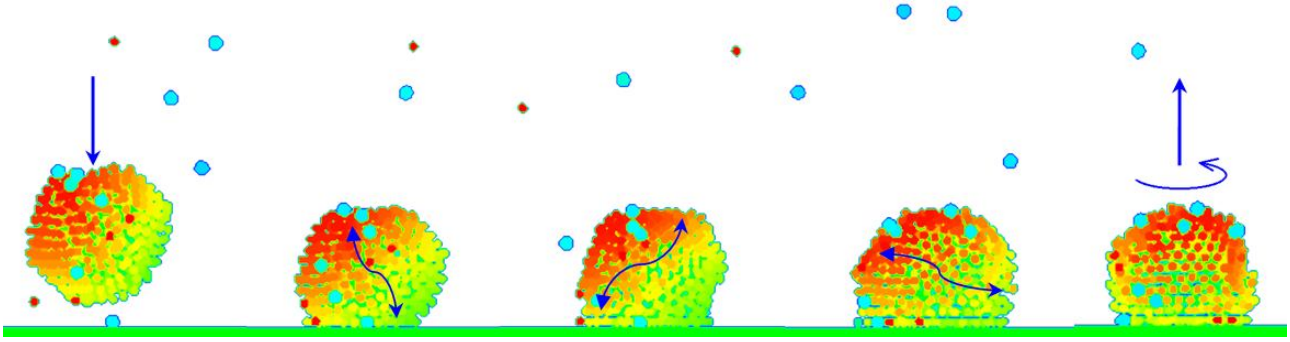

Figure 1: Water nano-particle behavior on a aircraft surface in an aerosol flow: initial stage of water accretion; Big blue circles– air molecules, other – water molecules

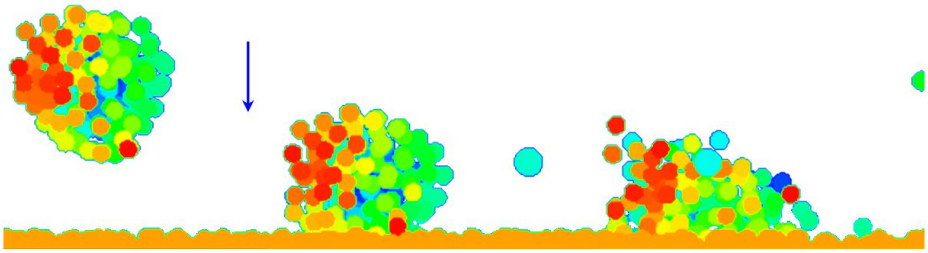

Figure 2: Water nano-particle wall-mass-heat exchange on a surface; heat crystal lattice oscillations correspond to a temperature minus 10 ^{o} C

Conclusions

This paper gives a brief review of our recent progress, showing that molecular simulations provide useful tools complementary to various experimental means in research of micro- and nanoscale particles.

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