Mathematical models of two-phase flows’ interaction with a solid body

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Abstract. Expressions for supercooled droplets’ crystallization parameters are proposed according to experimental results’ interpolation. Estimation of interphase boundary energy fluxes generation were obtained. Mathematical models of the non-spherical particles motion were developed.

1. Introduction

Experimental investigation and mathematical simulation of multiphase flow physics are essential in a wide spectrum of practical applications, in particular in a problem of aircraft icing [1–8]. Despite numerous experimental and numerical investigations, some physical peculiarities of supercooled droplets’ crystallization physics understanding as well as non-spherical particles motion simulation in non-uniform flows are not complete.

2. Supercooled droplets crystallization peculiarities’ modelling and experimental results

When supercooled water droplets in cloud impinge upon aircraft, icing may occur on surfaces, which declines the aircraft dynamic performance. Many studies have been done to explore the icing mechanism for the end purpose of improving the aircraft aviation safety.

In order to implement anticing facilities by means of turning into uncooled drops into solid ice, followed by their rebound from the surface one may estimate a characteristic distance, which would be enough for ultrasonic shaking. Note that a supercooled liquid may contain a significant amount of micro and nano ice crystals, whose presence do not change liquid properties, while shaking the crystals together to form patterned structures. The characteristic freezing time $\tau_f$ should not be longer than the characteristic time of approach droplets to the surface of the streamlined body. These times can be estimated from the following expression:

$$L_s (1 - a_m) \frac{4}{3} \frac{\rho_s}{\rho_p} \rho_p \tau_f^3 \equiv Nu 2 \alpha_m \lambda (T_f - T) = 2 \alpha_m \lambda (T_f - T) \left(2 + \frac{1}{2} \frac{\alpha_m}{\rho_s / \rho_p} \frac{1}{Re_p^2 Pr^3} \right).$$

Here $a_m$ is the radius of the microparticle (droplet), $L_s$ is the specific heat of crystallization, $Nu$ is the Nusselt number, $Re_p = 2 a_p \rho |V - V_p| / \mu$ is the Reynolds number of particle motion in a carrying gas ($V_p$ is particle’s velocity, $V$ is carrying gas velocity), $Pr$ is Prandtl number, $\rho$ and $\rho_p$ are air and water density respectively, $\alpha_m$ is ice crystals’ mass fraction (crystals appear after solidification front propagation), $\mu$ is dynamic gas viscosity, $T_f$ is temperature of freezing, $T$ is temperature of supercooled droplets. Experimental measurement of $a_m$ temperature dependence and corresponding interpolation of
experimental results one may take from [9]: \( \alpha_m(T) \approx \frac{\zeta(1-T/T_f)}{\sqrt{T/T_f}} \), where \( \zeta = (1.98 \pm 0.50) \). Since the Reynolds number \( \text{Re}_p \) of the particle motion relative to the gas is small

\[
\text{Re}_p \ll \frac{3L_a}{\tau_f \rho_p} \quad \Rightarrow \quad \frac{\text{Re}_p}{\text{Pr}} \ll \frac{1}{\tau_f} \quad \Rightarrow \quad \frac{\text{Re}_p}{\text{Pr}} \ll \frac{1}{\tau_f}.
\]

And the ratio of this time to characteristic time of a flow \( \tau_{\text{flow}} \) takes the following form:

\[
\frac{\tau_f}{\tau_{\text{flow}}} \approx \frac{3\lambda_a}{\tau_f} \left( \frac{\text{Re}_p}{\text{Pr}} \right)^{1/3} \ll 1.
\]

Here \( \text{Stk} \) is Stokes number, \( \text{Re}_0 \) is universal gas constant, \( \mu_m \) is air molar mass. This estimate shows that after the action of ultrasound and the passage of the crystallization front, a drop consisting of a mixture of crystals with water will not have time to significantly change the phase composition and solidify. Thus, the fight against icing of aircraft by ultrasonic action on supercooled droplets is problematic. The following physical parameters were accepted for the estimations: the droplet density \( \rho_p = 10^3 \) kg/m\(^3\), the specific heat of crystallization \( C_p = 0.33 \) MJ/kg, the flow velocity \( V_\infty = 100 \) m/s, the characteristic size of the streamlined body simulating the leading edge of the wing, \( R = 0.1 \) m. Estimates of the distance were made in [8], in which supercooled droplets should be subjected to ultrasonic action without taking into account the dependence of the mass fraction of ice crystals on the supercooling temperature.

A mathematical model of the stability of the supercooled state of droplets is proposed for their impact on the surface of a solid. In particular, an expression is proposed for the minimum droplet impact velocity necessary for the nucleation of crystallization, which has the following form:

\[
V_s = \sqrt{\frac{2L_a(T)}{\sigma \psi \rho}} \exp \left( -\frac{\psi \rho}{V_s^2 a_p / \sigma} \right).
\]

Here \( \psi \) is coefficient that depends on physical and chemical properties of liquid, \( \sigma \) is surface tension coefficient. Exponent index describes influence of surface tension on probability of crystallization.

In previous study [9], according to interpolation of experimental data the following expression for crystallization threshold was obtained: \( L_a(T) = L_a^0 \left( 1 - T / T_f \right)^{1/5} \); here \( L_a^0 = 4 \cdot 10^{-3} \) J/kg.

In present study, probabilities of supercooled water crystallization after mechanical influences were measured: \( p_1 \) – after one, \( p_2 \) – after two, \( p_3 \) – after more than two mechanical influences respectively. Experimental data were approximated by following equations:

\[
p_1 = \exp \left( -0.5V^2_{\text{imp}} / L_s^1 \right), \quad p_2 = 1 - \left( p_1 + p_3 \right). \quad \text{Here} \quad L_s^1 = 15 \text{ J/kg}, \quad L_s^2 = 2.5 \text{ J/kg} \quad \text{are constants.}
\]

\( K_s = 0.5V^2_{\text{imp}} / L_s^1 \) are nondimensional governing parameters.

The effect of accumulating the kinetic energy of the impact of a supercooled liquid on a solid surface, which is necessary for crystallization, is accumulated experimentally in the form of statistical diagrams which are published in previous studies. An explanation of the effect is associated with the existence of several "steps" in the investigated threshold of potential energy of intermolecular interaction.

It was previously mentioned that a process of crystallization may be accompanied with electromagnetic [10] and sound generation. To estimate the characteristic values of these energy fluxes \( q \) one may write the following energy balance equation:

\[
q \Delta S \Delta t = C \Delta m(T_f - T) - L_{is} \Delta m \alpha_m = \left( C(T_f - T) - L_{is} \alpha_m \right) \rho_f \Delta S \Delta t \quad \Rightarrow \quad q = \rho_f \left( C(T_f - T) - L_{is} \alpha_m \right).
\]
Here $\Delta m$ is element of mass, $\Delta S$ is element of area, $\Delta t$ is small interval of time, $u$ is the crystallization front velocity which depends on temperature [9], $C$ is water specific heat capacity. Here $u/u_0 = (1-T/T_f)^2$, where $u_0 = 280\pm30$ m/s.

Another approach to the calculation of radiation during a phase transition yields the following expression of the type of the Stefan boundary condition:

$$\nabla q + \lambda_u \frac{\partial T_u}{\partial n} - \lambda_s \frac{\partial T_s}{\partial n} = L_u \rho_i \alpha_i u(T)$$

Here $\lambda_u/\lambda_s = (1+\alpha_i \rho_i/\rho_s)^n$ is ratio of the coefficients of thermal conductivity of water-crystal mixture and water. The indices $l$ and $s$ mean liquid (water) and solid (ice), respectively, $n$ is normal to the interphase boundary. The first term in the last formula is the removal of the energy of phase heat by radiation. If we consider the problem of propagation of the crystallization front in the one-dimensional approximation, then the last expression takes the following form:

$$q \approx L_u \rho_i \alpha_i u \Delta X - \lambda_s \left[ (1+\alpha_i (\rho_i/\rho_s))^n - 1 \right] \left[ T_f - T \right]$$

Here $\Delta X \approx a_s - a_l = \frac{\mu_s}{N_A} \left( \frac{2}{\rho_s} - \frac{1}{\rho_i} \right) \approx 0.92 \text{ Å}$ is characteristic distance of molecules’ motion (in a process of crystallization front propagation) which is supported to be equal interphase boundary width, $m = 4$ according to experimental results’ interpolation.

The wavelength of the infrared radiation, which may take place in a process of crystallization could be estimated from the energy balance equation: $\lambda = h_P c N_A / L_v \mu \approx 20 \mu$m. Here $h_P$ and $N_A$ are Planck’s and Avogadro’s constants respectively, $c$ is the light speed.

3. Non-spherical particles’ motion modelling and experimental studies

Simulation of the nonstationary motion of bodies of complex shape in inhomogeneous media, particles of natural origin, nanodispersed flows where thermal fluctuations are significant, as well as the various effects in dusty plasmas, is of great scientific and practical interest in a wide range of fields of technology, economy, nature and life of human beings. Previous studies [9,11] demonstrate influence of particles’ shape on two-phase flow near a circumfluent body characteristics, in particular, on mass flow rate surface distribution, which is essential for aircraft icing calculation. In spite of a lot of different mathematical models for aerohydrodynamic characteristics of single non-spherical particles’ (e.g. [11,12]), simulation of the whole two-phase flow with non-spherical particles becomes problematic.

In [13], the following expression for lift force coefficient $C_L$, which acts on non-spherical particles is presented which depends on their orientation: $C_L/C_p = \sin^2 \theta \cos^2 \theta$. This formula is valid for Reynolds numbers of particle’s motion in a carrying gas up to $10^3$. In [14], authors presented a refinement of this dependence for larger values of the Reynolds number of a particle’s motion in a carrying gas

$$\frac{C_L}{C_p} = \frac{\sin^2 \theta \cos^2 \theta}{0.65 + 40 \text{Re}^{0.17}}$$

An attempt to introduce an orientational force for the two-dimensional motion of spheroids was undertaken in [9] by analogy with orientational forces in molecular dynamics [15]. For small Reynolds numbers of particles motion in a carrying media reference frame there is the following expression [8] for the force which acts on spheroids:

$$F(\text{Re},M) = F(\text{Re},\theta) = \frac{\rho \Omega^2}{2 \text{Re}_p} \left[ f_i (V - V_p) + f_z (V - V_p) \right] = 3 \pi \frac{\rho \Omega^2}{\text{Re}_p} [f_i \cos \theta + f_z \sin \theta].$$
Here $\theta$ is angle that characterizes non-spherical particle's orientation towards circumfluent flow, $f_\parallel$ and $f_\perp$ is force components [12]. Average force, which acts on spheroid, could be calculated from the following equation:

$$
\frac{\langle F(Re) \rangle}{3\pi (\mu/\rho) Re_p} = \frac{2}{\pi} \int_0^{\pi} \left[ f_\parallel^2 \cos^2 \theta + f_\perp^2 \sin^2 \theta \right] \sin \theta \, d\theta = \frac{1}{2} \left[ f_\parallel^2 \right] - 1 = \frac{2}{\pi} \left[ f_\parallel \right] \sqrt{1 + \epsilon^2 x^2} \int_{-1}^1 x^2 \, dx = f_x.
$$

Depending on $\epsilon$, the integral was take numerically and approximated by the following expression:

$$
I(\epsilon) = \frac{2}{\pi} \left[ f_\parallel^2 \right] - 1 \int_{-1}^1 \left[ 1 + \epsilon^2 x^2 \right] \, dx = 1 + 0.0072 \epsilon^4 - 0.07 \epsilon^3 + 0.2829 \epsilon^2 - 0.0043 \epsilon - 0.0009.
$$

Mean-deviation square from the mean average force is as follows:

$$
\frac{F_x}{|F_{\text{Stk}}|} = \frac{2}{\pi} \left[ f_\parallel^2 \right] - 1 \int_{-1}^1 \left[ f_\parallel^2 \cos^2 \theta + f_\perp^2 \sin^2 \theta \right] \sin \theta \, d\theta = \frac{1}{2} \left[ f_\parallel^2 \right] - 1 = \phi, \quad \text{Re}_p < 1.
$$

For higher Reynolds numbers the following expression is proposed to be used for orientational force calculation: $F_x^{\text{Re}_p > 0.1} = F_x C_D / C_{\text{Stk}}$. Here $C_D$ is drag coefficient (one may find models of $C_D$ in [8]), which depend on Reynolds and Mach numbers, $C_{\text{Stk}}^{\text{Stk}} = 24 / \text{Re}_p$ is Stokes drag coefficient.

### Table 1. Dimensionless parameters of non-spherical particles

| Physical quantity | Non-dimensional expression |
|-------------------|---------------------------|
| **Orientational force** | $F_x / F_{\text{Stk}} = \phi$ |
| **Scattering coefficient** | $S = \phi \rho / \mu \sqrt{\frac{F_x}{\rho} \sqrt{3\pi Re_x \phi}}$ |
| **Velocity** | $V_x / V_e = \frac{L}{a_p} \sqrt{\frac{\rho}{\rho_p} \phi \left( \frac{243}{16} \right)^{1/6}}$ |
| **Length** | $A_x = \frac{1}{\rho_p} \sqrt{\frac{\rho}{\rho_p} \phi \left( \frac{243}{16} \right)^{1/6}}$ |
| **Frequency** | $O_x / V_e = \frac{1}{a_p} \sqrt{\frac{\rho}{\rho_p} \phi \left( \frac{3}{4\pi} \right)^{1/6}}$ |
| **Stabilization coefficient** | $\delta_x / \rho V_e = \frac{1}{\rho \phi \left( \frac{3}{4\pi} \right)^{1/6}}$ |
| **Pressure** | $P_x / \rho V_e^2 = \frac{1}{\rho \phi \left( \frac{3}{4\pi} \right)^{1/6}}$ |

The complexity of mathematical modeling of nonstationary dynamics of multiple bodies in inhomogeneous flows and the pronounced probabilistic nature of their trajectories in gradient media under experimental investigation dictated the construction of new approaches in mathematical and numerical simulation of the dynamics of chaotic clouds of bodies of complex shapes. The equation for the change in the chaotic energy $W_x$ of non-spherical particles under the assumption that there are no phase transitions and temperature non-equilibrium is the following:
The first term in the right describes the production of chaotic energy, the second one describes the dissipation of this energy. Table 1 illustrates the calculated parameters of the gas (chaos) of non-spherical ice particles in inhomogeneous flows in a dimensionless form. In the stationary flow, integrating along the deterministic trajectories of the particles, one can rewrite the equation of energy transfer of chaos in the following form:

\[
\frac{\partial W}{\partial t} + (V - V_p) \nabla W = \frac{F_x \cdot V_x}{m_p} - \Gamma V \cdot V - V_p .
\]

Expressing the first term in terms of the Stokes number \( \text{Stk} = \frac{2\rho_p V^2}{9\mu h} a^2 \), one has an expression for the dimensionless parameter that characterizes the increase in the velocity of chaotic motion of particles (referred to the characteristic flow velocity \( V_\infty \)):

\[
\frac{dV}{ds} = a = \frac{\varphi}{\text{Stk}} \left( 1 - \frac{1}{3} \left( \frac{3}{4\pi} \right)^{1/6} \sqrt{\frac{\rho_p}{\rho}} \frac{\varphi}{\varphi} \right).
\]

According to this model, the motion of a non-spherical particle is stable when \( \frac{\rho_p}{\rho} > 3^{3/5} \sqrt{36\pi} \approx 14.51 \). Here \( h \) is characteristic length scale.

4. Conclusion

Estimations of a distance where supercooled droplets should be crystallized in order to make them solid before circumfluent body impingement were obtained. An effect of accumulating kinetic energy which is necessary for supercooled metastable liquid crystallization was revealed and presented in a form of experimental data interpolation expressions. A possible explanation of the effect was given. An expression for orientational force which acts on spheroidal article was derived. Mathematical model of non-spherical particles’ stochastic motion was proposed. Non-spherical particles’ chaos (gas) parameters were determined and represented in corresponding table. Experimental results of spheroidal particles’ scattering in a gravity field were obtained.

Acknowledgements

The work is supported by Russian Fund for Basic Research (project No 18-31-00485).

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