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Quasi-molecular modeling of a single supercooled large droplet impact

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ABSTRACT

A mesoscale model for droplet dynamics based on a quasi-molecular approach is proposed. It considers the interaction between quasi-molecules within a single liquid droplet, each quasi-molecule representing an agglomeration of a large number of actual water molecules. The goal is to improve the understanding of the dynamics of large droplet collisions over dry or wet surfaces at velocities typical of aeronautical applications. This detailed analysis will eventually be used to refine the macroscopic Eulerian description of the water impingement process by providing numerical correlations for splashing and bouncing phenomena relevant for in-flight icing applications. Based on the Equipartition Theorem, approaches for extracting macroscopic quantities such as temperature and transport coefficients from the quasi-molecular method are discussed. A proper choice of the free parameters of the model that leads to accurate values of the macroscopic properties is also addressed.

1. Introduction

In-flight ice accretion occurs on aircraft flying in clouds of supercooled water droplets. The performance degradation resulting from the contamination of aircraft surfaces can quickly become severe enough to cause incidents and accidents. Considerable loss in controllability and maneuverability has been reported as a result of icing conditions where the water droplets had diameters in the range of 50–400 μm (labeled as Supercooled Large Droplets, SLD) [1,2]. Depending on the flight conditions, SLD impacting on a solid surface are subject to a range of dynamic phenomena, such as sticking, splashing, break-up, partial or complete rebound, and deposition or spreading [3]. These phenomena make the impingement process of SLD much more complex than for smaller droplets. These large supercooled droplets may in fact result in water deposition well beyond the limits of Ice Protection Systems (IPS) that have been duly certified under the non-SLD Appendix C rules, resulting in hazardous in-flight conditions. Only recently, transport authorities have re-defined the requirements of the icing certification process by introducing the Appendix O to explicitly account for SLD environments [4].

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Most current SLD droplet dynamics data is based on empirical correlations, which are neither comprehensive nor detailed, because of the difficulty in studying these phenomena in experimental facilities under controlled conditions. Thus, there is a definite need to delve into the droplet dynamics, on a fine scale, in order to model them in a more general way and implant such models within the Lagrangian or Eulerian droplet impingement codes used to calculate impingement limits and ice shapes.

The aim of the present study is to formulate and propose a numerical model for droplet dynamics that will eventually produce numerical correlations for the SLD dynamics in order to provide accurate ratios of ejected to deposited water and the post-impact droplet diameter distribution and velocity vectors in three dimensions. The modeling of splashing, bouncing and break-up can be recast as a problem of tracking the deforming droplet boundary as the droplet interacts with a solid surface. Several numerical approaches have been proposed in the literature to address this problem, two of the most popular ones being the Volume of Fluid (VOF) and the Level Set methods. The VOF method [5,6] solves an advection equation for a volume fraction function that separates the liquid and gaseous phases. The Level Set method [7] implicitly describes the interface as the zero level set of an interface function which evolves in time according to a transport equation. When modeling the dynamics of the droplets under typical in-flight conditions, i.e. with velocities exceeding 100 m/s, these two methods for interface tracking encounter difficulties in mass conservation and smooth curvature prediction. They also require mesh refinement and very small time steps. Therefore, the studies using these methodologies have considered in most cases low-speed impact problems.

Studying droplet dynamics from a molecular point of view bears the advantage that water mass conservation is assured at all speeds and large deformations. Furthermore, there is no limitation on the particle displacement or surface tension magnitude. Also, using an equation to predict the surface tension is not required in a molecular method because this is already included as an intrinsic property in the effective interaction potentials between the molecules. The Molecular Dynamics (MD) approach permits a very detailed and precise description of the physics of the problem. Nevertheless, due to the high computational effort required by MD, the number of molecules that can be simulated is not large enough to accurately study SLD impact dynamics. In addition very small time steps are needed, in the order of 1 ps (10^{-12} s) and smaller. A typical SLD case consists of 10^{16}–10^{18} molecules simulated up to hundreds of milliseconds. In one of the largest MD simulations up to the date [8], 4.125×10^{12} molecules have been simulated on 146,016 cores with one time step taking roughly about 40 s. This means that with the current computational resources, MD modeling of a typical SLD dynamics case is hardly feasible. Another particle-based approach is the Smoothed Particle Hydrodynamics (SPH) [9-11]. SPH is a Lagrangian meshless particle method that approximates the quasi-incompressible Navier–Stokes equations. The equations of motion of the particles are determined from the continuum equations of fluid dynamics by interpolation from the particles. Although the SPH method is suitable for handling problems involving free surfaces and large deformations such as high velocity droplet impact, it suffers from the tensile instability leading to an unphysical clustering of particles [12]. This may eventually result in numerical instability during the droplet dynamics simulation. The methodology is still under development in terms of the pressure correction term, boundary treatment, surface tension models, and stability issues [13]. An interesting alternative to both MD and SPH is the Quasi-Molecular Dynamics approach (QMD) [14]. It has the advantages of MD in terms of physical representation but mitigates the computational cost by breaking down the water droplet into aggregates of large numbers of molecules, labeled quasi-molecules and by computing the constants in the equations of the interaction forces between the particles just once at the beginning of the simulation; the same equations for the interaction forces apply between the quasi-molecules during the entire droplet impingement process. Furthermore, in comparison to the SPH, QMD does not suffer from instability issues and does not require an additional equation to model surface tension.

Abdollahi et al. [15] previously extended the QMD application to the SLD impingement modeling on solid and liquid surfaces. The droplet shape and crown size were compared with the data in the literature to investigate the feasibility of employing the QMD for modeling a high speed droplet impact problem. The current study aims to improve these results by introducing a methodology to identify the optimum choice of the free parameters of the model that best represent the macroscopic properties of different materials. To this aim, a method for computing temperature and macroscopic transport coefficients from quasi-molecular data is considered following the Equipartition Theorem. Also, the computational efficiency has been improved to enable using more particles to reach a more detailed analysis of the impingement phenomenon. In the following sections, the quasi-molecular approach is briefly introduced, the methods to compute the macroscopic properties and the free variables of the model are proposed and the computational strategies are described. Finally, QMD results are compared to other numerical and/or published experimental data for the droplet impact problem.

2. Numerical methodology

QMD was originally introduced by Greenspan [14,16-18] in an attempt to bridge the gap between atomistic models and continuum approaches where the gaseous, liquid and solid phases are represented by a collection of “quasi-molecules”, each being an agglomeration of a large number of actual molecules. This method can be applied to study both steady and unsteady problems. Until now, the QMD has been applied to model droplet dynamics problems such as the pendant drop formation on a graphite solid surface and drop fall phenomena [18-20], two-dimensional very low-speed falling droplet impacts on both smooth and rough surfaces [21], and droplet–droplet collision dynamics [22,23]. The key to the QMD approach is the definition of the interaction potential energy between the particles. The particles dynamics is described by computing potential forces between particles according to this assumed potential energy and by solving Newton’s equations of motion for each particle. Greenspan