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Mass transfer mechanisms of rotary atomization: A numerical study using the moving particle semi-implicit method

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ABSTRACT

A particle-based meshless method, the moving particle semi-implicit (MPS) method, is employed in this study to simulate the process of liquid film breakup and atomization in a rotary atomizer. The computational framework incorporates a specially designed inlet flow model, a centrifugal force calculation, and a surface tension model to allow the simulation of the unsteady flow with extreme deformations. To improve efficiency, the searching algorithm of the MPS method is modified by eliminating redundant calculations. The computational framework is further utilized to systematically study the transition of the liquid from the bulk phase to a film, then to multiple belts, and finally to numerous droplets under the low pressure and flow rate conditions in the rotary atomization. Key mass transfer mechanisms underlying the atomization process are elucidated by a comprehensive analysis of the flow trajectories. The computational work is expected to improve the fundamental understanding of the rotary atomization process and facilitate future process optimization efforts.

1. Introduction

The atomization of liquids is a process of significant importance to many branches of industry. For example, a perfume needs to be atomized before use for best results; a fuel needs to be atomized before burning to enhance efficiency and reduce emission; in 3D printing, the fine powders (e.g. metal powders) may also be produced by atomization. Other applications of the atomization include the bubble atomizer, medical spraying agent, and spray coating of materials.

A liquid can be atomized in many different ways, e.g. by high-speed collision, air dynamic friction, sonic oscillation, and centrifugal forces etc. The collision-based atomization is widely used in liquid rocket engines, where a jet of fuel and a jet of oxygen are pressurized to collide at high speeds to allow high-quality mixture and atomization. The air dynamic atomizer breaks the liquid up by using the high-speed friction between the liquid and air. The ultrasonic atomizer is extensively used in humidifiers and some medical apparatuses, where the liquid is broken up under electronically induced high-frequency vibrations.

The present study aims to reveal the fundamental mechanisms of the rotary atomization using a meshless computational approach. In the rotary atomization process, the liquid is driven by centrifugal forces to go through a nozzle. During this process, the liquid is first stretched into a conical film, which then breaks into multiple belts and finally, to numerous droplets. To enable such a transition process, the centrifugal force must be large enough to overcome the surface tension, which can be very significant due to the large surface area of the ultra-fine droplets. Such anatomization process has been previously investigated by a variety of theoretical, experimental and computational fluid dynamics methods. For example, Couto et al. [1] proposed a theoretical approach to estimate the droplets' mean diameter based on a hypothesis on the thickness of a planar, disintegrating liquid sheet. By performing experiments in quiescent air conditions, Marchione et al. [2] systematically studied the size distribution of the droplets, the velocity profiles, and the cone angle of the spray as functions of time. In addition, a large number of experimental studies [3–8] have been devoted to investigating the performance of the liquid atomization by evaluating the cone angle and the droplets' size distribution using methods including the particle image velocimetry (PIV) [9–12].

Compared with the extensive theoretical and experimental explorations in the rotary atomization, numerical investigations

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Nomenclature

A	parameter of nozzle geometry	r_c	radius of the nozzle
d	dimension	w, w^{st1}, w^{st2}	Kernel functions
g	gravity acceleration/m·s^{-2}	α	angle of the cone
K	curvature	γ	surface tension force
Ks	increasing rate of the speed up ratio	Δ	dirac function
l_0	initial distance for neighboring particles	Δt, $\Delta t_{\max}$	time step/s
n^0	constant for particle number density	θ	Corresponding angle for unit surface
n^*	estimated particle number density	μ	coefficient of kinetic viscosity
n^{st1}, n^{st2}	new particles number densities	ξ	inlet area
P	pressure/Pa	ρ	density/kg·m^{-3}
r_e	cut off radius for particle interaction	Σ	surface tension coefficient/N·m^{-1}
$\mathbf{r}_i$, $\mathbf{r}_j$	position of particles	ϕ	scalar quantity
r_m	radius of the hollow cone	φ	nozzle coefficient

[13,14] have been quite limited, mainly due to the fact that classical mesh-based numerical methods can hardly handle the large deformation of the liquid from the bulk phase to hundreds and even thousands of discrete droplets. The breaking of the liquid into droplets poses great challenges to the mesh-based methods, particularly in simulating the interaction between unlinked domains. Among the few existing numerical investigations, the methods or tools that were used include OpenFOAM [15], large eddy simulation [16], boundary element method [17,18] and VOF [19]. Making a general survey of their important contributions, we could found that most of these methods are mesh-based, and they trace the free surfaces in the entire flow field by calculating certain parameters on the mesh. Nevertheless, the mesh usually does not match the exact shape of the free surfaces, leading to low accuracy and low efficiency, especially for unsteady flow. Moreover, none of these mesh-based methods could be used to simulate the atomization process directly; the calculations often build upon certain pre-calculation and/or mesh adjustment, which are complex and time consuming. Due to the limitations, these studies have hardly been able to present the full physical process of the bulk-film-belt-droplet transition and discuss the underlying mechanisms in detail.

In view of these challenges associated with the previous methods, this study employs a particle-based meshless approach, i.e. the moving particle semi-implicit (MPS) method [20–22], to simulate the rotary atomization process. Using discrete particles to model continuum fluids, the MPS method is particularly suitable for simulating the atomization process involving complex unsteady flow of arbitrarily large deformations. The computational framework is improved by incorporating a specially designed inlet flow model, a centrifugal force model, and a surface tension model to allow the simulation of the unsteady flow with extreme deformations. Using the computational framework, this study systematically investigates the rotary atomization process [23,24]. Key mass transfer mechanisms underlying the atomization process are revealed by using the stained method and the trajectory tracing method.

2. Moving particle semi-implicit (MPS) method

In the MPS method, the computational cell is discretized with numerous identical particles, and the interaction between any two particles within a cutoff distance is governed by a kernel function. The governing equations for incompressible fluids include a gradient model, a Laplacian model, and an incompressible model, which can be further converted into a Poisson's Equation with pressure as the unknown. By solving this equation at any time step, the pressure, velocity, and position for each of the particles are updated, based on which the next step of calculation is conducted.

2.1. Governing equations

The mass and momentum conservation for an incompressible flow are formulated as follows:

$$\frac{D\rho}{Dt} + \rho\nabla\cdot\mathbf{u} = 0 \tag{1}$$

$$\rho\frac{D\mathbf{u}}{Dt} = -\nabla p + \mu\nabla^2\mathbf{u} + \rho\mathbf{g} \tag{2}$$

where $\mathbf{u}$, p, ρ, μ, $\mathbf{g}$ are the velocity vector, pressure, density, viscosity of the fluid and acceleration of gravity, respectively.

2.2. Particle interaction model

The kernel function (or weight function) is defined as:

$$w(r) = \begin{cases} \frac{r_e}{r} - 1 & r < r_e \\ 0 & r \geqslant r_e \end{cases} \tag{3}$$

where $r = |\mathbf{r}_j - \mathbf{r}_i|$ is the distance between the i_{th} and j_{th} particles. The cutoff distance r_e is chosen to be the 2.1 times the averaged distance between the nearest neighboring particles in the initial configuration (l_0). Therefore, the particle number density in the MPS method which is similar to the density in general physics is defined as

$$n_i = \sum_{j\neq i} w(r) \tag{4}$$

The particle density n^0 remains a constant when the particle is inside the incompressible fluid.

2.3. Gradient and Laplacian models

For any scalar variable ϕ, the gradient and Laplacian models can be written in the form of [25]:

$$\langle\nabla\phi\rangle_i = \frac{d}{n^0}\sum_{j\neq i}\frac{\phi_j - \phi_i}{|\mathbf{r}_j - \mathbf{r}_i|^2}(\mathbf{r}_j - \mathbf{r}_i)w(|\mathbf{r}_j - \mathbf{r}_i|) \tag{5}$$

$$\langle\nabla^2\phi\rangle_i = \frac{2d}{n^0}\sum_{j\neq i}\frac{\phi_j - \phi_i}{|\mathbf{r}_j - \mathbf{r}_i|^2}w(|\mathbf{r}_j - \mathbf{r}_i|) \tag{6}$$

where $d = 3$ for a three-dimensional problem. Temporal velocities and positions of the particles are obtained by solving the governing equations. Then, the temporal particle number density n_i^* is calculated explicitly by adding the action of external forces, for example the gravity. In order to reinforce the incompressible condition, n_i^* needs to be corrected back to n^0. The gradient and Laplacian models