Numerical simulation of a two-component jet atomization

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Abstract. Numerical modelling of the breakup of a jet consisting of two immiscible liquids outflowing into the atmosphere has been carried out. For this, the modified three-fluid VOF method has been implemented in the Basilisk open-source package. The jet outflows from a swirl nozzle, in which the liquids are mixed. The mixing of liquids in a swirl nozzle is investigated. The fields of velocities and mass fractions of the components, as well as the size distribution of droplets, are obtained. It is shown that the distribution of droplets in the outer region of the flow is non-uniform as a result of insufficient mixing inside the nozzle.

1 Introduction

Spraying is often modelled as a two-stage process. During the primary breakup, the liquid exiting the spray nozzle outlet breaks up into droplets due to the instability that develops on the surface of the liquid. Instability can be caused by shear stress due to interaction with the surrounding atmosphere (Kelvin-Helmholtz instability) or normal stress (Rayleigh-Taylor non-stability). The formed droplets undergo further breakup with the formation of even smaller droplets as a result of secondary atomization.

Secondary breakup plays a significant role in many practical applications, such as fuel flow atomization in diesel and gasoline engines. Several widely-used simplified computational models, such as the TAB model or the Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) atomization model, have been developed based on insights obtained from secondary breakup studies. The secondary breakup of commonly used liquids, such as water or kerosene, serves as a useful test case for numerical models.

Water can be found in fuel in three forms: dissolved in the fuel, as water-in-fuel emulsions, or as free water. Dissolved water is invisible to the naked eye and is considered a component of jet fuel that vaporizes during combustion. Suspended water appears as a dull, hazy, or cloudy appearance that takes time to coalesce or settle down. Free water, being denser than fuel, forms a separate layer at the bottom of fuel tanks. Water-in-fuel emulsions and free water are regarded as fuel contaminants and are controlled through rigorous quality control measures.

Previously, numerical simulation of the breakup of a swirling jet in a stationary atmosphere was performed [1]. The simulation was carried out by numerical solution of the Navier-Stokes equations using the Basilisk open-source code package (www.basilisk.fr). The interfacial surface was tracked using the VOF method. To account for non-resolved small-scale velocity fluctuations, the LES method was used according with Vreman subgrid-scale model [2].

Fig. 1. Atomization of a swirling jet.

It is shown that on the axis of symmetry near the nozzle outlet from which the swirling jet flows out, a clearly defined recirculation zone free of liquid is formed. The grid convergence was studied up to a cell size of 6 μm and it was shown that the droplet size distributions are significantly different for different grid resolutions, even for large droplets. This indicates that the scales associated with the interface are extremely sensitive to the size of the computational cells. In other words, even the resolution of the Kolmogorov scale does not guarantee absolute convergence in droplet sizes due to interface effects. These effects are especially noticeable in problems with thin liquid layers, which take place during the outflow of swirling jets.

In the present work, a test simulation of the atomization of a two-component jet consisting of immiscible liquids (water, oil) was performed. For this purpose, a three-fluid fluid flow model based on the
Navier-Stokes equations and the VOF method was developed and implemented in the Basilisk package.

2 Numerical methods

To simulate the jet flow, we used the Basilisk open-source code (www.basilisk.fr), which numerically solve the Navier-Stokes equations in conjunction with the VOF method.

2.1 Governing equations

Simulation is carried out of the incompressible Navier-Stokes equations, supplemented by the equation for the liquid content:

\[
\rho \left( \frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} \right) = \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + f_s
\]

\[
\frac{\partial u_i}{\partial x_i} = 0
\]

where \( \rho \), \( u_i \) and \( x_i \) represent the mixture density, velocity components and coordinates, respectively; \( t \) is time variable; \( p \) is pressure; \( \mu \) is dynamic viscosity.

The viscous stress tensor is defined as:

\[
\sigma_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

The surface tension force \( f_s \) is based on the CSF model [3]. The model assumes the existence of separate interface for each phase and the existence of independent surface tension forces that are summed up at the contact of any two phases:

\[
f_s = (\sigma_{ij} \kappa_{1j} + \sigma_{ij} \kappa_{2j} + \sigma_{ij} \kappa_{3j}) \delta \cdot n_s
\]

The Dirac function \( \delta \cdot n_s \) is assumed non-zero only at the liquid-gas or liquid-liquid interface. The surface-tension coefficient, curvature, and normal to the interface are denoted as \( \sigma \), \( \kappa_3 \), \( -\nabla \cdot n_s \), and \( n_s = \nabla c_i / |\nabla c_i| \), respectively. The indexes show the relation to the corresponding liquid. At the interface between liquid 1 and liquid 2, the following relation is fulfilled: \( \kappa_1 = -\kappa_2 \) and \( \kappa_3 = 0 \).

In the context of the three-fluid formulation for multiphase flows, three different phases are distinguished by the values of characteristic function \( c_i(x, t) \), whose time evolution satisfies the following transport equation:

\[
\frac{\partial c_i}{\partial t} + u_j \frac{\partial c_i}{\partial x_j} = 0, \quad i=1,2
\]

The physical properties of the mixture depend on the characteristic function:

\[
\rho = c_1 \rho_1 + c_2 \rho_2 + (1-c_1-c_2) \rho_3
\]

\[
\mu = c_1 \mu_1 + c_2 \mu_2 + (1-c_1-c_2) \mu_3
\]

Equations are discretized and solved using the open-source continuum dynamics simulation code Basilisk [4, 5, 6] with a momentum conserving scheme (MCVOF) [7]. The computations were performed using finite-volume discretization with the second order central-difference schemes for space derivatives and the second order implicit time derivative scheme.

2.2 Computational domain

Dimensionless variables were used in the calculation. Thus, when calculating the properties of liquids and gases, dimensionless quantities were used: the Reynolds number \( Re = 500 \) and the Weber number \( We = 50 \). The computational domain is a cube with a side of 3. A vortex nozzle is placed close to the left boundary of the computational domain, which has a length of 0.7. The nozzle is shown in Figure 2.

The densities of the liquids were equal to 1, while the gas density was 1/1000. The dynamic viscosity of the liquid was calculated based on the given Reynolds number and was \( 4 \times 10^{-4} \). Similarly, the dynamic viscosity of the gas was calculated and was \( 4 \times 10^{-7} \). The surface tension coefficient was calculated using the Weber number and was \( 4 \times 10^{-3} \) for liquids and \( 4 \times 10^{-6} \) for the gas.

![Fig. 2. Vortex nozzle.](image)

The jet flows out through a hole with a diameter of 0.1 into the air atmosphere from a vortex nozzle, in which interaction and swirling of fluid flows (water, kerosene) take place.

2.3 Boundary conditions

Two one-component jets flow out of the left domain boundary through the holes 0.2 in diameter with fixed velocities of 1. The inlets are connected tangentially to the internal chamber of the nozzle. Thus, a swirling flow is organized inside the nozzle. The jets enter the mixing chamber in the vortex nozzle, as shown in Figure 3.

On the right boundary of the computational, the condition of constant static pressure equal to zero is set.
At all other boundaries, the conditions of zero gradient for pressure, volume fractions, and velocity fields are set.

For the solid boundaries the immersed boundary method was used. The boundary was defined as a null isosurface of distance field to the 3D model. The 3D model was composed of connected triangles stored in .stl file format. The distance field was calculated as a distance to the closest triangle. The distance to the triangle was defined as a distance to its closest element (edge, vertex, or face). The attractive feature of such representation is the lack of need to manually create a geometry-capturing computational mesh.

**2.4 Mesh refinement**

Spatial discretization of the computational domain is performed using cubic cells. The grid is adaptively refined by hierarchical splitting of each cell into 8 equal cells of half-size, using a special algorithm that estimates the local error in the approximation of the gradients of the calculated values. The refinement procedure is repeated dynamically at each time step of the simulation thus ensuring the local fine-resolution criteria. The minimum achieved cell size corresponds to 0.012 in dimensionless units. The maximum refinement level may be specified depending on the computed distance to the solid model.

**3 Results**

Using the implemented model, the simulation of the outflow of a two-component jet into the air atmosphere was performed. Figure 4 shows that near the nozzle the jet consists of two parts of unmixed liquids. Further downstream, as a result of instability, the jet breaks up first into ligaments, and then into droplets of various sizes. It can also be seen that the droplets of different liquids are unevenly distributed over the volume, which is apparently due to insufficient mixing of liquids in the nozzle. The periodic zones of different liquids are observed in the far field of the flow.

Figure 5 shows how the liquid is mixed inside the nozzle. It can be seen that there are large areas containing only one type of liquid. Of course, this effect will depend on dimensionless outflow parameters such as Reynolds number and Weber number. In addition, the quality of the computational grid can also affect the mixing of the fluid. Further research will be focused on these aspects. The current study is intended to demonstrate the performance of a three-fluid model for simulating the outflow of a two-component jet together with solid boundaries defined by immersed boundaries method on a rectangular grid with dynamic mesh refinement.
liquids from the nozzle occurs in the form of twisted helical bundles, which then break up in the external environment.

4 Conclusion

A three-fluid model was developed and implemented in the open-source Basilisk code to simulate the outflow of a two-component jet into the air atmosphere from the solid nozzle defined by immersed boundary method. The model is based on the creation of an interface for each phase and the existence of independent surface tension forces that are summed up at the contact of any two phases.

During the simulation two jets of different fluids are mixed inside the swirl nozzle forming helical vortex structures. Which then flow out through the nozzle outlet and undergo the primary atomization into droplets.

It is shown that the droplets in the outer region of the jet are unevenly distributed due to insufficient mixing of the liquids inside the nozzle. Changing the outflow parameters (Reynolds number, Weber number) can change the nature of mixing and make the distribution of droplets more uniform.

The study was funded by the Russian Science Foundation grant No. 22-79-10246.

References