Simulation of the liquid fuel spraying based on Eulerian-Lagrangian model

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Abstract. The paper presents test results of the method for numerical simulation of liquid fuel spraying based on the Eulerian-Lagrangian model. This model describes the fluid flow inside the injector and directly behind it using the Euler-VOF method, while the dispersed medium (droplets) formed at a certain distance from the injector is described using the Lagrange approach. When using the VOF (volume of fluid method), the dynamical adjustment of the calculation grid at the phase interface is applied. Turbulence is modeled by the large eddy simulation (LES) method. The research results were compared with the data of direct numerical simulation (DNS) [1]. The calculation results based on the Eulerian-Lagrangian model show an acceptable agreement with the data of direct numerical simulation in terms of the main characteristics of the spraying. Thus, the structure of the two-phase flow, the parameters, and shape of the drops, as well as the speed and direction of their movement are determined qualitatively correctly.

1. Introduction

Liquid spraying is widely used in modern technology [2-5]. Extremely important is the atomization in heat power engineering when combusting liquid fuels. Liquid fuel combustion methods are very diverse, however, for all methods, the stage of fuel atomization is mandatory. Fuel spraying results in an increase of the total contact surface between the media, it enhances significantly heat transfer of atomized fuel with a gas medium and improves fuel drops mixing with the oxidizer that significantly contributes to the enhancement of the combustion process.

Currently, the world is actively engaged in research of promising suspended fuels for energy production, which consist of water, pulverized coal or processed waste fuel, chemical additives, as well as oil refinery waste. Such fuel is called organic coal-water fuel (OCWF) [6-8]. Wastes of coal mining and enrichment have a sufficiently high calorific value however their widespread use in energy production is constrained by the lack of energy-efficient and environmentally friendly technologies related to the use of OCWF. Creating such technology requires conducting a comprehensive scientific study. To control the disintegration process of liquid fuels, obtain the opening angle of the torch and disperse fuel composition depending on the geometric characteristics of the injector, it is necessary to carry out experimental and computational studies.

The great importance of liquid fuels spraying, when solving a wide range of technical problems, has led to the creation of a large number of various designs of injectors that meet the specific requirements of the particular tasks. The efficiency of the pneumatic injector for spraying of OCWF is determined by
the organization of gas flows. In this regard, the task of developing an effective and reliable numerical method to describe liquid fuel spraying in advanced burner devices is especially relevant.

The conducted analysis of the literature has shown that today the most realistic results on the simulation of spraying at an acceptable computational cost can be obtained using a hybrid Eulerian-Lagrangian Spray Atomization (ELSA) model [9-13].

The aim of the present work is to test a numerical technique for simulation of primary and secondary spraying of liquids based on the Eulerian-Lagrangian model.

2. Problem statement and research methods

As a test example, the model problem of kerosene jet spraying into the surrounding environment through an injector with a diameter of 100 µm at a velocity of 100 m/s was considered [1]. The properties of the liquid and the environment are shown in Table 1. Despite this is a model task, it allows verifying whether the model is implemented correctly.

Table 1. Task options.

| Liquid injection | Turbulent intensity | Turbulent length scale | Velocity | Injector diameter |
|------------------|---------------------|------------------------|----------|-------------------|
|                  | 5%                  | 10 µm                  | 100 m/s  | 100 µm            |

| Property         | Surface tension     | Liquid density         | Gas density | Liquid viscosity  |
|------------------|---------------------|------------------------|-------------|------------------|
|                  | 0.06 kg/s²          | 696 kg/m³              | 50 kg/m³   | 0.0012 kg/m/s    |

For numerical simulation of liquid fuel spraying, a Eulerian-Lagrangian Spray Atomization model based on a combination of VOF and DPM methods was implemented in the Fluent software package. This model describes the fluid flow inside the injector and directly behind it using the Euler approach, while the dispersed medium formed at a certain distance from the injector is described using the Lagrange approach. The conversion of Eulerian drop (VOF) to a discrete drop (DPM) occurs when it reaches a shape close to spherical. For the simulation of turbulence when calculating the flow using the VOF method, the large-eddy simulation LES technique was employed. This technique requires the solution of the “filtered” Navier-Stokes equations to describe turbulent flows. For the closure, the Wall-Adaptive Large Eddy (WALE) model was used. Also, a hybrid RANS/LES turbulence model, namely, DES k-w SST, was applied.

In this paper, we used the dynamic grid refining in the two-phase area (Fig. 1). Areas of the liquid phase boundaries are tracked using a refined grid, and when converted into a discrete drop, the grid returns to its original dimensions. This significantly reduces the required computing resources for such a costly task.

Figure 1. Computational grid: a) dynamic adaptation, b) condensation of the grid at the two phases interface.
The problem was solved in a three-dimensional unsteady formulation. The geometric configuration of the computational domain was a cylinder with a diameter of 0.6 mm and a length of 2.2 mm. A fixed value of the liquid velocity was set at the inlet. Free outflow conditions were set at the outlet. The Cartesian grid was used for the calculation. The time step was determined based on the condition CFL=2. This restriction leads to the fact that the value of the time step is about $1 \times 10^{-8}$ s.

3. Results and discussion
The calculation results were compared with the data of direct numerical simulation obtained in [1]. The drop spraying and crushing pattern for this task are shown in Fig. 2. The jet structure and the spraying shape obtained in the calculation are qualitatively similar to the results obtained by direct numerical simulation.

![Figure 2](#)

**Figure 2.** Instantaneous field of the liquid phase isosurface: 1 – LES calculation with the VOF model, 2 – DNS (VOF) calculation presented in [1].

When calculating this problem using the VOF method, taking into account the dynamic adjustment of the grid, the calculated grid contained about six million cells. The simulation results obtained by the VOF method are shown in Figs. 3-5. Quantitative and qualitative comparison of the major characteristics of the two-phase medium with the DNS data shows good agreement on the distribution of the liquid volume fraction. The LES method more correctly describes the liquid phase spraying in comparison with the DES method.

![Figure 3](#)

**Figure 3.** The averaged field of the liquid volume fraction in the central section: 1 – LES (VOF) based calculation of the authors; 2 – The authors’ calculation using DES k-w SST (VOF); 3 – DNS (VOF) based calculation from [1].
Figure 4. Distribution of the averaged liquid volume fraction along the jet axis: 1 – LES (VOF) based calculation; 2 – DES k-w SST (VOF) based calculation; 3 – DNS (VOF) based calculation from [1].

Figure 5. Radial distribution of the liquid volume fraction at a distance from the input equal to 5D, 10D, and 20D; 1 – LES (VOF) based calculation; 2 – DES k-w SST (VOF) based calculation; 3 – DNS (VOF) based calculation from [1].

Figures 6–7 show the calculation results obtained using the method of conversion of Eulerian droplets into discrete drops (VOF to DPM), and the LES method. The calculated grid, in this case, was about four million cells since the discrete phase does not require strong grid detailing. Figure 7 presents
a qualitative comparison of the simulation results with DNS data in the form of a sprayed cloud of droplets detached from the main jet. Comparative analysis shows that the concentration of droplets and the shape of the discrete cloud are similar to the results obtained in [1].

Figure 6. Visualization of the liquid phase based on the Eulerian and Lagrangian approach, the size of discrete droplets is shown in m.

Figure 7. Results of the Eulerian-Lagrangian calculation: 1 – Visualization of the jet based on the Eulerian and Lagrangian approach with LES; 2 – a cloud of discrete drops, LES (DPM); 3 – a cloud of drops, DNS (VOF) [1].

Conclusion
A numerical method to simulate the spraying of liquid fuel using Eulerian-Lagrangian model and the dynamic adjustment of the calculation grid has been tested for the model problem of the spraying of kerosene into the surrounding environment. The calculation results obtained show an acceptable
agreement with the data of direct numerical simulation in terms of the major spraying characteristics. The Eulerian-Lagrangian method in combination with VOF and DPM models allows determining the structure of a two-phase flow qualitatively correctly, as well as to deduce drops parameters such as the size, speed, and their movement direction. This technique allows reducing the required computational resources by reducing the number of computational cells by 30-40% through its optimization based on the use of dynamical adjustment of the grid. In the future, several real-life tests will be considered and the calculation results will be compared with the full-scale experiment.

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