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Towards high-fidelity multi-scale simulation of spray atomization

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Abstract

Liquid jet atomization is an important process in internal combustion engine. This paper presents a multi-scale approach coupling a Eulerian interface-tracking method and a Lagrangian particle tracking method to simulate liquid atomization processes. This method aims to capture the complete spray atomization process, particularly primary and second breakup, paving the way for high-fidelity simulation of spray atomization in the dense spray zone and spray combustion in the dilute spray zone. The Eulerian method is based on the Coupled Level-Set and Volume-of-Fluid (CLSVOF) for interface tracking, which can accurately simulate the primary breakup process. For the coupling approach, the Eulerian method only describes large droplet and ligament structures, while small-scale droplet structures are removed from the resolved Eulerian description and transformed into Lagrangian point-source droplets. The Lagrangian method is thus used to track small droplets and their further secondary breakup and collision. In this study, two-dimensional simulation of liquid jet atomization is performed. We will analyse Lagrangian-droplet formation and motion due to the coupling and the atomization characteristics using the multi-scale approach.

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Keywords: multi-scale, CLSVOF, point particle, spray atomization

1. Introduction

Liquid jet atomization plays a significant role in achieving efficient and clean combustion in internal combustion engines. It is a complex process, which can be divided into three regimes [1,2]. The first is the liquid core zone in which the liquid area is very dense and appears as a continuum fluid; the second is the dispersed flow zone where the liquid can be approximated as disperse particles; the last is the transition zone. In order to simulate accurately and efficiently the spray process in different zones, some efforts have been made in recent years and some multi-scale methods have been proposed, such as ELSA [3], the CLSVOF (or the Volume-of-Fluid method (VOF)) and Lagrangian particle-tracking methods [4-7]. Eulerian methods like VOF, Level Set and CLSVOF have been used to track or capture liquid-gas interfaces in the primary breakup regime (the liquid core zone), and the Lagrangian droplet-tracking

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method has been used to trace dispersed small droplets in the dilute spray zone. The coupling procedure between the two methods is the focus of this paper.

Proposing a multi-scale method for two-phase flow is challenging. Our main contribution of this paper is to demonstrate the achievement of the transformation of little droplets from a Eulerian structure to a Lagrangian particle and the performance of the coupled method based on the combination of CLSVOF (Eulerian) and KIVA (Lagrangian) in simulating a liquid jet process.

2. Numerical methods

2.1 Solvers

A coupled Level Set (LS) and Volume of Fluid (VOF) method CLSVOF [8] is used to capture and evolve gas-liquid interfaces. Gas–liquid interfaces are captured by the level-set method. To improve the volume conservation, a modified VOF method called the Multi-interface Advection and Reconstruction Solver (MARS) is incorporated. The detailed numerical method and its validation can be found in [8]. We use KIVA [9] as the Lagrangian solver, in which droplet velocity in the computation domain is determined by the drag force $F_{i,d}$ on the droplet, which is in turn determined by the relative velocity between the liquid droplet and the gas phase.

2.2 Eulerian-Lagrangian droplet transition

The droplet transition from a Eulerian structure to a Lagrangian particle is divided into three steps [4]. First, isolated droplets need to be identified and their mass, velocity and temperature are determined. In our work, we use a neighbour searching algorithm to identify an isolated liquid structure [4]. Second, we set up the conversion criteria for the Eulerian-Lagrangian transition. Whether or not a Eulerian structure will be transformed into a Lagrangian particle is determined by its critical volume and the critical length of a thin ligament. In this work, we use two different grids, one for CLSVOF and another for KIVA. The critical volume is set to be the KIVA cell volume in order to meet the requirement that the droplet dimension should be (much) smaller than the cell size in a Lagrangian point-particle method. Therefore the conversion criterion is $V_{eulerian} < V_{kivagrid}$, where $V_{eulerian}$ and $V_{kivagrid}$ are the Eulerian droplet volume and the KIVA grid cell volume, respectively. In order to accurately calculate the further breakup process of a largely deformed thin ligament with the Eulerian description despite that the Eulerian droplet volume meets the first criterion, the second criterion is $\alpha \geq R_{max}/max\left[\Delta x, \left(\frac{3}{4\pi}V_{eulerian}\right)^{1/3}\right]$.

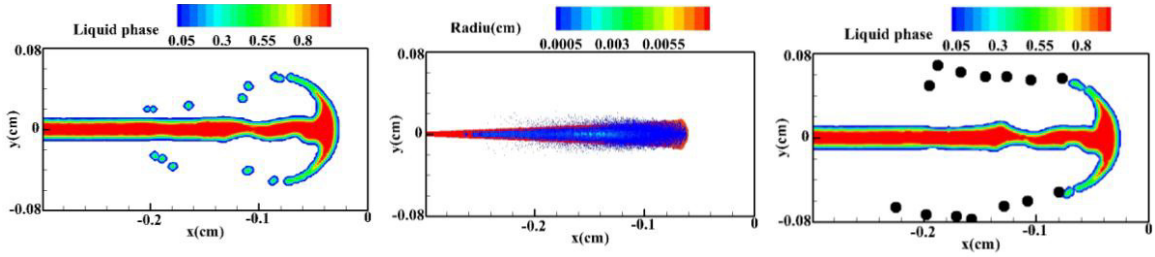
where R_{max} is the maximum distance from the edge of a Eulerian droplet structure to the centre of mass of the Eulerian droplet. The criterion parameter α is equal to 4. Third, remove the isolated droplets that meet the conversion criteria from the Eulerian description. At the same time the removed droplets are transformed to Lagrangian particles with determined droplets mass and velocity.

3. Results

In this paper, the two-dimensional computational domain is 0.6cm x 0.3cm with grid numbers 300 x 150 for CLSVOF and 150 x 75 for KIVA, respectively. The nozzle diameter is 0.016cm and the injection velocity is 100m/s. The liquid fuel is n-Heptane. Numerical results have been obtained for this case by using the Eulerian CLSVOF method [8], the Lagrangian point-particle tracking method in KIVA, and the hybrid Eulerian-Lagrangian multi-scale method developed for the present study. The Eulerian approach produces direct simulation results, which can be used as benchmark. The Lagrangian method is model based. The KH-RT breakup model is used in KIVA. The developed numerical method is a high-fidelity

multi-scale approach combining direct simulation and modelling, aiming to have advantages of both accuracy and cost.

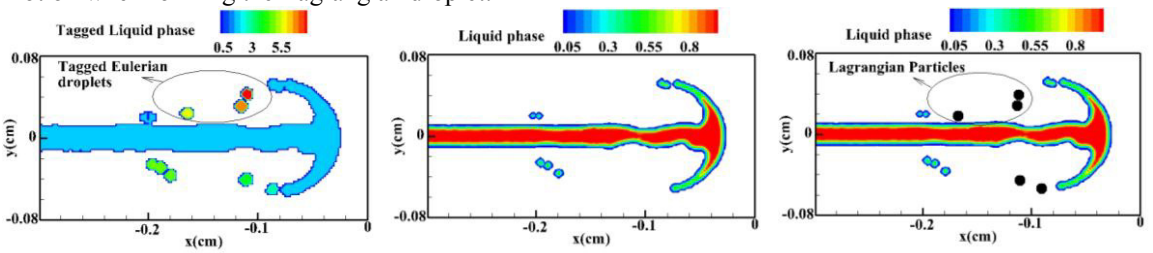
The results produced by the three methods are shown in Fig. 1. It can be seen that different methods have their distinct features. The liquid penetration length appears very similar among the three. Comparing the CLSVOF method (Fig. 1a) with the Lagrangian method with a breakup model (Fig. 1b), using CLSVOF can capture more detailed and precise spray breakup dynamics, such as the umbrella-like liquid head formed due to the liquid jet impact on the ambient gas. At the same time, atomized droplets are produced. In contrast, the Lagrangian method generates a lot of little droplets as expected. In Fig. 1c, the black dots represent Lagrangian droplets. The difference of the droplet distribution between Fig.1 a) and c) is largely due to the modelled Lagrangian drag force. To reduce the difference is our future work.



a) CLSVOF b) KIVA c) CLSVOF + KIVA

Fig. 1 Comparison between CLSVOF, KIVA and the developed coupled method. The color labels represent liquid phase volume fraction in (a) and (c), and droplet radius in (b).

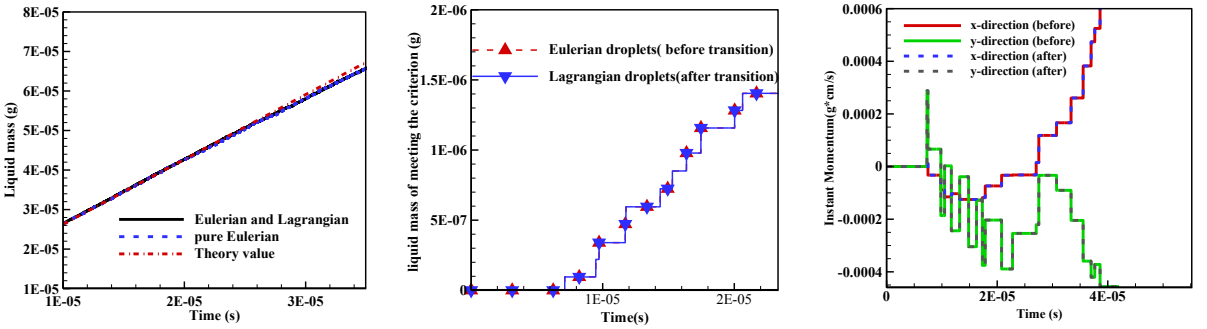
As mentioned in Section 2, there are three steps involved in the Eulerian-Lagrangian transformation. Figure 2 presents the transition process in detail. According to the neighbour searching algorithm, different liquid structures are tagged with different numbers, as shown in Fig. 2a. In Fig. 2b, the isolated little droplets meeting the transition criterion are removed from the Eulerian description, but larger droplets are retained. Figure 2c shows the instantaneous transition process without considering the droplet motion when forming the Lagrangian droplet.



a) Tagging isolated droplets b) Removing isolated droplets c) Generating Lagrangian particles (black dots) on the KIVA coarse grid

Fig. 2 Three steps of droplet transition from using the Eulerian to Lagrangian method

To check the quality of the numerical transition process, Fig. 3 shows the comparison of droplet mass and momentum before and after the transition procedure. Figure 3a presents the evolution of the change of the overall liquid mass with time. It can be seen that the coupled method and the Eulerian method have the same overall liquid mass. A small percentage of the liquid mass is lost due to the Eulerian method (CLSVOF) in comparison with the theoretical value. Figures 3b and 3c prove the accuracy of the transition process by checking the conservation of the mass and momentum of isolated droplets before and after the transition.



a) Overall liquid mass b) Isolated droplets mass c) Isolated droplets momentum

Fig. 3 Mass and momentum conservation before and after the transition

4. Conclusion

The present study has presented a multi-scale hybrid Eulerian-Lagrangian approach to simulating liquid jet atomization processes. The detailed transition process from the Eulerian to Lagrangian description is conducted in three steps. The instantaneous mass and momentum are found to be consistent before and after the transition. In our future work, secondary breakup, collision and coalescence of Lagrangian particles will be considered to improve the numerical accuracy of the coupled method. In addition, the transition from the Lagrangian back to the Eulerian description of a droplet is also an important subject.

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References

[1] Hoyas S, Pastor JM. Khuong-Anh, D., Mompó-Laborda, J.M.,Ravet, F. Application and evaluation of the Eulerian-Lagrangian spray atomization (ELSA) model on CFD diesel spray simulations, SAE 2011-37-0029, 2011.

[2] Hoyas S, Gil A, Margot X, Khuong-Anh D, Ravet F. Evaluation of the Eulerian–Lagrangian Spray Atomization (ELSA) model in spray simulations: 2D cases, Mathematical and Computer Modelling, 2013, 57 (7), pp. 1686-1693.

[3] Wang Y, Lee WG, Reitz RD, Diwakar R. Numerical simulation of diesel sprays using an eulerian-lagrangian spray and atomization (elsa) model coupled with nozzle flow, SAE Technical Paper 2011-01-0386, 2011.

[4] Arienti M, Li X, Soteriou M, Eckett C, Sussman M, Jensen R. Coupled level-set/volume-of-fluid method for simulation of injector atomization, Journal of Propulsion and Power, 2012, 29 (1), pp. 147-157.

[5] Li, X., Soteriou, M. High fidelity simulation of the spray generated by a realistic swirling flow injector, Atomization and Sprays, 2013, 23 (11), pp. 1049-1078.

[6] Herrmann, M. A parallel Eulerian interface tracking/Lagrangian point particle multi-scale coupling procedure, Journal of Computational Physics, 2010, 229 (3), pp. 745-759.

[7] Tomar G, Fuster D, Zaleski S, Popinet S. Multiscale simulations of primary atomization, Computers & Fluids, 2010, 39 (10), pp. 1864-1874.

[8] Shinjo, J., Umemura, A. Simulation of liquid jet primary breakup: Dynamics of ligament and droplet formation, International Journal of Multiphase Flow, 2010, 36 (7), pp. 513-532.

[9] Alamos, L. KIVA-3V: A block-structured Kiva program for engines with vertical or canted values. LA-18818-MS, 1997.