

Development of a multiphase turbulent flow solver for rocket injector atomization simulation

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1 Introduction

In rocket engines, injectors are used to supply the liquid fuel and oxidizer into the combustion chamber. Such liquid reactants undergo atomization, vaporization, and combustion processes. Figure 1 presents the physical processes of liquid reactants in the combustion chamber.

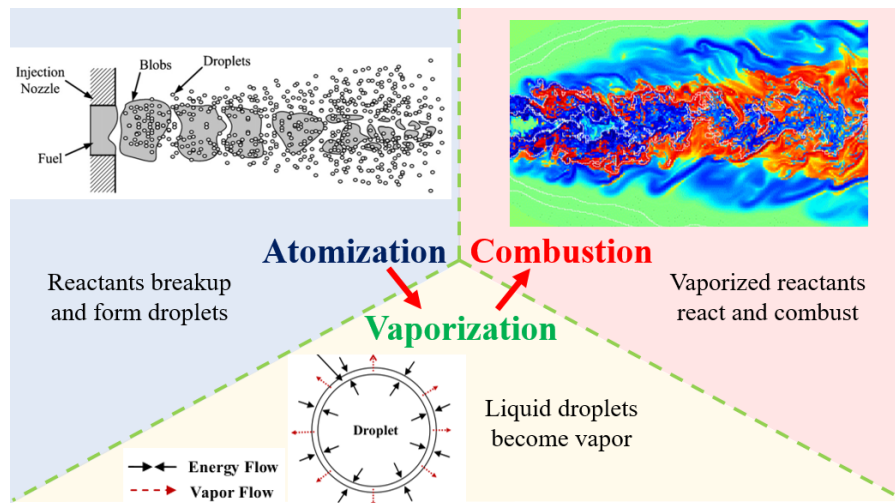


Figure 1: Physical processes in the combustion chamber [1-3]

The liquid fuel and oxidizer breakup and form droplets in the atomization process. In the vaporization process, liquid droplets get some heat in the combustion chamber and become vapor. Vaporized reactants react and combust in the combustion process. On the other hand, simulations on the combustion chamber of rocket engines have often been performed focusing on only the combustion process. Most simulations assumed that the injected reactants immediately become a flammable mixture of gases, then combustion occurred while neglecting the atomization and vaporization processes. Still, it is necessary to consider the full processes (atomization, vaporization, and combustion) to design reliable and efficient injectors and combustors. Henceforth, a solver which can simulate atomization, vaporization, and combustion processes needs to be developed.

The development framework consists of the followings. In the atomization process, the reactants exist in two phases: liquid and gas. Their physical properties are discontinuous across the interface between these liquid and gas phases. The vaporization process is modeled by considering the energy conservation law. Lastly, chemical kinetics calculation is required in the combustion process.

For the first step of the development framework, a solver for the atomization process is developed. In order to tackle the aforementioned challenges, two existing solvers are chosen: PeleLM [4-6] and IRL [7,8]. As the ultimate goal is to solve combustion, PeleLM is the most suitable candidate as the code solves variable density incompressible, reacting Navier-Stokes equation in the adaptive mesh refinement framework. Furthermore, the volume of fluid (VOF) method is necessary to interpret interfaces of multiphase flows. Thus, Interface Reconstruction Library (IRL) is coupled with PeleLM to solve the VOF with Piecewise Linear Interface Calculation (PLIC) method to develop a multiphase solver in the base of PeleLM.

Furthermore, surface tension has considerable effects on spray breakup in the atomization process. Computing interface curvature from volume fraction is important to estimate the surface tension. There are three techniques for estimating curvature from VOF. These techniques are the convolved VOF (CV) technique [9], the reconstructed distance function (RDF) technique [10], and the height function (HF) technique [11,12]. Cummins et al. [10] compared these techniques and concluded that the CV and RDF techniques do not achieve the accuracy level of the HF method. Thus, in this work, an improved HF technique [12] is used to calculate the curvature to develop the solver for the atomization process.

2 Numerical methods

To develop a multiphase flow solver, the new scalar field α (volume of fluid) needs to be defined. If α is 0, there is no tracking fluid inside the cell and if α is 1, the cell is full with the tracking fluid.

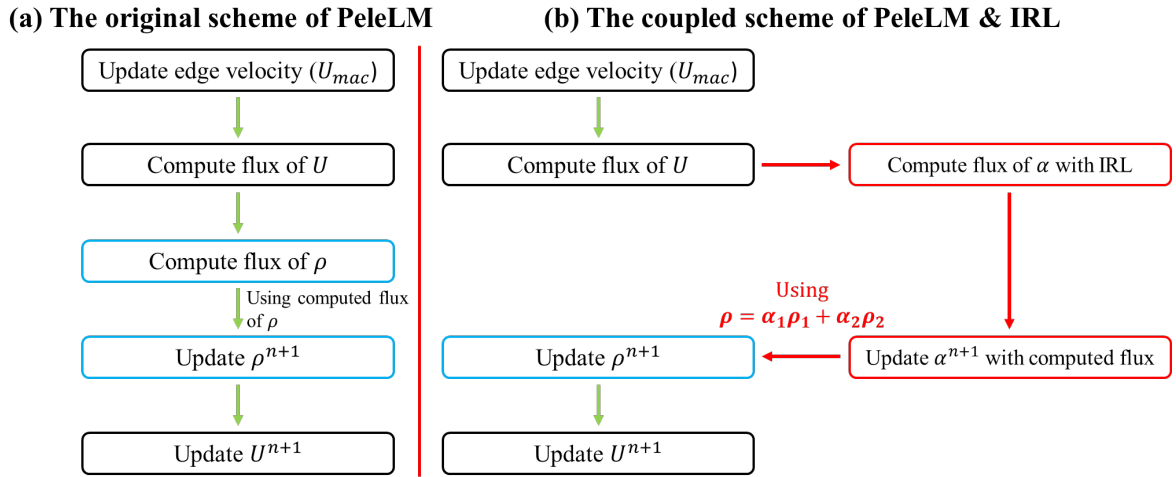


Figure 2: (a) The original scheme of PeleLM. (b) The coupled scheme of PeleLM and IRL.

Figure 2 presents the original scheme of PeleLM and the coupled scheme of PeleLM and IRL. In the coupled flow solver, the flux of α is calculated with IRL. Then, the next time step α^{n+1} is updated with computed flux. Lastly, the next time step density is updated using α^{n+1} .

The viscosity coefficient also changed with α . At the beginning of each time step, the viscosity coefficient of the whole cell is updated using the following equation [13].

$$\mu = \mu_l \alpha + \mu_g (1 - \alpha),$$

where the subscripts l and g denote liquid and gas, respectively.

In the continuum surface force model (CSF) [14], the surface tension force is calculated at the interface with the following equation.

$$\vec{F} = \sigma\kappa\vec{n},$$

where σ is the surface tension coefficient, κ is the curvature, and \vec{n} is the interface normal vector.

In this work, \vec{n} is obtained from the gradient of α using the method of Youngs [15]. Then, the improved HF technique [12] is used to calculate the curvature. Finally, the surface tension force is introduced in the momentum equation by force term.

3 Validation results

To verify the coupling of PeleLM and IRL, two test cases were conducted: (i) translation and rotation of Zalesak’s disk and (ii) three-dimensional deformation of a sphere droplet. To see just the IRL effect, the viscosity coefficient and surface tension force are set to zero at tests (i) and (ii).

To verify the surface tension force introduced in the momentum equation, one test case was conducted: (iii) the sphere droplet test. To see the surface tension force effect only, the viscosity coefficient is set to zero at test (iii).

3.1 Validation 1: Translation and rotation of a Zalesak's disk

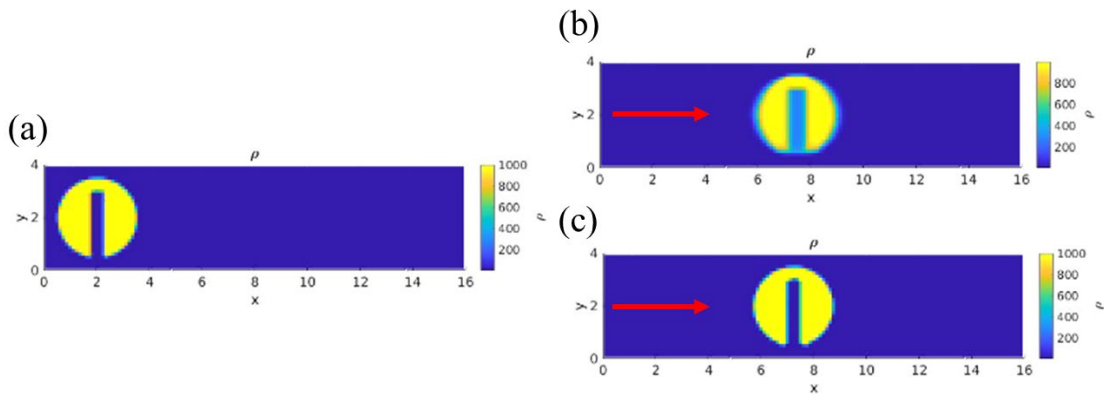


Figure 3: Test case 1a – translation of the Zalesak's disk. (a) Initial shape. (b) Translated disk without coupling IRL. (c) Translated disk with coupling IRL.

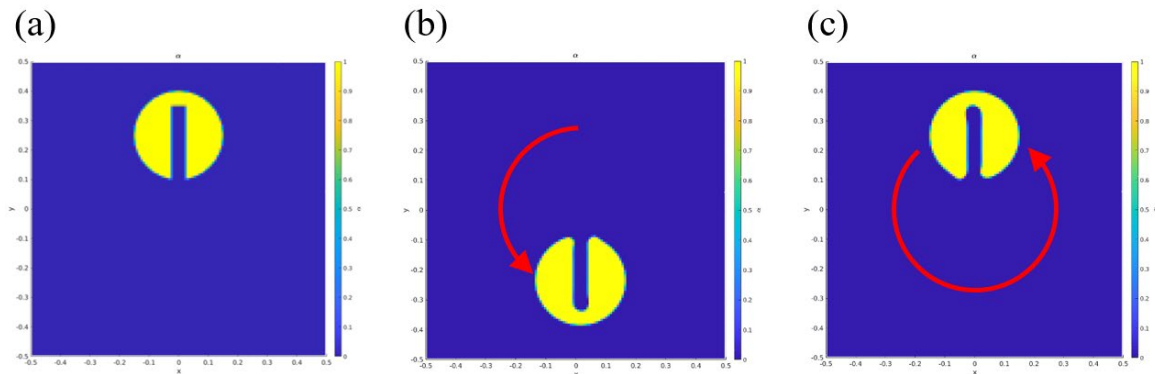


Figure 4: Test case 1b – rotation of the Zalesak's disk. (a) Initial shape. (b) Rotated by 180 degree. (c) Rotated by 360 degree.

Figure 3 shows the result of the translation of the Zalesak's disk with and without coupling IRL. By comparing figure 3 (b) and (c), coupling IRL with PeleLM captures the interface of the liquid and gas phase more clearly than without coupling. Figure 4 shows the result of the rotation of the Zalesak's disk with coupling IRL. The interface of the liquid and gas phase is well maintained during the rotation with a minor loss of capturing the sharp-edged interface.

3.2 Validation 2: 3D deformation of a sphere droplet

Figure 5 shows the result of the three-dimensional deformation of the sphere droplet. Given a prescribed velocity field, the sphere droplet has the maximum deformation at $t = 1.5$ s (figure 5 (b)) and the sphere droplet is reversed back to un-stretched at $t = 3$ s (figure 5 (c)) [7]. The prescribed velocity field is

$$u = 2 \sin^2(\pi x) \sin(2\pi y) \sin(2\pi z) \cos(\pi t/3),$$

$$v = -\sin(2\pi x) \sin^2(\pi y) \sin(2\pi z) \cos(\pi t/3),$$

$$w = -\sin(2\pi x) \sin(2\pi y) \sin^2(\pi z) \cos(\pi t/3).$$

The sphere droplet reverses back to the initial shape without significant changes during stretching and un-stretching. Therefore, coupling IRL with PeleLM captures a clearer interface of liquid and gas phases.

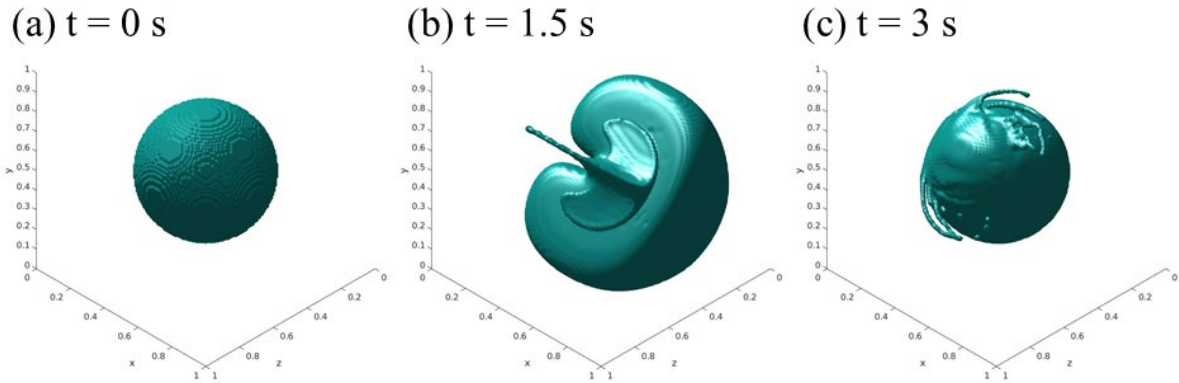


Figure 5: Test case 2 – three-dimensional deformation of a sphere: (a) Initial shape. (b) Deformed shape after stretching. (c) Deformed shape after un-stretching.

3.3 Validation 3: pressure inside a stationary droplet

The radius of the sphere is 1 mm and the surface tension coefficient is 0.07 N/m. The initial velocity is zero and the densities inside and outside the droplet are 1000 kg/m^3 and 1 kg/m^3 . The initial pressure is not set to a steady state condition because of the limitation of the PeleLM scheme.

Figure 6 (b) shows the pressure inside the sphere droplet. If the sphere droplet is in a steady state, the ideal pressure is

$$\Delta P = \frac{2}{R} \sigma = 140 \text{ Pa.}$$

In the sphere droplet test, the maximum pressure is 135 Pa. The unsteady initial state is regarded to have caused the difference. The difference is around 3.6 %, indicating the surface tension force works well in the momentum equation.

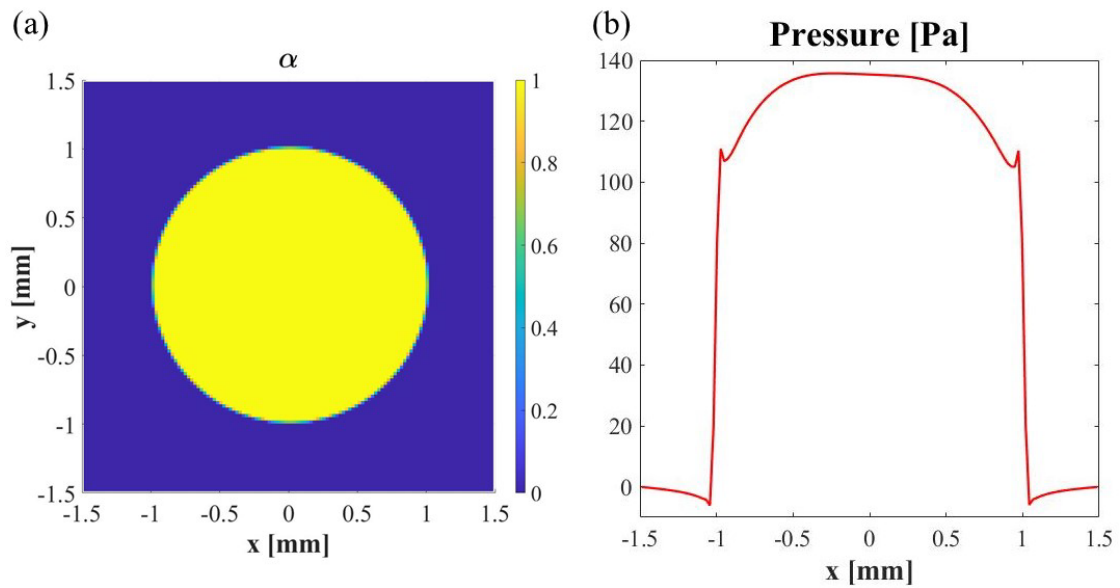


Figure 6: (a) The α field cross-section view of the sphere droplet. (b) The pressure inside the sphere droplet.

The solver is sufficient to test the verification case of atomization of liquid jet spray by adding the viscosity coefficient effect.

4 Conclusions

To design reliable and efficient injectors, it is necessary to consider the full and detailed processes (atomization, vaporization, and combustion). In this work, a multiphase flow solver for the atomization process is developed. A library of the volume of fluid (VOF) scheme for simulating multiphase flows, IRL, is coupled with the variable density incompressible, reacting Navier-Stokes equation solver, PeleLM. Furthermore, surface tension is implemented by using the improved height function (HF) technique.

To verify the solver, multiple validation simulations were conducted to test the code-coupling and the surface tension implementation. The shapes of Zalesak's disk and a sphere droplet remain unchanged by the prescribed velocity field. Moreover, the interface of the liquid and gas phases is well maintained. In the validation simulation for the surface tension force, the resulting pressure increase inside the sphere droplet is similar to the theoretical value within a 3.6 % error.

In future work, the developed solver will be used to simulate the full atomization and fluid-collision processes of rocket injectors. Furthermore, vaporization physics will be implemented to develop a complete atomization-vaporization-combustion solver.

Acknowledgments

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References

- [1] Jiang X, Siamas GA, Tagus K, Karayiannis TG. (2010). Physical modelling and advanced simulations of gas-liquid two-phase jet flows in atomization and sprays. *Prog. Energ. Combust.* 36(2):131.
- [2] Ragab R, Wang T. (2012). An investigation of liquid droplet evaporation model used in multiphase flow simulation. *ASME International Mechanical Engineering Congress and Exposition* 45233:485.
- [3] Lu T, Yoo C, Chen J, Law C. (2008). Analysis of a turbulent lifted hydrogen/air jet flame from direct numerical simulation with computational singular perturbation. *46th AIAA aerospace sciences meeting and exhibit* (p. 1013).
- [4] Nonaka A, May S, Almgren AS, Bell JB. (2011). A three-dimensional, unsplit godunov method for scalar conservation laws. *SIAM J. Sci. Comput.* 33(4):2039.
- [5] Day MS, Bell JB. (2000). Numerical simulation of laminar reacting flows with complex chemistry. *Combust. Theor. Model.* 4(4):535.
- [6] Nonaka A, Bell JB, Day MS, Gilet C, Almgren AS, Minion ML. (2012). A deferred correction coupling strategy for low mach number flow complex chemistry. *Combust. Theor. Model.* 16(6):1053.
- [7] Owkes M, Desjardins O. (2014). A computational framework for conservative, three-dimensional, unsplit, geometric transport with application to the volume-of-fluid (VOF) method. *J. Comput. Phys.* 270:587.
- [8] Chiodi R, Desjardins O. (2022). General, robust, and efficient polyhedron intersection in the Interface Reconstruction Library. *J. Comput. Phys.* 449:110787.
- [9] Williams MW. (2000). Numerical methods for tracking interfaces with surface tension in three-dimensional mold-filling processes. University of California, Davis.
- [10] Cummins SJ, Francois MM, Kothe DB. (2005). Estimating curvature from volume fractions. *Comput. Struct.* 83(6-7):425.
- [11] Sussman M. (2003). A second order coupled level set and volume-of-fluid method for computing growth and collapse of vapor bubbles. *J. Comput. Phys.* 187:110.
- [12] Lopez J, Zanzi C, Gomez P, Zamora R, Faura F, Hernandez J. (2009). An improved height function technique for computing interface curvature from volume fractions. *Comput. Methods Appl. Mech. Engrg.* 198(33-36):2555.
- [13] Zhang Z, Shin D-H. (2020). Effect of ambient pressure oscillation on the primary breakup of cylindrical liquid jet spray. *Int. J. Spray Combust.* 12:1756827720935553.
- [14] Brackbill JU, Kothe DB, Zemach C. (1992). A continuum method for modeling surface tension. *J. Comput. Phys.* 100:335.
- [15] Youngs DL. (1984). An interface tracking method for a 3D Eulerian hydrodynamics code. Technical Report AWRE/44/92/35.