



# Implementation of Surface Tension on a Reacting Flow Solver, PeleLM

## Preprint

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## 1. Introduction

In liquid rocket engines, the fuel is supplied to the combustion chamber in the liquid state through injectors. Such fuel undergoes atomization, vaporization, and combustion processes. To design reliable and efficient injectors, it is required to understand the full processes. This research is part of an effort to develop a full atomization-vaporization-combustion solver from first principles. As an initial step to tackle the atomization process, a multiphase flow solver is under development. For the development, a library of the volume of fluid scheme for multiphase, IRL [1-2], is coupled with a reacting Navier-Stokes equation solver, PeleLM [3]. Furthermore, as the surface tension has considerable effects on spray breakup, surface tension is implemented in the momentum equation using the continuum surface force model (CSF) [4] and the improved height function (HF) technique [5].

## 2. Numerical Methods

In the coupled PeleLM-IRL solver, the scalar field  $\alpha$  (volume fraction of fluid) is defined. If  $\alpha$  is 0, there is no tracking fluid inside the cell, and if  $\alpha$  is 1, the cell is full with the tracking fluid. Instead of solving the continuity equation of density, a flux of  $\alpha$  is calculated with IRL in the coupled PeleLM-IRL solver. Then, the next time step  $\alpha^{n+1}$  is updated with computed flux. The density is estimated by  $\rho = \rho_l \alpha + \rho_g (1 - \alpha)$ , where the subscripts  $l$  and  $g$  denote liquid and gas, respectively.

In the CSF model [4], the surface tension volume

force is calculated by  $\vec{F} = \sigma \kappa \vec{n}$ , where  $\sigma$  is the surface tension coefficient,  $\kappa$  is the curvature which is calculated by the improved HF technique [5], and  $\vec{n}$  is the interface normal vector which is obtained from the gradient of  $\alpha$ . Finally, the surface tension is introduced in the momentum equation by the external force term.

## 3. Verification Results

To verify the implementation of surface tension, two test cases were conducted. In both test cases, the liquid density is 1,000 kg/m<sup>3</sup> and the gas density is 1 kg/m<sup>3</sup>. The dynamic viscosity coefficient is set to 0.01 N·s/m<sup>2</sup> and the surface tension coefficient is 0.07 N/m.

### 3.1 Verification 1: Stationary circular droplet

The objective of the test case is to confirm that the surface tension implementation leads to the correct pressure difference inside a circular droplet. As shown in Fig. 1a, a circular droplet of the radius of 1 mm is placed on the simulation domain as an initial condition, then unsteady simulations were conducted on three different grid resolutions ( $\Delta x = \Delta y = 23, 47, \text{ and } 94 \mu\text{m}$ ).

Fig. 1b shows the resulting pressure distribution along the centerline on the fine grid. The pressure inside the circular droplet is fairly uniform, and the average pressure is 66, 67.1 and 67.5 Pa for the coarse, medium, and fine grids respectively. Considering the theoretical value of 70 Pa, the fine grid solution provides a small error of 3.6 %.

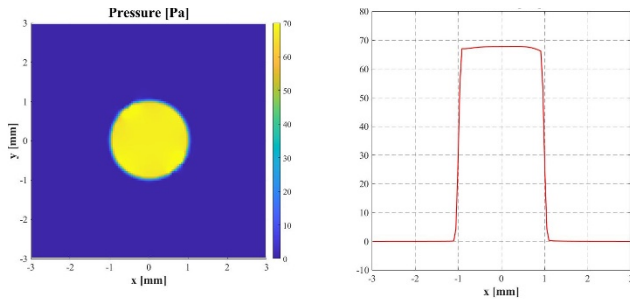


Fig. 1. The result of the stationary droplet test: (a) The pressure field. (b) The pressure along the  $y = 0$  line.

### 3.2 Verification 2: Oscillating elliptical droplet

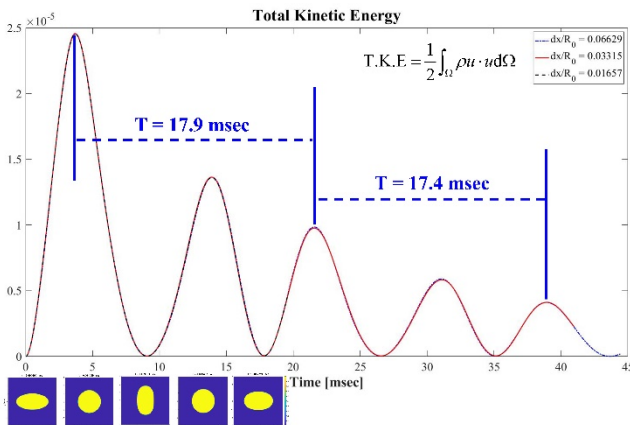


Fig. 2. The total kinetic energy of oscillating droplet test case with various grid sizes.

An elliptical droplet is given by  $x^2/4 + y^2 \leq 1$ , whose units are in mm. Fig. 2 shows the evolution of the total kinetic energy (T.K.E). Rayleigh [6] derived the analytic solution for the oscillation period when the amplitude is small. The analytical solution value is 16.3 msec, while the first and second periods are 17.9 msec and 17.4 msec, respectively from the simulation. The differences (9.8% and 6.7%) are decreasing over time as the amplitude becomes smaller.

### 4. Conclusion

The surface tension is implemented in the coupled PeleLM-IRL solver using the continuum surface force model and the improved height function technique.

Two validation cases were performed. Firstly, a stationary circular droplet test was conducted. The resulting pressure difference inside the droplet is similar to the theoretical value with a 3.6 % difference. Secondly, an oscillating elliptical droplet test was conducted. Total kinetic energy (T.K.E) is used to quantify the oscillating period. The amplitude of T.K.E decreases due to viscosity and the period is similar to the analytical solution [6] with a 9.8 % error.

In future work, the liquid jet atomization will be

simulated using the developed solver. Furthermore, vaporization physics will be implemented.

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