Multiphase Homogeneous Mixture Model On Metal Combustion With Eulerian To Lagrangian Transformation

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1 Introduction

Underwater vehicles have been continuously developed since the 1940s [1]. The vehicles mainly used solid propellants, but due to their low propulsion efficiency, it has been developed in the direction of using additives rather than using solid propellant alone [2]. As an additive, a metal fuel that has a high energy density and reacts well with water is used; for example, Be, Al, and Mg can be candidate as metal fuels. However, Be is limited due to toxicity, so aluminum and magnesium have become the most attractive metal fuels. In addition, since aluminum and magnesium generate hydrogen when it reacts with water, it has the advantage of being environmentally friendly. However, in the case of aluminum, it is difficult to use it alone because the oxide layer is so hard that it takes too much energy to break it. On the other hand, although magnesium has a lower energy density than aluminum, it is suitable as a metal fuel due to its relatively soft oxide shell and low boiling point [3].

In this study, a numerical model that include all three phases is developed to perform metal fuel combustion with water injection. A homogeneous mixture model is used to analyze the liquid and gas phase, and the Adaptive Mesh Refinement (AMR) technique and the Eulerian to Lagrangian (E2L) transformation method are implemented for efficient calculation. The converted droplet and metal fuel are tracked through the Lagrangian Particle Tracking (LPT) method. Also, the droplet breaks up through the KH-RT secondary break-up model. The Abramzon evaporation model is employed for the droplet evaporation. And the empirical correlation for burn time was implemented for calculating evaporation rate of the metal fuel. The evaporated mass, momentum, and energy source terms are coupled with Eulerian phase. Evaporated liquid and metal fuel react in the gas phase, and gas phase combustion is calculated by the Arrhenius equation using the magnesium global mechanism.

2 Numerical Method

2.1 Governing Equations

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In this study, the mass, momentum, energy, and mass fraction conservation equations are considered and can be expressed as

$$\frac{\partial \boldsymbol{Q}}{\partial t}+\frac{\partial \boldsymbol{F}}{\partial x}+\frac{\partial \boldsymbol{G}}{\partial y}+\frac{\partial \boldsymbol{H}}{\partial z}=\frac{\partial \boldsymbol{F_v}}{\partial x}+\frac{\partial \boldsymbol{G_v}}{\partial y}+\frac{\partial \boldsymbol{H_v}}{\partial z}+\boldsymbol{S_f}$$

$$\boldsymbol{Q}=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho w\\ \rho E\\ \rho Y_i\end{bmatrix},\quad \boldsymbol{F}=\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ \rho uw\\ (\rho E+p)u\\ \rho Y_i u\end{bmatrix},\quad \boldsymbol{G}=\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ \rho vw\\ (\rho E+p)v\\ \rho Y_i v\end{bmatrix},\quad \boldsymbol{H}=\begin{bmatrix}\rho w\\ \rho uw\\ \rho vw\\ \rho w^2+p\\ (\rho E+p)w\\ \rho Y_i w\end{bmatrix}$$

$$\boldsymbol{F_v}=\begin{bmatrix}0\\ \tau_{xx}\\ \tau_{xy}\\ \tau_{xz}\\ u\tau_{xx}+v\tau_{xy}+w\tau_{xz}+k\dfrac{\partial T}{\partial x}\\ 0\end{bmatrix},\quad \boldsymbol{g_v}=\begin{bmatrix}0\\ \tau_{yx}\\ \tau_{yy}\\ \tau_{yz}\\ u\tau_{yx}+v\tau_{yy}+w\tau_{yz}+k\dfrac{\partial T}{\partial y}\\ 0\end{bmatrix},\quad \boldsymbol{H_v}=\begin{bmatrix}0\\ \tau_{zx}\\ \tau_{zy}\\ \tau_{zz}\\ u\tau_{zx}+v\tau_{zy}+w\tau_{zz}+k\dfrac{\partial T}{\partial z}\\ 0\end{bmatrix}$$

$$\boldsymbol{S_f}=\begin{bmatrix}\dot{\rho}_s\\ \dot{F}_{s,x}\\ \dot{F}_{s,y}\\ \dot{F}_{s,z}\\ \dot{Q}_s\\ \dot{S}_s\end{bmatrix}=\begin{bmatrix}\dot{m}_d\\ \dot{m}_d u_d-\dfrac{4\pi}{3}\rho r^3\dfrac{du_d}{dt}\\ \dot{m}_d v_d-\dfrac{4\pi}{3}\rho r^3\dfrac{dv_d}{dt}\\ \dot{m}_d w_d-\dfrac{4\pi}{3}\rho r^3\dfrac{dw_d}{dt}\\ \dot{m}_d h_{fs}-h\pi d^2\left(T-T_p\right)\\ \dot{m}_d\end{bmatrix}$$

The source term, S_f, is the source vector due to the droplet and solid particle two-way coupling.

2.2 Thermodynamic Properties

The multi fluid mixture (MFM) model is used to analyze both the liquid and the gas phases in the Eulerian field [4]. The MFM model can use several types of equation of state(EOS) at the same time. NASG and ideal EOS is implemented in the liquid and gas phase, respectively. Then, the mixing model calculates the mixture properties with species thermodynamic properties. In the NASG EOS, pressure and energy are calculated as follows.

$$p=Tc_v\frac{\gamma-1}{1/\rho-b}-p_\infty$$

$$e=\frac{p+\gamma p_\infty}{\gamma-1}\left(\frac{1}{\rho}-b\right)+q$$

2.3 Eulerian to Lagrangian(E2L) Transformation

The homogeneous mixture model handles the liquid and the gas phases in Eulerian field. Therefore, the grid size is depending on the smallest droplet size to be captured. The computational load becomes, however, so much burden to capture proper droplet size in the Eulerian field because the droplets appearing as a result of the first and secondary breakup are several tens of micro-sized in general. In

order to overcome the burden, the breakup of the liquid column is computed for the certain level of the droplet size in the Eulerian field, and then the droplets generated as a result of ligament breakup are converted into Lagrangian particles. There are two conversion criterias: size, sphericity. Size criteria must satisfy the following:

$$V_{Eulerian} \leq V_{cri} = \frac{4}{3}\pi R_{cri}^3$$

Where R_{cri} is critical droplet size which is set as 120 um in this study. Sphericity should satisfy the following[5]:

$$\alpha = \frac{R_{max}}{\max\left[\Delta x, \left(\frac{3}{4\pi}V_{Eulerian}\right)^{1/3}\right]}$$

Where R_{max} represents the maximum distance from center of mass to liquid surface. If the sphericity is less than 4, it is converted, and this is set to a large value to convert the droplet after the primary break-up. If the above two conditions are satisfied, it is removed from the Eulerian field and converted to a Lagrangian particle.

2.4 Break-up Model

Since most of the droplets converted by E2L transformation are droplets after the primary breakup, the secondary breakup can occur. In this study, the KH-RT secondary breakup model is applied, and the main equations can be found in reference [6]. All sphericity of each droplet is acquired in the E2L transformation process, additional weights are set for RT breakup acceleration. By dividing the breakup time required for RT breakup by sphericity value, so that the secondary breakup can occur mor quickly.

2.5 Magnesium Combustion Model

In order to model the magnesium combustion, reaction rate based empirical correlation is applied for enhancing computational efficiency. Miller et al. summarized various magnesium combustion results in terms of diameter and effective oxidizer concentration [7]. The proposed expression is as follows:

$$\tau = \frac{Cd^2}{X_{ox}^{0.9}(1 + 0.25Re^{0.5})}$$

Where

$$C = \begin{cases} 0.007, & P_c = 1\ atm \\ 0.02, & P_c > 4\ atm \end{cases}$$

Through the above formula, a more accurate analysis is possible by deriving the mass evaporation rate corresponding to the change in the surrounding environment of the metal fuel particle.

2.6 Numerical Method

The flux scheme such as Harten-Lax-van Leer (HLLC) [8] to the mass flux term and simple low dissipation AUSM 2 (SLAU2) [9] to the pressure flux term are applied. The Vanleer limiter is applied to the high-order reconstruction scheme, and the flux-blending interface-capturing scheme (FBICS) limiter [10] is applied to the mass fraction when calculating flux to prevent numerical diffusion of the phase interface. Also, polyhedron-based AMR technique is applied to analyse more detailed phenomena in the phase interface.

3 Numerical Results

The computational domain is similar to general rocket chamber, and a donut-shaped manifold is attached to inject water. For computational efficiency, the domain is configured in the form of a 18 degree sector. At the gas inlet, combustion gas due to grain combustion and magnesium particles are injected. Fig. 1 shows the breakup of the injected water coming out of the four inlets and E2L converted Lagrangian particles. It can be seen that the Eulerian field water breaks into small droplets due to the various instabilities caused by the crossflow interaction. In particular, the water injected from the front and rear injectors of donut-shaped manifold shows distinct breakup characteristics. In the case of the front injector, ligament is affected by one direction flow, either up or down. On the other hand, in the case of the rear injector, the flow accelerated along the manifold compresses the ligament both up and down at the same time. As a result, the rear injector ligament develops into a thin liquid sheet, resulting a high breakup performance.

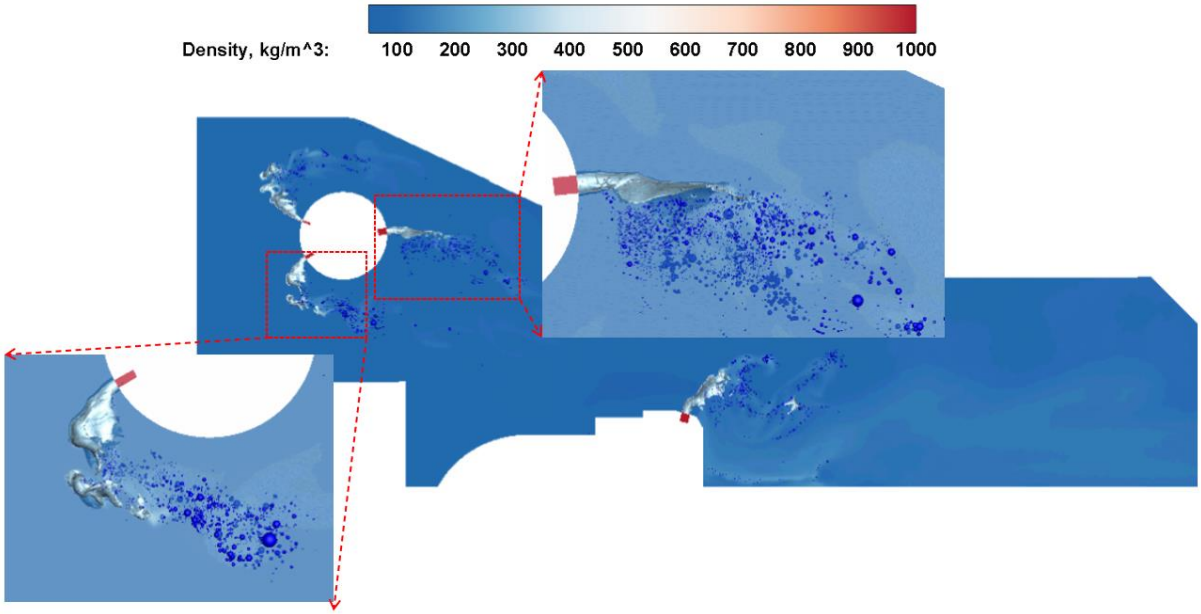

Figure 1 Density field and liquid surface(white) with E2L converted Lagrangian particle(blue)

Fig. 2 shows the combustion results of water and magnesium reaction. The converted Lagrangian particle evaporates and switches to water vapor that reacts with magnesium fuel so that the temperature rises rapidly to 4000 K like combustion gas temperature, which contributes vaporizing the secondary water injected downstream. The secondary water injection serves to protect the structure by reducing the combustion temperature and increases both the mass and momentum of the exhaust gas that enable to increase thrust.

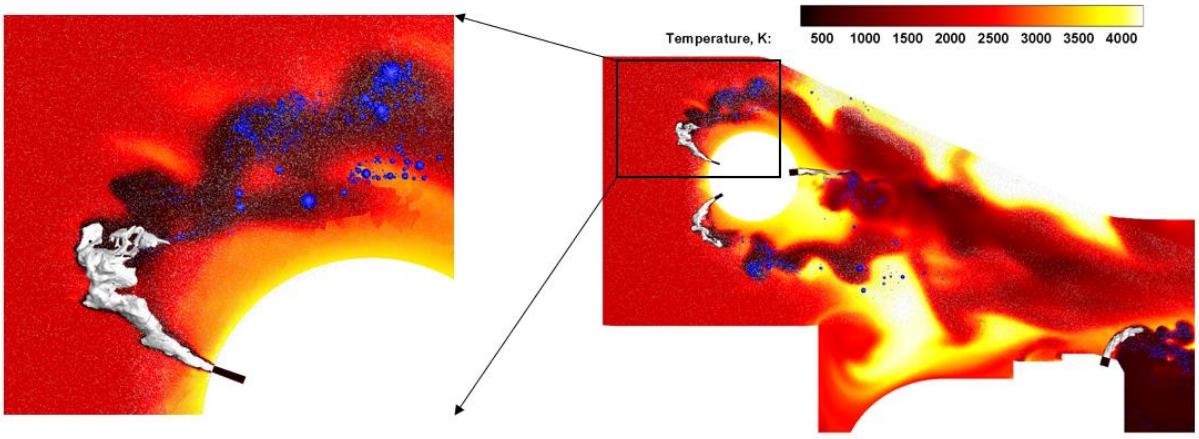

Figure 2 Temperature distribution with liquid surface, water particles, and Mg particle

4 Conclusion

In this study, a numerical model that include all three phases is developed to perform metal fuel combustion analysis. A homogeneous mixture model is used to handle the liquid and gas phase, and the Lagrangian Particle Tracking model is employed for the metal fuel which is a solid particle. In addition, efficient calculation is performed by applying AMR and E2L technique. The water and magnesium particle are vaporized by applying the Abramzon evaporation model and burn time empirical correlation, respectively. Vaporized water and magnesium react with global magnesium mechanism using Arrhenius equation.

As a result of the analysis, surface instability develops on the liquid surface due to the interaction between the liquid column and the crossflow, which causes the liquid column to break up into small droplets. In addition, because of the flow direction change by the manifold structure, the water injected from the rear of the injector is compressed by the flow and spreads in the form of thin sheet. The droplets produced by the breakup evaporate by the high temperature gas flow, and the water vapor reacts with magnesium fuel so that the temperature rises rapidly to 4000 K like combust gas temperature. The high-temperature combustion gas is cooled by the secondary water injection which protect the structure and increase the thrust.

Acknowledgements

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