Numerical Study on an Euler-Euler model for Liquid-Gas Two-Phase Detonation in n-Heptane/Air Mixture

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Introduction

Detonation is a fast and powerful combustion process characterized by high-pressure shock waves and supersonic flame propagation, offering high combustion efficiency [1–5]. In two-phase detonation involving liquid fuels, the interaction between shock waves and chemical reaction zones becomes more complex. Key factors such as the equivalence ratio and the size of fuel droplets play a critical role in determining the stability and propagation characteristics of the detonation wave [6–10]. To better understand and predict these complex interactions, various computational approaches have been utilized. The Eulerian–Eulerian (EE) model has been widely adopted for its efficiency in large-scale simulations by treating both gas and liquid phases as continuous media. For example, Nicolas et al. (2012) [11] demonstrated EE-based results comparable with experimental observations by Benmahammed et al. (2013) [12]. However, despite its strengths, the EE model suffers from limitations in capturing detailed droplet–gas interactions and tracking the motion of individual particles [13–15]. In this study, we conduct 2D numerical simulations of n-heptane–air detonation using the EE model to analyze the effects of fuel droplet distribution and equivalence ratio under high-temperature and high-pressure ignition conditions. The current simulations focus on evaluating the impact of droplet size distributions on detonation wave regularity and structure. Furthermore, to enhance the fidelity of localized phenomena such as droplet breakup and evaporation, a hybrid EE–EL model is being developed as a future extension. The Eulerian–Lagrangian (EL) approach enables detailed tracking of individual droplets, albeit with higher computational costs, making the hybrid framework a promising compromise between accuracy and efficiency. The results provide valuable insights into the coupling effects between droplet dynamics and combustion wave stability, offering potential for optimized fuel spray design in applications such as rotating detonation engines (RDEs). The hybrid model framework is expected to play a key role in bridging the gap between real-world physics and numerical predictions.

Numerical Method

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The EE model is employed to describe the macroscopic behavior of the continuous gas-phase field, capturing the evolution of pressure, temperature, species concentration, and detonation wave propagation. Simultaneously, it is utilized to resolve the discrete motion and phase transition of liquid droplet and solid particles, tracking their velocity, size distribution, evaporation, and interaction with the surrounding gas. The hybrid model integrates these two approaches by coupling mass, momentum, energy, and chemical source terms, ensuring consistent and accurate exchange of information between the gas and droplet phases. The special attention is given to the modeling of key interactions, including drag forces, heat transfer, and fuel evaporation, which are critical for accurately predicting detonation behavior. A detonation tube, which is the computational zone for this study, is illustrated in Fig. 1.

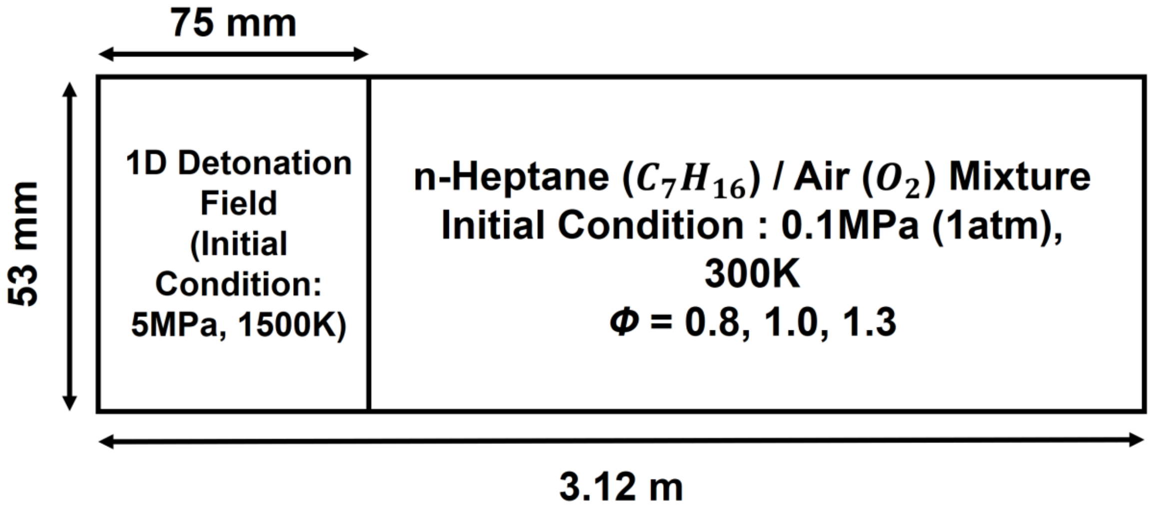

Figure 1: Detailed detonation channel dimension.

The ignition zone was computed by applying the EE model to the 1D detonation field. It is where a detonation is initialized, chaotic and rapid reactions between fuel and oxidizer begin, and strong pressure waves are generated. Since the reaction is very intense, the EE model is applied because the identification of the reaction rate and heat transfer mechanism is more important than the identification of the fine fuel distribution and interactions between fuels. The diffusion region is then applied with the EE-EL hybrid model. The center of the channel is where the detonation wave spreads stably, and the evaporation of droplets and their interaction with the gas play an important role. In particular, the droplet size distribution and evaporation rate affect the waveform and stability of detonation. Therefore, the EE model is applied to the center of the channel to model the interaction between droplet motion and gas in detail. The EL model is used near the wall because the droplet density is low and the gas flow plays a more important role. Here, the height of the center, which is the application section of the EL model, is changed to optimize the accuracy and computational resources. Additional initial values and parameters are listed in Table 1.

Table 1: Detailed inital values of detonation environment

Type	Value	Type	Value
Initial Pressure (P_0)	0.1 MPa	Initial Temperature (T_0)	300 K

Ignition Pressure (P_2)	5 MPa	Initial Temperature (T_2)	1500 K
Equivalence Ratio (Φ)	0.8, 1.0, 1.3		
The number of sample size	1, 5, 13, 15		
Diameter of droplet	30 μm		

Results and Discussion

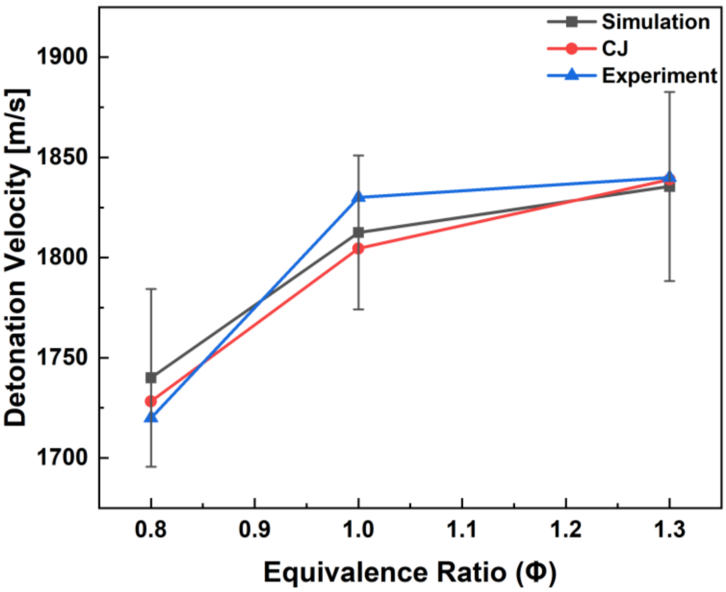

Figure 2: 2D EE model detonation velocity comparison results.

Figure 2 depicts the results of the 2D numerical simulation based on the Eulerian–Eulerian (EE) model that demonstrated a high degree of agreement with the experimental results, with a deviation of less than 3% in detonation velocity. This confirms the model's validity in capturing two-phase detonation behavior under high-temperature and high-pressure conditions. Additionally, it was observed that the detonation velocity increases with the equivalence ratio (Φ). This is primarily due to the enhanced chemical reactivity in fuel-rich conditions. As the equivalence ratio increases, the availability of fuel relative to oxidizer increases, which leads to higher heat release rates and elevated flame temperatures. Consequently, the energy driving the detonation front becomes stronger, resulting in faster propagation speeds. However, it is also important to note that excessively rich mixtures can lead to incomplete combustion and instability. Thus, there exists an optimal range of Φ where both high detonation velocity and stability can be achieved.

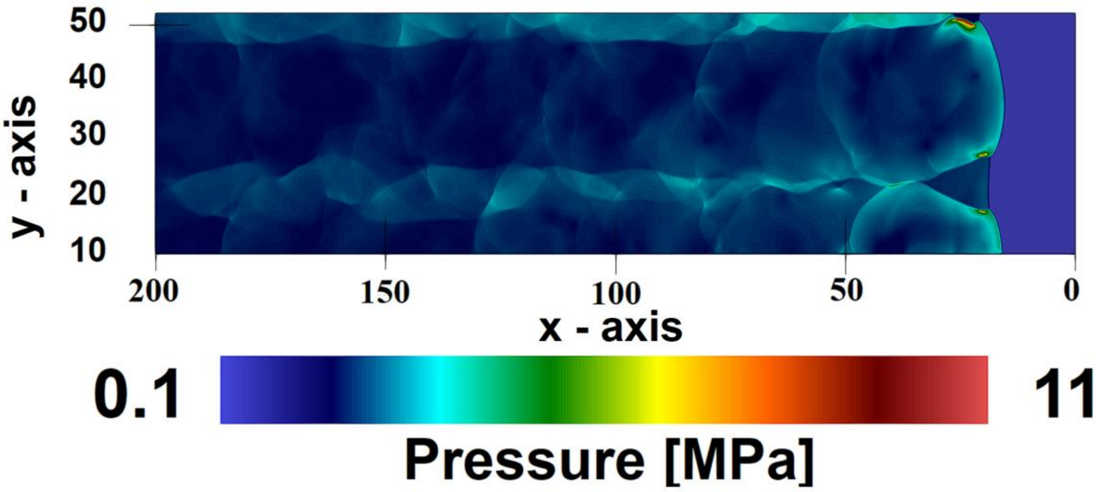

Figure 3: 2D EE model detonation result contours of instantaneous pressure.

The numerical results for the 2-dimensional (2D) detonation tube, especially the the result of the instantaneous pressure and temperature contours are shown in Fig. 3. These contours are the results at the location of 200 mm from the end of the channel, where detonation propagates with high pressure and temperature due to shock waves after the initial ignition. In the process, the leading shock wave is observed to rapidly increase at pressure and temperature, and the chemical reaction that provides the energy to sustain the shock wave continues. In the case of pressure profile, the Mach stem, incident shock, triple point, and transverse wave are observed. And, the temperature of the liquid fuel reaches at a high temperature very quickly and it can be confirmed that the reaction takes place.

In the final stage, the stability parameter is applied to evaluate the stable and continuous diffusion of detonation. This follows the equation (1):

$$X = \epsilon_I \frac{\Delta_I}{\Delta_e} \quad (1)$$

The X stands for the stability parameter of Eq. 1, where ϵ_I, Δ_I, Δ_e are for global activation energy, induction length, and energy pulse width, respectively. The stability parameter's dependence on droplet size and equivalence ratio is discussed by linking microscopic dynamics to macroscopic detonation behavior. To validate the proposed hybrid framework, the numerical results are compared against the experimental data of Benmahammed et al. (2013) [12] for detonation waves propagating in liquid-fueled environments. Key metrics such as detonation velocity, pressure profiles, and detonation cellular structure, are evaluated showing strong agreement with the experimental observations. The present study also evaluates computational challenges, such as ensuring numerical stability during gas-droplet interaction and mitigating the increased computational cost of coupling EE and EL models. The strategies to address these challenges, including parallel computing and adequate meshing, are discussed.

Conclusions

In conclusion, this study demonstrates the potential of a hybrid Eulerian–Eulerian and Eulerian–Lagrangian (EE–EL) modeling approach for analyzing multiphase detonation phenomena. Preliminary simulations using the EE model have shown that droplet size distribution and equivalence ratio significantly influence the stability and structure of the detonation wave. Building upon these findings, the proposed hybrid EE–EL framework aims to enhance simulation fidelity by capturing both the macroscopic wave behavior and detailed droplet-gas interactions. This approach is particularly valuable for applications in aerospace propulsion systems, such as rotating detonation engines (RDEs) and supersonic combustors, where precise control over combustion dynamics is essential. Future work will expand this framework to include three-dimensional simulations and incorporate additional physical processes such as droplet fragmentation, secondary atomization, and real spray dispersion patterns to improve the predictive capability and practical relevance of the model.

Acknowledgments

This research was conducted on the SQUID supercomputer of the Cybermedia Center of Osaka University.

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