

Numerical study on Ethanol/Air two-phase detonation

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1 Introduction

Weber[1] and Cramer[2] were the first to perform spray detonation experiment. Their experiments were conducted in a vertical shock tube with several spray nozzles on the tube wall. Dabora et al.[3] reported that detonation velocity is lower than the ideal Chapman-Jouguet value and it decelerates due to the big droplet size. Borisov et al.[4] investigated a model of two-phase detonation including droplet breakup and vapor processes theoretically. They considered a droplet deformation and stripping mechanisms. It becomes difficult to get steady detonation, since the evaporation of droplets is delayed when droplets are greater than 10 μ m. Furthermore, the stripping mechanism caused in such a long reaction zone that the heat losses from zone should lead to detonation failure. Bowen et al.[5] investigated detonation using decane which droplet diameter was estimated about 2 μ m, then droplet shattering and stripping could be neglected.

In this study, we numerically analyze two phase detonation using ethanol/ air to comprehend the fuel concentration effect on the detonation cell width.

2 Numerical method

2.1 Governing equations

A compressible Euler equation is used as a governing equation. Discretization of the governing equation is the followings: the Harten-Yee TVD scheme is used for the gaseous phase; the Godunov-type MUSCL Hancock TVD scheme for the liquid phase; and the 2nd order accuracy Strang-type fractional step for the time integration. Since the system equations are inhomogeneous an adaptive mesh refinement method is applied for the numerical grid system. This method is that the finer grid system is set by a condition of density gradient in a grid to get a higher space resolution and has a merit of constructing a system to concentrate grids at a shock wave and detonation wave with fewer grid numbers. Figure 1 shows a schematic diagram of moving grid system used in the present analysis to reduce the numerical cost.

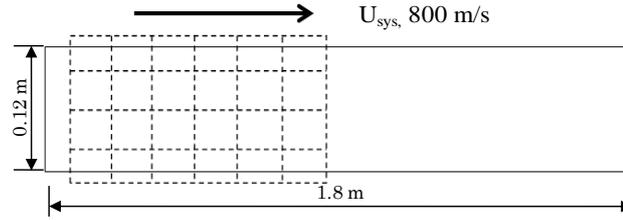
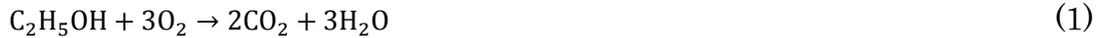


Fig.1 A schematic diagram of the moving grid system used in the present calculation. The width is 0.12 m and the length is 1.8 m.

2.2 Chemical reaction model

There are several ethanol detailed reaction models. Most of them have several hundred elementary reaction steps and computational cost is too expensive. Then the present computation uses a one step overall reaction model developed by Westbrook and Dryer[6] as follows;



$$\omega_1 = k_1 [\text{C}_2\text{H}_5\text{OH}]^{0.15} [\text{O}_2]^{1.5} \quad (2)$$

$$k_1 = 1.5 \times 10^{12} \exp\left(\frac{12600}{RT}\right) \quad (3)$$

where ω_1 is the reaction rate and k_1 is the reaction constant of ethanol.

2.3 Evaporation model

In this two-phase model, when the droplet is heated by a surrounding gas, it evaporates. After it evaporation, it starts to burn in the gas phase. In our computations a simplified combustion law of d^2 -type is employed. The mass transfer factor Δc which droplet evaporates and transfers from liquid phase to gas phase is explained as:

$$\Delta c = \frac{3\rho_l\phi_l}{\tau} (1 + 0.276\sqrt{\text{Re}}) \quad (4)$$

where ρ_l is the fuel density, ϕ_l the liquid phase volume percent, Re the Reynolds number, τ the characteristic time for combustion, which is expressed as:

$$\tau = K_r d_0^2 \quad (5)$$

where d_0 is a diameter of initial droplet and K_r combustion rate constant, which is expressed as:

$$K_r = \frac{\rho_l C_{pg}}{8\lambda \ln(1+B)} \quad (6)$$

where C_{pg} is the specific heat of gas, λ is the thermal conductivity, and B is the transfer number. The mass transfer number B is proportional to the amount of ethanol in the mixture and droplet diameter.

3 Results and discussion

Figure 2 shows the relation of detonation cell width with the fuel concentration at the droplet size of $3\mu\text{m}$. Those results were obtained from 10 detonation cells. The circles are their average value, the error bar implies the maximum and minimum value. The average cell width increases for the higher fuel concentration. And Figure 3 shows the trace of maximum pressure at the fuel concentration of (a) 0.03, (b) 0.06 and (c) 0.12 kg/m^3 . It found from (a) and (b) that the detonation cell width is larger when fuel concentration is higher. In the case of (c), there are unsteady small cells. And in the higher fuel concentration case, the trace of detonation cell line is significantly thicker, since the evaporation needs a longer time when the fuel concentration is higher and transverse wave is stronger because the induction time was longer. Figure 4 shows the gas phase temperature distribution at the fuel concentration of 0.13 kg/m^3 . This condition is that detonation does not propagate. It is found that behind shock, temperature is lower. Therefore there are the heat losses because of evaporation behind the shock. The amount of change to the vapor phase increases and the evaporation energy becomes higher.

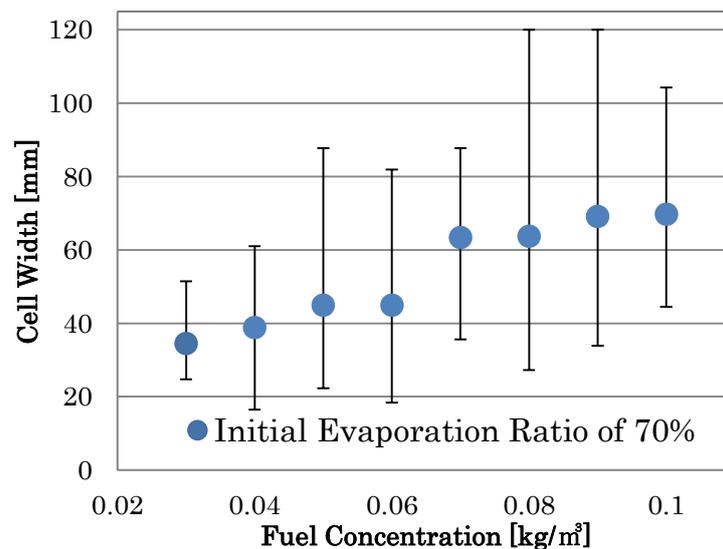
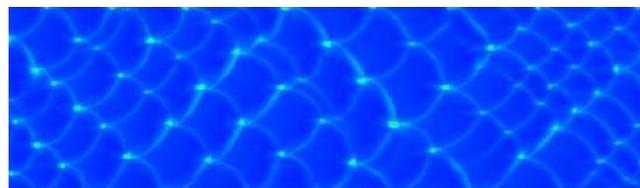
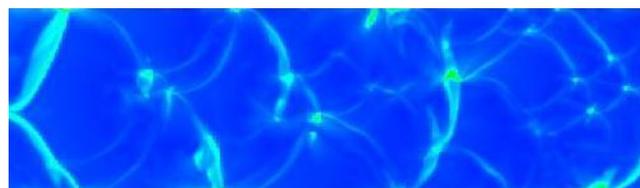


Fig.2 Detonation cell width with different fuel concentration at $3\mu\text{m}$ of droplet



(a) Fuel concentration 0.03 kg/m^3



(b) Fuel concentration 0.09 kg/m^3

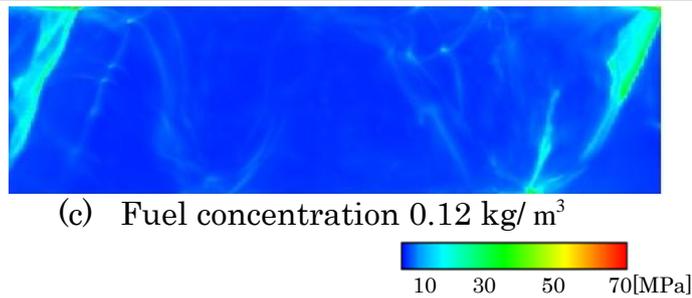
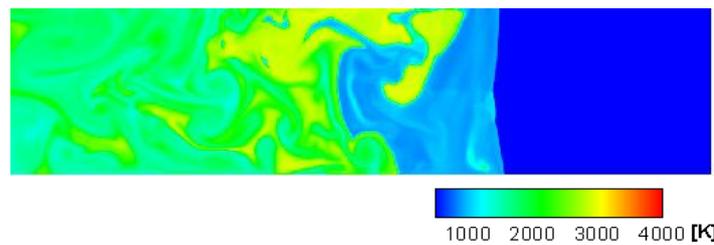


Fig.3 Trace of the maximum pressure of gas.

Fig.4 Temperature distribution of gas phase at fuel concentration 0.13 kg/m^3

4 Conclusion

We studied the relationship between the detonation cell width and the liquid fuel concentration from 0.03 to 0.13 kg/m^3 at the droplet size of $3 \mu\text{m}$ and the initial evaporation ratio of 70%. Analyzing the liquid and gas two-phase detonation using Ethanol/Air, its detonation cell width is bigger as fuel concentration is richer. However in the case at the fuel concentration of 0.13 kg/m^3 , the detonation does not propagate, hence this value could be the upper limit.

Acknowledgments

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References

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