Multiscale modeling on shock-cool flame interaction with DME/Air mixture

E Fan, Tianhan Zhang Department of Mechanics and Aerospace Engineering, SUSTech Shenzhen, Guangdong, China

Abstract

In this study, we numerically model the interaction between a planar shock wave and spherical cool flames using an adaptive mesh refinement solver at various shock strengths. For weak incident shocks (M = 1.2, 1.6, 2.1), cool flames are compressed by the shock, and their unsteady evolution is similar to the typical shock-light bubble interaction phenomenon. However, for a strong incident shock (M = 2.6), cool flames transition to hot flames shortly after the interaction, significantly affecting the evolution of the flame front.

1. Introduction

Studies on low-temperature chemistry (LTC), cool flame dynamics, and the transition regime between the cool and hot flames are essential to facilitate next-generation engine design. For high-performance engines, high compression ratio leads to high pressures, where the reduction of ignition delay time and the formation of temperature and concentration gradients following low-temperature ignition (LTI) may result in super-knock, which is widely accepted to be caused by deflagration-to-detonation (DDT) process [1].

In this study, we employ the finite volume method to investigate the interaction between a planar shock and spherical cool flames, assuming axisymmetry for simplicity. The computational domain is initially filled with DME/Air mixtures at the stoichiometric ratio of 500 K and 1 atm. Prior to the interaction, cool flames are prepared by igniting the premixture with a 2 mm radius hot spot at 1100 K. Following ignition, a planar shock wave is introduced according to the Rankine-Hugoniot relations when the flame radius reaches 1 cm. The shock Mach number is varied between 1.1 and 2.6.

We solve the compressible multi-component reactive flow using the adaptive mesh refinement (AMR) solver ECOGEN::Fire [2], which has been validated for reacting shock-bubble interactions and detonation problems. The inviscid fluxes are solved using the HLLC solver and MUSCL schemes, while the viscous fluxes are solved using a 2nd-order central scheme, and a 2nd-order Runge-Kutta scheme is used for the temporal advancement. The chemical process is solved through a splitting approach using the CANTERA package [3]. To model the DME/Air mixture, we adopt a 39-species skeletal mechanism

E. Fan

[4]. The minimum grid size at the shock and flame fronts is around 62.5 mm, which achieves grid convergence, as proposed by Zhang et al. [5].



2 Results and Discussion

Figure 1: Contour plots for the shock-cool flame interaction at different incident shock strengths. In each subfigure, the upper regions depict the temperature, and the lower regions depict the HRR.

Figure 1 shows the instantaneous temperature and heat release rate (HRR) contours at various incident shock strengths. The incident shock propagates from the left side of the computational domain. Before reaching the right boundary of the domain, cool flames are observed in the M = 1.2, 1.6, and 2.1 cases. However, in the M = 2.6 case, cool flames transition to hot flames at 46 µs when the flame temperature reaches around 1700 K. In cases where cool flames persist ($M \le 2.6$), unsteady flame evolutions display typical shock-light bubble interaction phenomena. As the burnt gas is lighter than the unburnt one, the transmitted shock is divergent, and shock waves distort the spherical flame into a vortex tube. For the M = 1.2 case, the upstream flame fronts are initially flattened by the compression of shock waves (200 μ s), and two lobes begin to form, which continue to grow and connect through a thin strand (800 μ s), later the flame vortex becomes separated (1066 μ s). For the M = 2.1 case, the streamwise reaction zone is long, which may be due to the degeneration of the secondary vortex [6] by low-temperature reaction. In the M = 2.6 case, hot flames occur 46 µs after the incident shock has fully passed the flame fronts. The hot flame fronts propagate inside the lighter bubble, which is mostly filled with the products of cool flames. After the transition to hot flames, a pair of vortices appear but remain connected in the computational domain. The small-scale structures in the vortex disappear due to the significant HRR in hot flames.

29th ICDERS - July 23-28, 2023 - Siheung

E. Fan

3 Conclusion

In this numerical study, we have found that the interaction between a planar shock and cool flame can lead to a transition to hot flame at an appropriate shock strength. In future work, we will conduct a detailed analysis, including an examination of the fuel consumption rate, heat release rate, and unsteady shock-cool flame interaction at the initial stage.

References

[1] Y. Ju, C. B. Reuter, O. R. Yehia, T. I. Farouk, and S. H. Won, "Dynamics of cool flames," *Progress in Energy and Combustion Science*, vol. 75, p. 100787, Nov. 2019, doi: 10.1016/j.pecs.2019.100787.

[2] E. Fan, J. Hao, B. Guan, C. Wen, and L. Shi, "Numerical investigation on reacting shockbubble interaction at a low Mach limit," *Combustion and Flame*, vol. 241, p. 112085, Jul. 2022, doi: 10.1016/j.combustflame.2022.112085.

[3] D. G. Goodwin, R. L. Speth, H. K. Moffat, and B. W. Weber, *Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes.* 2018. doi: 10.5281/zenodo.1174508.

[4] A. Bhagatwala, Z. Luo, H. Shen, J. A. Sutton, T. Lu, and J. H. Chen, "Numerical and experimental investigation of turbulent DME jet flames," *Proceedings of the Combustion Institute*, vol. 35, no. 2, pp. 1157–1166, 2015.

[5] W. Zhang, M. Faqih, X. Gou, and Z. Chen, "Numerical study on the transient evolution of a premixed cool flame," *Combustion and Flame*, vol. 187, pp. 129–136, Jan. 2018, doi: 10.1016/j.combustflame.2017.09.009.

[6] D. Ranjan, J. Oakley, and R. Bonazza, "Shock-Bubble Interactions," *Annual Review of Fluid Mechanics*, vol. 43, no. 1, pp. 117–140, Jan. 2011, doi: 10.1146/annurev-fluid-122109-160744.