Two-dimensional detonation propagation in partially prevaporized *n*-heptane sprays

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Abstract

Detonation is a shock-induced combustion wave with high-energy release rate and high pressure. Due to the promising application in propulsion, such as the pulse detonation engine (PDE) and the rotating detonation engine (RDE), the detonation structures and its propagation characteristics have been investigated by many researchers. In previous studies, most work are mainly focused on the detonation propagation in gaseous fuel/oxidizer mixtures. However, realistic hydrocarbon liquid fuels should be used in future practical applications, due to their higher energy density and easier storage. Therefore, it is necessary to study the behaviors of detonation propagation in liquid fuel/oxidizer mixtures.

In the present work, two-dimensional detonation propagation in partially prevaporized *n*-heptane sprays is studied by using Eulerian–Lagrangian method. For the gas phase, the Navier–Stokes equations, together with the equations of species mass fractions, are solved. The liquid phase is modeled as a spray of spherical droplets tracked by the Lagrangian method. The inter-droplet interactions are neglected with the assumption of dilute sprays, i.e. volume fraction < 0.001. The calculations are based on a developed solver *RYrhoCentralFoam* in the framework of the open-source code OpenFOAM-5.0. A two-step kinetic model [1] is adopted for the n-heptane/air combustion. A rectangular computational domain (as shown in Fig. 1) is used. The length (*x*-direction) and height (*y*-direction) of the domain are 300 mm and 20 mm, respectively. The initial pressure and temperature of *n*-heptane/air mixtures are 0.5 atm and 300 K, respectively. Hot spots with high temperature (2000 K) and pressure (50 atm) are used to ignite the detonation wave.

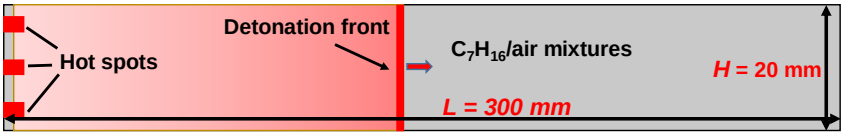

Fig. 1 Computational domain of two-dimensional detonation propagation.

The present work includes two parts. In the first step, the two-step *n*-heptane/air reaction mechanism is first validated by using the SD Toolbox [2] in terms of pressure and temperature at the Chapman–Jouguet (CJ) and von-Neumann (VN) conditions. The results are compared with that of a skeletal mechanism [3] and show good agreement. The two-dimensional detonation waves propagating in

gaseous *n*-heptane/air mixtures are investigated to further verify the computational code and chemical mechanism. It is shown that the two-dimensional detonation propagation speed and cell size are close to the theoretical value from the SD Toolbox. In addition, the detailed detonation structures are captured in the two-dimensional detonation simulations with proper mesh size. In the second step, the two-dimensional detonation propagating in partially prevaporized *n*-heptane sprays is simulated with different pre-vaporization degrees, diameters, and number density of droplets. The effects of the pre-vaporization degrees, diameters, and number density of droplets on the detonation propagation speed, structures, instability, and cell size are discussed and analyzed.

Reference:

[1] C.K. Westbrook, F.L. Dryer, Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames, Combust. Sci. Technol. 27 (1981) 31–43.

[2] Joe Shepherd, Shock and Detonation Toolbox, Https://Shepherd.Caltech.Edu/EDL/PublicResources/Sdt/.

[3] S. Liu, J.C. Hewson, J.H. Chen, H. Pitsch, Effects of strain rate on high-pressure nonpremixed n-heptane autoignition in counterflow, Combust. Flame. 137 (2004) 320–339.