

# Initiation characteristics of wedge-induced oblique detonations in partially pre-vaporized n–heptane sprays

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## 1 Introduction

The oblique detonation wave (ODW) is one kind of extreme combustion which can be induced by a wedge in an incoming, supersonic combustible mixture. Due to compression of the leading shock, ODWs can achieve high thermal efficiency. As a pressure-gain combustion, ODWs have the potential application to ram accelerators [1] or oblique detonation engines (ODEs) [2,3]. In the previous studies, many basic foundations for ODWs in gaseous mixtures such as the initiation structures [4] and wave angles have been established. Besides, some theoretical analysis of ODWs have also been performed with gaseous mixtures [5,6]. These issues of ODWs in liquid fuels such as kerosene or n–heptane mixtures have seldom been reported. However, liquid fuels have the advantages of higher energy density and easier storage and have been widely used in existing propulsion systems [7]. It is necessary to expand the fundamental knowledge of ODWs in liquid fuels as a scientific foundation to facilitate liquid fuels applications in ODE.

For the liquid-gas two-phase ODWs, some works have been performed to study the oblique detonation wave systems. Ren et al. [8] carried out a numerical study of ODWs in two-phase kerosene-air mixtures using the Eulerian–Lagrangian method for the first time to best of our knowledge and the initiation features of two-phase ODWs with different droplet diameters of inflow liquid kerosene are investigated, demonstrating that as increasing droplet diameter, the morphology of ODWs changes from the abrupt wave system to the smooth wave system and the initiation lengths will decrease. Soon afterwards, Ren et al. [9] investigated the effect of the equivalence ratio of the liquid kerosene fuels on ODWs and found that the evaporative cooling effects have more influence in the fuel-lean side, but the heat release effects predominate in the fuel-rich side. However, these above-mentioned investigations used a two-step global chemical reaction model to simulate the detonation combustion and it cannot mimic the accurate heat release processes and reaction rates of all species. Recent researches have demonstrated that the initiation structures are strongly dependent on the chosen reaction models [10]. Besides, the liquid droplets in previous studies is usually assumed to be no pre-vaporized, which does not accord with the practical scenario. Considering the application of ODWs in airbreathing engines in which the airstream is compressed by the inlet and the gas temperature is far large than ambient temperature, the liquid fuel

droplets will be partially evaporated before entering the combustion chamber. Hence, the effects of partially pre-vaporized liquid fuel on ODWs should be considered to facilitate liquid fuels applications in ODE.

Using the hybrid Eulerian–Lagrangian method, the ODWs in partially pre-vaporized n–heptane sprays and air mixtures are numerically simulated to study their structural features with different liquid droplet diameters in this study. The initiation structures of ODWs in dilute sprays present unsteady process, including the appearance of the hot spots, re-formation of new normal detonation waves and the normal detonation waves moving backward. Furthermore, to quantify the scales and the unsteady behaviors of ODWs with different diameters, the initiation lengths are tested. The present results revealing that the initiation lengths of ODWs in partially pre-vaporized n–heptane droplets increase with small diameters and decrease with large diameters, different from those in liquid kerosene and air mixtures and never been reported before. This change of the initiation lengths is well explained by proposing a non-dimensionalized parameter of the amount of transferred heat caused by droplets evaporation and the analyzation of the heat transfer rates along the streamlines. Besides, the main factor caused this unsteady behavior is discussed through calculation of the theoretical initiation lengths.

## 2 Physical Models and Numerical Methods

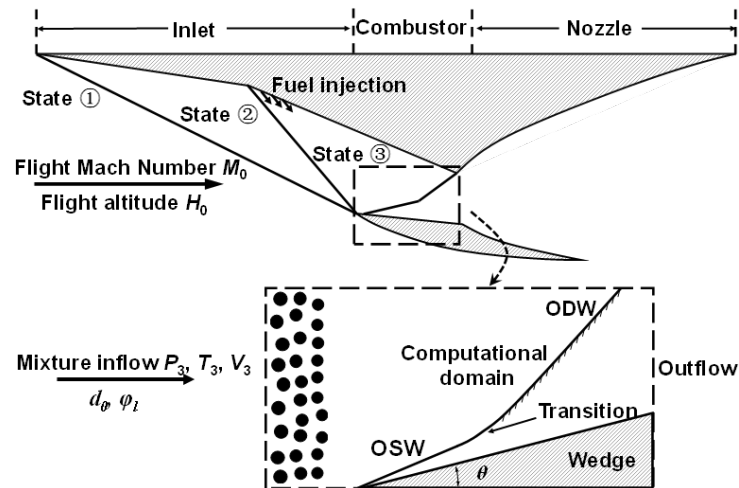


Fig. 1. Schematics of oblique detonation engine and computational zone.

The schematic of an ODE is used in this work and as shown in Fig. 1, in which the wedge-induced ODW is present. The engine inlet wave configuration is proposed by Dubebout et al. [11] and employed in later researches [12]. Following this configuration, the high-altitude air inflow is assumed to be compressed by two equal-strength oblique shock waves (OSWs) to minimize the entropy increase. Due to the lack of referential engines so far, the injection process is not modeled here. Similar to previous studies [13,14], the inflow fuel-air is assumed to be well-premixed. The supersonic homogeneous inflow reflects on the two-dimensional wedge to generate an OSW and the high post-shock temperature triggers an exothermic chemical reaction and then induces ODW initiation downstream. As shown in Fig. 1, the computational zone used in this study is represented by the region enclosed by the dashed lines. The structured grids are used and the mesh is uniform distribution along the x- and y-direction.

In this study, the hybrid Eulerian–Lagrangian method is employed. The Eulerian gas and Lagrangian liquid droplet governing equations are solved by a compressible two-phase reacting flow solver, RYrhoCentralFoam [15,16]. It is developed from rhoCentralFoam in OpenFOAM 6.0. For the gas phase, the multi-species Navier–Stokes equations are solved. The liquid phase is modeled as a spray of spherical droplets tracked by Lagrangian method. The inter-droplet interactions are neglected since

dilute sprays (volume fraction  $< 0.001$  [17]) are considered. The hybrid Eulerian–Lagrangian method used here has been carefully validated for two-phase detonation [18–21], including the numerical study of two-phase ODEs [18], which will not detailed repeat it here. Moreover, the liquid fuel of n-heptane is considered and the chemical kinetics model used in this study is a skeletal mechanism of 44 species and 112 reactions [22] for n-heptane/air combustion.

For the boundary conditions, inflow condition is used for the left boundary of the computational zone and the zero gradient condition is used for the right and upper boundaries. Some early studies [23] have pointed out that boundary layer effects are negligible under very high Reynolds number. Some recent studies [24,25] have demonstrated that the boundary layer may change the ODW structures, but the effects are weak and limited near the wedge in some cases with thick boundary layers. For the cases in this study, the thickness of boundary layer near the ignition position is below 5.0% of the induction zone height and the Re number is on the order of  $10^6$ . Hence, following previous ODW studies, the slip reflecting boundary condition is used and the effect of the boundary layer will be investigated in the future work. On the right of the left boundary, the wedge starts from the  $x = 0.01$  m. Because of the multi-scale nature of the phenomena, the computational zone and mesh scale are adjusted respectively.

To consider the specific flight conditions, the controlling parameters of pre-detonation mixtures are the flight altitude  $H_0$  and Mach number  $M_0$ . According to the standard atmosphere, the pressure  $P_0$  and temperature  $T_0$  of free inflow are determined by  $H_0$  and the velocity  $V_0$  which is obtained from Mach number  $M_0$  and the local sonic speed  $a_0$ . The air inflow is assumed to be compressed by two equal-strength OSWs and based on Rankine–Hugoniot relation with a total deflection angle of  $20^\circ$ , the flow parameters after the compression are calculated and taken as the inflow parameters before the ODW. In this study,  $H_0$  and  $M_0$  are fixed as 30 km and 9.0. Based on the methods introduced above, the pre-detonation parameters are calculated and the inflow temperature  $T_3$ , pressure  $P_3$  and velocity  $V_3$  are 697 K, 28554 Pa and 2535 m/s, respectively. The cases with pure gas and partially pre-vaporized n-heptane/air mixture are both simulated and the total equivalence ratio is 1.0 for all the cases. The liquid fuel is modeled as mono-dispersed droplets and the droplets equivalence ratios are 0.3 and the gas equivalence ratios are 0.7 for all two-phase cases. The distribution of liquid droplet diameters  $d_0$  is considered to be uniform at left boundary and ranging from 1 to 25  $\mu\text{m}$ . The initial temperature of droplets is fixed as 300 K for all cases. The angle of the wedge that supersonic inflow reflects on is fixed as  $27^\circ$ .

### 3 Results and discussion

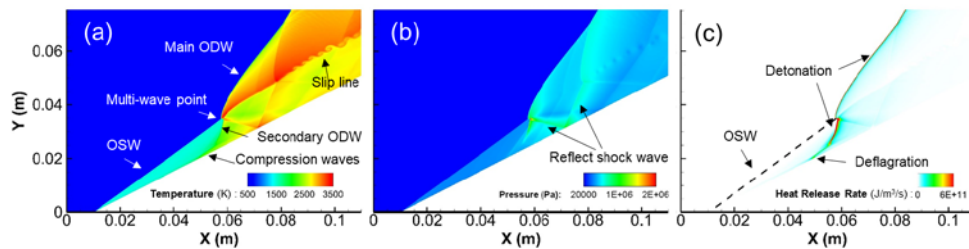


Fig. 2. Temperature (a), pressure (b) and heat release rate (c) fields in the pure gas mixture.

The case in the pure gas mixture of n-heptane/air is simulated as the base case first, as shown in Fig. 2 by temperature, pressure and heat release rate. First of all, the ODW is initiated in a short distance at such condition and the position of the OSW–ODW transition is around 0.06 m. The OSW–ODW transition is an abrupt type and the OSW and main ODW is connected by a multi-wave point. From the multi-wave point, the reflect shock wave and slip line extend downstream. In the initiation region upstream, the compression waves caused by the heat release of deflagrations arise from the wedge and

converge to a secondary ODW. Despite of different chemical reaction mechanisms, this morphology is a typical wave system named ‘TYPE III’ in ref. [21].

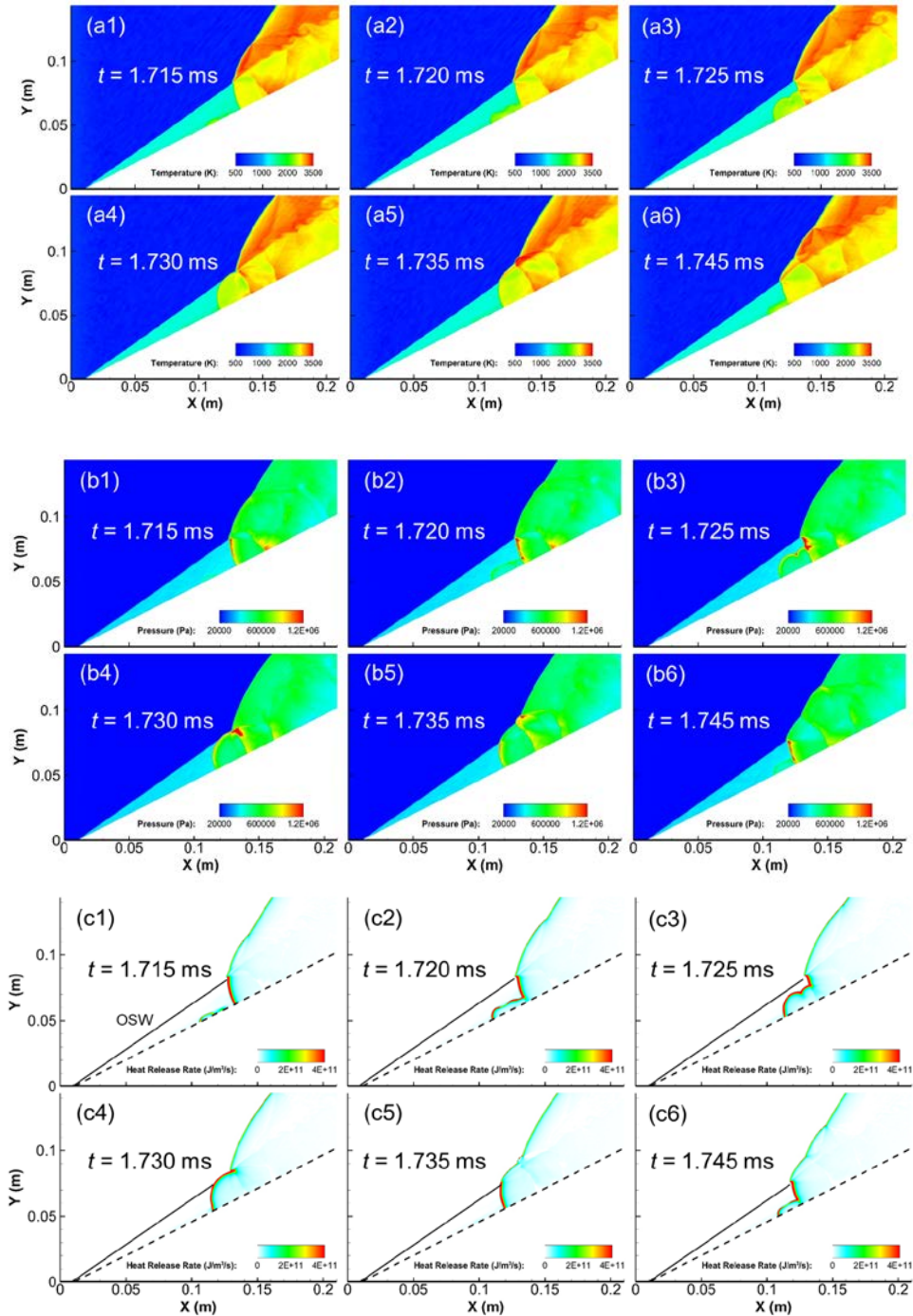


Fig. 3. Temperature (a), pressure (b) and heat release rate (c) fields in partially pre-vaporized  $n$ -heptane sprays with  $d_0 = 2 \mu\text{m}$ .

The ODWs in partially pre-vaporized  $n$ -heptane/air mixture are simulated. The ODW with  $n$ -heptane sprays of droplet diameter  $d_0 = 2 \mu\text{m}$  presents an unsteady behavior and as shown in Fig. 3 and temperatures, pressures and heat release rates of six different times are displayed to illustrate the variation of the wave structure. When  $t = 1.715 \text{ ms}$ , as shown in Fig. 3(a1), the OSW–ODW transition

is abrupt. Notably, the OSW–ODW transition position is around 0.13 m, longer than that of the case in pure gas mixtures due to the endotherm of droplet evaporation. The OSW and ODW is connected with a multi-wave point. Beneath the multi-wave point, a normal detonation wave (NDW) with large heat release is displayed in Fig. 3(c1). This morphology is similar with the wave system named ‘TYPE IV’ in ref. [23]. Differently, in front of the NDW, some high temperature hot spots with small heat release appear near the wedge. As shown in Fig. 3(a2-a4), 3(b2-b4) and 3(c2-c4), the hot spots trigger the exothermic chemical reaction and a new wave with the intensity of detonation in the induction zone. The new detonation wave moves upward to the OSW and backward to the downstream simultaneously, resulting in a new NDW beneath the OSW and a triple point on the ODW surface as displayed in Fig. 3(a5), 3(b5) and 3(c5). Subsequently, as shown in Fig. 3(a6), 3(b6) and 3(c6), the new NDW move backward and some new hot spots in front of the new NDW appear again. These new hot spots will transfer into a new NDW in successive times. In generally, this unsteady process with hot spots appearing and the new NDW re-forming repeats in the ODWs with partially pre-vaporized *n*-heptane/air mixture.

## 4 Conclusions

In this study, the ODWs in stoichiometric *n*-heptane-air mixtures with equivalence ratio of liquid fuel 30% and different liquid droplet diameters are simulated by using the Eulerian–Lagrangian method with a skeletal chemical mechanism. The results suggest that the initiation structures of ODWs with partially pre-vaporized *n*-heptane sprays are unsteady, and the unsteady process includes the appearance of the hot spots, re-formation of a new normal detonation wave (NDW) and the NDW moving backward. The scale of ODWs is quantified by the initiation lengths, and it is found that the fluctuation of the initiation lengths is relevant to this unsteady behavior.

For the cases with small inflow droplet diameters, the initiation lengths of ODWs increase with initial droplet diameter, which is different from the previous study [25]. Based on the analysis of a non-dimensionalized parameter of the amount of transferred heat, it is found that the reduction of initiation lengths is caused by the increase of transferred heat of droplets evaporation. However, for the cases with large droplet diameters ( $d_0 > 8 \mu\text{m}$ ), the initiation lengths decrease with the initial droplet diameters due to the reduction of the heat transfer rate behind the induction oblique shock wave, and a corresponding high-temperature zone accelerates the induction chemical reaction of the inflow gas mixtures.

The main reason that causes this unsteady behavior is analyzed by comparing the fluctuation amplitudes of the theoretical lengths and the numerical initiation lengths. It is found that the fluctuations of the post-shock temperatures caused by evaporation of dilute sprays dominate this unsteady behavior, while other parameters such as the have little impact. Moreover, when the temperatures fluctuate at a low-temperature range, the fluctuation amplitude of initiation lengths will be large and the initiation structure of ODWs will be more unsteady.

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