Modelling Rotating Detonative Combustion Fueled by Partially Pre-vaporized $n$-Heptane Sprays

Majie Zhao and Huangwei Zhang*

Department of Mechanical Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117576, Republic of Singapore

Abstract

Eulerian–Lagrangian simulations are conducted for two-dimensional Rotating Detonative Combustion (RDC) fueled by partially prevaporized $n$-heptane sprays. The influences of droplet diameter and total equivalence ratio on detonation combustion and droplet dynamics are studied. It is found that small $n$-heptane droplets (e.g. 5 µm) are completely vaporized around the detonation wave, while intermediate $n$-heptane droplets (e.g. 20 µm) are consumed in or behind the detonation wave, with the escaped ones be continuously evaporated and deflagrated. The detonated fuel fraction is high when the droplet diameters are small or large, reaching its minimal value with diameter being 20 µm. The detonation propagation speed decreases with increased droplet diameter and is almost constant when the diameter is larger (> 30 µm). The velocity deficits are 2—18% compared to the respective gaseous cases. Moreover, the propagation speed increases as the total equivalence ratio increases for the same droplet diameter. It is also found that the detonation propagation speed and detonated fuel fraction are considerably affected by the pre-vaporized gas equivalence ratio. Mixed premixed and non-premixed combustion modes are seen in two-phase RDC. The droplet distributions in the RDE combustor are significantly affected by the droplet evaporation behaviors.

Keywords: Rotating detonation combustion, $n$-heptane spray, partial pre-vaporization, reactant mixing, combustion mode, droplet diameter

* Corresponding author. E-mail: huangwei.zhang@nus.edu.sg. Tel: +65 6516 2557.
1. Introduction

Rotating Detonation Engine (RDE), as one of the pressure-gain combustion technologies, has the great potential to be commercialized. It has numerous advantages over other detonation engines (e.g. pulse detonation engines), including compact configuration, high frequency, high specific power output, and continuous existence of Rotating Detonation Waves (RDWs) [1,2]. In previous studies, gaseous fuels are mainly tested, including hydrogen and simple hydrocarbons [1–5]. However, a critical step towards practical RDE applications is to adapt liquid fuels, due to their higher energy density and easier storage.

The early studies on two-phase rotating detonation combustion (RDC) can date back to 1970s [6]. Various liquid fuels were tested by Bykovskii et al.[3], including kerosene, gasoline and diesel fuels over a range of operating conditions, and their results show that the RDW velocity and frequency decreases with the flow rate of the two-phase mixtures. They further studied the liquid kerosene / air mixture with addition of hydrogen or syngas [7,8], and highlighted the role of these additives in achieving stable RDWs. Moreover, they evaluated the effects of the heterogeneous mixtures on the overall RDE indices (e.g. specific impulse) [8]. The feasibility of liquid-fueled RDEs has also been confirmed by Kindracki [9]. In his experiments, successful RDW propagation with liquid kerosene was achieved through adding hydrogen and increasing the chamber temperature [9].

However, due to the limitations of the experimental techniques, detailed information insides the RDE channel is difficult to be measured, including the flow structure, combustion mode and droplet transient characteristics. Numerical simulation provides an alternate tool for studying the two-phase RDE. For instance, quenching mechanism in RDC with liquid JP-10 was studied recently by Hayashi et al. [10]. Our work aims to investigate the influences of liquid n-heptane properties (e.g. droplet diameter and pre-vaporization) on rotating detonation combustion and droplet evolutions in the combustor. Two-dimensional RDC model will be used and the liquid fuel is injected into a model RDE with a lean pre-vaporized n-heptane / air mixture.
2. Mathematical and physical models

2.1 Governing equations

In the present investigations, Eulerian–Lagrangian method is adopted to study the two-phase RDC. For the gas phase, the Navier–Stokes equations, together with the equations of species mass fractions, are solved [11]. 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 [12]) are considered. Also, the shock-induced break-up is not considered here, and its effects on RDC are small, which are shown in Supplemental Material. The equations of mass, momentum and energy for the liquid phase respectively read [12]

\[
\frac{dm_d}{dt} = -\dot{m}_d, \quad (1)
\]

\[
\frac{du_i, d}{dt} = \frac{F_{ld}}{m_d} \quad (2)
\]

\[
c_{p,d} \frac{dT_d}{dt} = \frac{Q_{s} + Q_{lat}}{m_d} \quad (3)
\]

where \( t \) is time. \( m_d = \pi \rho_d d^3 / 6 \) is the mass of a single droplet, where \( \rho_d \) and \( d \) are the droplet density and diameter, respectively. \( u_i, d \) is the droplet velocity component in \( i \)-th direction, \( c_{p,d} \) is the droplet heat capacity, and \( T_d \) is the droplet temperature. Infinite thermal conductivity of the droplet is assumed since small droplets are investigated.

The evaporation rate, \( \dot{m}_d \), in Eq. (1) is calculated with Abramzon and Sirignano model [13]

\[
\dot{m}_d = \pi d \rho_f D_f S_h ln(1 + B_M) \quad (4)
\]

where \( \rho_f \) and \( D_f \) are the density and mass diffusivity at the film and estimated based on one-third rule between the gas and liquid quantities [13]. This model is also used in other two-phase detonation simulations [14]. The modified Sherwood number \( \widetilde{S_h} \) is calculated as \( \widetilde{S_h} = 2 + [(1 + Re_d Sc)^{1/3} \max (1, Re_d)^{0.077} - 1] / F(B_M) \), with the Schmidt number being \( Sc = 1.0 \). \( F(\vartheta) = (1 + \vartheta)^{0.7} \ln(1 + \vartheta) / \vartheta \) is introduced to consider the variation of the film thickness due to Stefan flow.
effects [13]. Here $\theta$ represents the Spalding mass transfer number $B_M = (Y_{FS} - Y_{F\infty})/(1 - Y_{FS})$ or the Spalding heat transfer number $B_T$. $Y_{FS}$ and $Y_{F\infty}$ are the fuel vapor mass fractions at the droplet surface and gas phase, respectively. $Y_{FS}$ is calculated from its corresponding mole fraction $X_{FS}$, which is obtained from saturation pressure $P_{sat}$ based on Raoult's Law [15].

Only Stokes drag is included in Eq. (2), and modelled as $F_{i,d} = \frac{18 \mu_g C_d Re_d}{\rho_d d^2} m_d |u_{i,d} - u_{i,g}|$ [16]. $C_d$ is the drag coefficient and estimated using the Schiller and Naumann model [17]. $Re_d \equiv \rho_d d |u_{i,d} - u_{i,g}|/\mu_g$ is the droplet Reynolds number, where $\mu_g$ is gas dynamic viscosity and $u_{i,g}$ is the gas velocity component in $i$-th direction.

In Eq. (3), $\dot{Q}_c = h_c A_d (T_g - T_d)$ denotes the convective heat transfer between gas and liquid phases. Here $A_d$ is surface area of a single droplet. $h_c$ is the convective heat transfer coefficient, and estimated using the correlation of Ranz and Marshall [18] through the modified Nusselt number, i.e. $\overline{Nu} = 2 + [(1 + Re_d Pr)^{1/3} \max (1, Re_d)^{0.077} - 1]/F(B_T)$, where $k_g$ is the gas thermal conductivity and $Pr$ is the gas Prandtl number (assume to be unity here). Furthermore, $\dot{Q}_{lat}$ in Eq. (3) accounts for the heat transfer caused by the latent heat of evaporation.

Two-way coupling between gas and liquid phases are considered, in terms of mass, momentum, energy and species exchanges. Therefore, the source terms for the gas phase equations read ($V_c$ is cell volume and $N_d$ is the droplet number in a cell)

$$S_m = \frac{1}{V_c} \sum_1^{N_d} \dot{m}_d, \quad S_{i,F} = -\frac{1}{V_c} \sum_1^{N_d} F_{i,d}, \quad S_e = -\frac{1}{V_c} \sum_1^{N_d} (\dot{Q}_c + \dot{Q}_{lat})$$

$$S_{Y_m} = \begin{cases} S_m & \text{for the liquid fuel species,} \\ 0 & \text{for other species.} \end{cases}$$

(6a)

(6b)

2.2 Liquid-fueled RDE model

Figure 1 shows a two-dimensional (2D) rectangular domain, to mimic an annular RDE combustor. The soundness of 2D RDE modelling has been confirmed by numerous previous work (e.g. [11,19]).
The length ($x$-direction) of the domain is 280 mm (the equivalent diameter is around 90 mm), whereas the height ($y$-direction) is 100 mm. These scales are used in our previous RDE modelling [11], and are also comparable to those of laboratory-scale RDE combustors [20].

Fig. 1. Computational domain and boundary condition in two-dimensional RDE with $n$-heptane sprays. Background contour: gas temperature (200-3,000 K) of Case 2a (see details in Section 2.2).

The red zone with high pressure and temperature is used for RDW initiation at $t = 0$.

The boundary conditions are marked in Fig. 1. The outlet is assumed to be non-reflective. Periodic boundaries at the left and right sides are enforced, such that the RDW can continuously propagate inside the domain. The $n$-heptane liquid droplets are injected into the domain through 56 discrete inlets at the top head as schematically shown in Fig. 1. They are carried by premixture of air and $n$-heptane vapour, which is used to model the droplet partial pre-vaporization occurring in the upstream manifold before they enter the combustor. In the practical liquid fueled RDE experiments, some level of premixing is desirable to increase the detonability of the liquid propellant [3,9].

The wall surfaces between the discrete spray injectors are assumed to be non-slip, impermeable and adiabatic. The area ratio (in 2D case, length ratio) of the injector and wall is fixed to be 2:3. This ratio is selected based on our numerical experiments of droplet-free RDC with the same configuration, and it is found that with this ratio the RDW can propagate stably, without detonation front de-stabilization and chaotic propagation. The focus of this work is liquid fuel droplets effects on RDC and therefore it would
be favorable to rule out the above highly unsteady phenomena.

Four case groups parameterized by total equivalence ratio, \( \phi_t = \phi_g + \phi_l \), are considered, as listed in Table 1. Unless otherwise stated, the equivalence ratio of the premixed carrier gas is assumed as \( \phi_g = 0.6 \), whilst the liquid equivalence ratio \( \phi_l \) varies from 0.2 to 1.4, corresponding to \( \phi_t = 0.8–2.0 \) in Cases 1–4. Here \( \phi_l \) is defined as the mass ratio of the droplets to the oxidizer normalized by the mass ratio of \( n\text{-C}_7\text{H}_{16} \) vapor to air under stoichiometric condition. In each group, various initial diameters of mono-dispersed droplet \( d_0 \) are considered, ranging from 2 to 80 \( \mu \text{m} \). Three cases from Group 2 (i.e. \( \phi_t = 1.0 \)) will be studied in detail in Section 3, and respectively have \( d_0 = 5, 10 \) and 20 \( \mu \text{m} \). Hereafter, they are termed as Case 2a, 2b and 2c, respectively. In all the studied cases, the volume fractions \( \alpha \) of the injected spray are below 0.001 (see Table 1), confirming the dilute characteristics of the sprays.

| Case group | Total equivalence ratio \( \phi_t \) | Diameter \( d_0 \) (\( \mu \text{m} \)) | Volume fraction \( \alpha \) |
|------------|---------------------------------|---------------------------------|-----------------|
| 1          | 0.8                             |                                 | 0.00014         |
| 2          | 1.0                             | 2–80                            | 0.00028         |
| 3          | 1.5                             |                                 | 0.00064         |
| 4          | 2.0                             |                                 | 0.00099         |

Table 1. Liquid fuel spray information.

2.3 Numerical method

Both gas and liquid phase (i.e. Eqs. 1–3) equations are solved by a multi-component, two-phase, and reactive solver, \textit{RYrhoCentralFoam} [21], with two-way interphase coupling in terms of mass, momentum, energy and species (i.e. Eq. 6). For gas phase, it has been validated for gaseous supersonic flows and detonative combustion problems [11,21]. Satisfactory accuracies are achieved in capturing
supersonic flow discontinuity, detonation propagation speed, and detonation cell size. More information about the numerical schemes and solution strategies can be found in Refs. [11,21].

![Graph showing time evolution of droplet diameter and evaporation coefficient versus initial gas temperature.](image)

Fig. 2. (a) Time evolution of droplet diameter and (b) evaporation coefficient versus initial gas temperature. Experimental data from Ref. [22].

For the liquid phase, i.e. Eqs. (1)−(3), they are solved using first-order implicit Euler method, which is sufficiently accurate with the time step used in this work (about 10⁻⁹ s). The evaporation model [13] for droplet evaporation in RYrhoCentralFoam solver is validated here. Figure 2 shows the comparisons of diameter evolution against the measured data of single droplet (initial diameter \(d_0 = 1.285 \text{ mm}\)) evaporation under high ambient temperature (973 K) and pressure (2.0 MPa) [22]. From Fig. 2(a), the evaporation model well reproduces the diameter evolution. The duration initial expansion, caused by the heat conduction from the surrounding gas, is slightly over-predicted, but the evaporation coefficient (\(C_V\), slope of \(d^2 \sim t\) curve) corresponding to the steady evaporation (> 1.2 s) is reasonably predicted. The evaporation coefficients over a range of RDC relevant operating conditions (i.e. elevated pressures and temperatures) are further compared in Fig. 2(b) and the results demonstrate that the errors for the predicted \(C_V\) are generally less than 15%. Validations of the same model [13] under spray detonation conditions are also made in Ref. [14], and their results also confirm the accuracies of this model in
predicting droplet evaporation under RDC conditions.

The domain in Fig. 1 is discretized with 352,800 Cartesian cells. The cell size in the $x$-direction is uniform at 0.2 mm, whereas in the $y$-direction it increases from 0.1 mm at the top head to 1 mm at the outlet. Mesh sensitivity analysis of Case 2a (5 µm) are performed and the results (not included) show that the sensitivity of the major flow features (including RDW speed, slip line, contact surface and oblique shock wave) to a finer resolution (0.05–0.1 mm) is marginal. Similar resolutions (0.1–0.2 mm) are widely used in previous RDC modelling [11,23,24]. In addition, the above resolution is still larger than the considered droplet diameters, which can ensure that the gas phase quantities near the droplet surfaces (critical for estimating the two-phase coupling, e.g. evaporation) can be well approximated using the interpolated ones at the location of the sub-grid droplet [14].

One-step reaction of 5 species [25] is used for $n$-heptane detonation. Figure 3 shows the detonation propagation speeds in $n$-C$_7$H$_{16}$(gaseous) / O$_2$ and $n$-C$_7$H$_{16}$(droplets) / air mixtures and the accuracies of the one-step mechanism are examined through comparing the results with those from a skeletal mechanism [26] and experimental data [27,28]. Apparently, the results of gaseous $n$-C$_7$H$_{16}$ with one-step mechanism agree well with the experimental data and also those using the skeletal mechanism. Moreover, the detonation propagation speeds in mono-sized (5 µm) $n$-C$_7$H$_{16}$ droplet mists calculated with two mechanisms are very close, but both are slightly over-predicted (error 10.7%) relative to the experimental data [28]. This may be because the actual experimental conditions in gas–droplet detonations, e.g. uniformity of droplet distribution, are not quantified and therefore difficult to be fully reproduced in the simulations. In general, the accuracies of the global chemistry for calculating $n$-C$_7$H$_{16}$ / air detonation propagation are satisfactory. Further comparisons with one-step and skeletal mechanisms in 2D RDC are also made, including detonation propagation speed, detonated fuel fraction and mean droplet diameters. Excellent agreements are observed, which are available in Supplemental Material.
Fig. 3. Detonation propagation speeds with one-step and skeletal mechanisms. Experimental data from Refs. [27,28].

A rectangular region (280 mm × 12 mm) close to the head end are initialized with stoichiometric \( n \)-heptane / air mixture, whilst the rest domain is filled with air. A rectangular hot pocket (1 mm × 12 mm, see red zone in Fig. 1) with high temperature (2,000 K) and pressure (40 atm) is used to ignite the detonation wave. In this study, the total temperature \( T_0 \) and total pressure \( P_0 \) of the injected fuels are assumed to be 300 K and 10 atm, respectively. Variations in either of them affect the RDC dynamics [11], but are not studied in this work. The inlet pressure, temperature and velocity in the flow field are modelled based on the correlations between the top head pressure and total pressure [24,29]. The interphase kinetic equilibrium is assumed due to small droplets considered [12], with which the droplet injection velocity are equal to that of the carrier gas. Therefore, spray injection is activated if, and only if, the top head gas pressure is lower than the total pressure.
Fig. 4. (a) Droplet volume fraction, (b, d) evaporation rate (kg/m³/s), (c) HRR (J/m³/s), (e) n-C₇H₁₆ mass fraction, and (f) temperature (K) for Case 2a. Black lines: pressure iso-lines of (a, b) 1–15 MPa and (c)–(f) 1 MPa. Domain size for (a, b): 280 mm × 100 mm. (c)–(f) correspond to zone Z1 in (b).

Droplets colored with their temperatures are visualized in (c) and the inset of (a).

3. Results and discussion

3.1 Droplets effects on RDC

Figure 4 shows the distributions of droplet volume fraction \( \alpha \), evaporation rate \( S_{C_7H_{16}} \), Heat Release Rate (HRR), n-heptane mass fraction \( Y_{C_7H_{16}} \) and temperature \( T \) for Case 2a (\( \phi_t = 1 \) and \( d_0 = 5 \mu m \)). The present simulation captures the main RDC structures, including the detonation front, oblique shock wave, and deflagration surface, as shown from Figs. 4(b), 4(c) and 4(f). They are similar to the structures of the purely gaseous RDC [24]. Due to the dispersed droplets, new features arise. Specifically, the n-heptane droplets are distributed in the triangular fuel refill zone, confirmed by the high volume fraction \( \alpha \) in Fig. 4(a). In most of the refill zone, n-C₇H₁₆ mass fraction is close to that in the carrier gas, i.e. 3.82%, indicated the limited evaporation in the interior of the refill zone because of
the low injection temperature. Nevertheless, all the droplets are vaporized along the deflagration and detonation fronts due to local high temperature, and large evaporation rate $S_{C_7H_{16}}$ can be seen there (see Figs. 4b and 4d). This directly leads to high $n$-C$_7$H$_{16}$ concentration around them (Fig. 4e). Ribbon-shaped zones ahead of detonation wave with high $n$-C$_7$H$_{16}$ concentration can be seen in Fig. 4(e), which correspond to the recirculation zone due to the walls between the spray injectors. However, this $n$-C$_7$H$_{16}$ non-uniformity does not affect the RDW stability, and it steadily propagates at a mean speed of about 1,537 m/s. It is about 16.0% lower compared to the purely gaseous RDC speed, i.e. 1,830 m/s. Although the droplets are depleted inside the fuel refill zone, however, finite $n$-C$_7$H$_{16}$ gas can also be found along the slip line (Fig. 4e). Limited deflagrative combustion occurs there, with small amount of heat release (Fig. 4c).

Plotted in Figure 5 are the counterpart results from Case 2c with $\phi_\ell = 1$ but larger initial diameter, i.e. $d_0 = 20$ μm. The main RDC structures are similar to those in Fig. 4, and the RDW propagation is also stable with the speed of 1,519 m/s, about 1.2% lower than that of Case 2a. This is about 16.9% lower than the purely gaseous RDC result. However, besides in the refill zone, there are still a large number of $n$-heptane droplets behind the detonation wave (see Fig. 5c), between the slip line and deflagration surface, which is characterized by the high volume fraction there. Besides droplet evaporation along the deflagrative and detonation fronts, even stronger evaporation (hence higher $S_{C_7H_{16}}$, greater than 4000 kg/m$^3$/s) proceeds immediately behind the RDW. However, the local $n$-C$_7$H$_{16}$ concentration does not increase accordingly, which may be due to the distributed deflagration combustion behind the RDW. Moreover, the mean droplet residence time in the refill zone is about 67 μs for Case 2c, much smaller than that in the whole domain (about 91 μs). However, for Case 2a with droplets fully evaporated in the refill zone, the mean droplet residence time in the refill zone is about 42 μs.
Fig. 5. (a) Droplet volume fraction, (b, d) evaporation rate (kg/m$^3$/s), (c) heat release rate (J/m$^3$/s), (e) $n$-C$_7$H$_{16}$ mass fraction, and (f) temperature (K) for Case 2c. (c)–(f) correspond to zone Z2 in (b).

Droplets colored with their temperatures are visualized in (c). Color bars same as in Fig. 4.

Figure 6 shows the detonation wave speed $D$ as a function of $d_0$ (2–80 μm) for different total equivalence ratios $\phi_t$ (0.8–2.0). For comparisons, the results of gaseous RDC with $\phi_g = \phi_t$ (i.e. fully pre-vaporization before injection) are also plotted. In general, the wave speeds from liquid fueled RDC are 2%–18% lower than those of the corresponding gaseous RDE. These deficits are slightly lower than that in the previous liquid kerosene RDE experiments, i.e. 20–25% [30]. The velocity deficits in two-phase RDC may be associated with the non-uniform distributions (see Figs. 4e and 5e) of $n$-C$_7$H$_{16}$ vapours in the refill zone (see Figs. 4 and 5), due to the dispersed droplets and insufficient reactant mixing therein [23,30]. Moreover, for the same $\phi_t$, $D$ first decreases with initial droplet diameters. This is because smaller droplets are expected to have shorter evaporation time [22], and therefore the composition of mixture ahead of the detonation wave is closer to the stoichiometric condition. For a fixed droplet diameter, larger $\phi_t$ indicates the more liquid fuel supply since the pre-vaporized $n$-C$_7$H$_{16}$
equivalence ratio is fixed to be 0.6. Therefore, more droplets tend to generate more vapor in the refill zone and therefore larger $D$. However, when $d_0$ exceeds 30 µm, the droplet size effects on detonation propagation speed become marginal. This is reasonable because larger droplets would not markedly affect the gas composition ahead of the RDW due to their limited evaporation in the refill zone and hence negligible kinetic contributions towards the detonable gas.

![Graph](image)

Fig. 6. Detonation wave speed as a function of initial diameter and total equivalence ratio. Open circles: gaseous RDC; solid circles: two-phase RDC.

The presence of the evaporating droplets behind the RDW has been observed in Fig. 5. Local deflagration combustion of $n$-C$_7$H$_{16}$ vapours may occur under some favorable conditions, thereby deteriorating the overall fuel utilization in RDE. Figure 7 shows the detonated fuel fraction $\psi$ under different $d_0$ and $\phi_t$. It is estimated based on the volume-averaged $n$-C$_7$H$_{16}$ consumption rates conditioning on HRR greater than $10^{13}$ J/m$^3$/s, which deemed to be detonative combustion [11]. Overall, when the droplet diameter is small, i.e. $d_0 < 20$ µm, $\psi$ decreases with increased $d_0$. Small droplets can be fully vaporized around the detonation front, thereby a higher $\psi$. When $d_0 > 20$ µm, increased $d_0$ leads to high $\psi$. As seen in Fig. 5, large droplets continue evaporating in the denoted gas. However, with increased droplet size, the droplets take longer time to finish the evaporation and release the vapor, and
therefore their kinetic effects on the RDC become weaker. The droplets with large $d_0$ cannot be fully vaporized in the RDE chamber and then exit through the outlet, and the deflagration combustion behind RDW is weakened due to the less fuel vapor. As such, detonated fuel fraction increases again with $d_0$. 20 μm is a critical diameter corresponding to a minimal detonated fuel fraction based on our simulations.

![Diagram showing detonated fuel fraction as a function of initial droplet diameter and total equivalence ratio.](image)

Fig. 7. Detonated fuel fraction as a function of initial droplet diameter and total equivalence ratio.

In Figs. 6 and 7, the pre-vaporized $n$-C$_7$H$_{16}$ equivalence ratio is fixed to be $\phi_g = 0.6$. Figure 8 further shows the wave speed ($D$) and detonated fuel fraction ($\psi$) with $\phi_g = 0.5$ and 0.8. Same as in Figs. 6 and 7, the total equivalence ratio is $\phi_t = 1.0$. For a given $\phi_g$, the trends of $D$ and $\psi$ are similar to those of $\phi_g = 0.6$ shown in Figs. 6 and 7. It can also be found that $D$ increases with gas equivalence ratios $\phi_g$ with the same $d_0$. Note that the wave speeds with different $\phi_g$ and $d_0$ are always much smaller (6%–24%) than that of purely gaseous RDW with the same total equivalence ratio, i.e. $\phi_t = 1.0$, due to the heterogeneous nature of the reactants. Figure 8(b) show that the critical diameter corresponding to the minimum detonated fuel fraction increases with $\phi_g$, i.e. about 10, 20 and 30 μm for $\phi_g = 0.5$, 0.6 and 0.8, respectively. Moreover, when $d_0$ is smaller than the critical diameter, increased gas equivalence ratio would lead to high $\psi$. However, for $d_0$ greater than the critical diameter,
ψ of $\phi_g = 0.5$ is higher than that of $\phi_g = 0.6$, but slightly lower than that of $\phi_g = 0.8$. This may be due to the less deflagrated vapor with lower detonation temperature of $\phi_g = 0.5$ than that of $\phi_g = 0.6$.

![Graph](image)

Fig. 8 (a) Detonation wave speed and (b) detonated fuel fraction as functions of initial diameter and pre-vaporized gas equivalence ratio.

### 3.2 Combustion mode

Figure 9 shows the distributions of Flame Index (FI) and HRR for Cases 2a and 2c. The flame index is $\text{FI} = (\nabla Y_F \cdot \nabla Y_O) / (|\nabla Y_F||\nabla Y_O|)$, where $Y_F$ and $Y_O$ represent the mass fractions of gaseous $n$-heptane and oxidizer, respectively. It is often used to identify the premixed (FI = +1) and non-premixed (FI = -1) combustion modes [31]. Premixed modes occur along the detonation and inner layer of the contact surface, but non-premixed combustion is observable along the outer layer of the deflagration surface and the slip line (see Figs. 9a and 9c). Recall that, for Case 2a, both $n$-heptane vapor and droplets are completely consumed by the RDW (see Fig. 4). However, for Case 2c, there are still surviving droplets in the detonated gas. The $n$-heptane vapor evaporated from these droplets mixes and reacts with
the oxidant due to the high pressure and temperature, leading to lots of spotty diffusion flames, as shown in Figs. 9(c) and 9(d).

![Fig. 9. (a, c) Flame index and (b, d) HRR (J/m³/s) for Cases 2a and 2c. Domain: 280 mm×45 mm.](image)

**3.3 Droplet dynamics in RDE**

Figure 10 shows the profiles of arithmetic mean diameter ($D_{10}$) and Sauter mean diameter ($D_{32}$) along the height of the RDE. Cases 2a, 2b and 2c are considered, including 5, 10 and 20 μm. Here $D_{10}$ and $D_{32}$ are calculated based on the droplets in the same height interval for all the computed instants. Although the mean RDW height is about 0.025 m (the dashed line), however, droplets distributed with $y < 0.025$ m does not necessarily mean that they lie in the refill zone since the droplets are collected along the entire $x$ direction for a fixed height. Very close to the inlets (i.e. $y = 0$), various levels of the diameter deficit (4%–40%) can be seen for all the diameters. This is caused by the fast evaporation of the newly injected droplets ($y \approx 0$) since they interact with the hot detonated gas once they are injected, as shown in the inset of Fig. 4(a).

For small droplets, e.g. $d_0 = 5$ and 10 μm, their $D_{10}$ and $D_{32}$ are almost constant for $y < 0.025$ for all the three cases, indicating limited evaporation in the refill zone. These droplets of $d_0 = 5$ μm are then fully vaporized around the detonative fronts (around 0.025 m) due to the local high temperature. However, for $d_0 = 10$ μm, residual droplets exist beyond the RDW height. They may continue evaporating along
the slip line, and completely depleted around 0.05 m, around half of the RDE height.

For \( d_0 = 20 \) µm, \( D_{10} \) and \( D_{32} \) monotonically decrease from the top head, and even at the burner exit (i.e. \( y = 0.1 \) m), there are still some small-sized droplets (about 1 µm). The decrease with \( y < 0.025 \) m is caused by the evaporation of the residual droplets behind the RDW. The droplets dispersed beyond \( y > 0.025 \) m would continue evaporating in the detonated gas, and the vapor is burned through distributed zones, as shown in Figs. 5 and 9. If the RDE is integrated with turbines, these exiting fuel droplets may affect the normal operation of the entire propulsion system [2]. Therefore, from spray RDE design perspective, besides the conventional requirements (e.g. minimum diameter) [3], critical RDE chamber heights for liquid fuels should be carefully designed to achieve better liquid fuel utilization.

4. Conclusions

Two-dimensional RDE’s with partially pre-vaporized \( n \)-heptane sprays are simulated with Eulerian–Lagrangian method. Emphasis is laid on the influences of droplet diameter and total equivalence ratio on rotating detonation combustion. The results show that the small \( n \)-heptane droplets are completely consumed around the detonation wave, while for larger ones, the droplets can continue
evaporating behind detonation wave. The detonation propagation speed decreases with increased droplet diameter, and beyond a critical diameter (about 30 µm), it almost does not change with droplet diameter. The detonated fuel fraction first decreases and then increases with the droplet diameter. It is also found that the detonation propagation speed and detonated fuel fraction change considerably with the pre-vaporized gas equivalence ratio. Mixed premixed and non-premixed combustion modes exist in the two-phase RDC. The droplet distributions in the RDE combustor are considerably affected by the droplet evaporation behaviors.

Acknowledgement

This work used the ASPIRE 1 Cluster from National Supercomputing Centre, Singapore (NSCC) (https://www.nscc.sg/).

References

[1] P. Wolański, Detonative propulsion, Proc. Combust. Inst. 34(1) (2013) 125–158.
[2] V. Anand, E. Gutmark, Rotating detonation combustors and their similarities to rocket instabilities, Prog. Energy Combust. Sci. 73 (2019) 182–234.
[3] F.A. Bykovskii, S.A. Zhdan, E.F. Vedernikov, Continuous spin detonations, J. Propuls. Power. 22(6) (2006) 1204-1216.
[4] B.A. Rankin, D.R. Richardson, A.W. Caswell, A.G. Naples, J.L. Hoke, F.R. Schauer, Chemiluminescence imaging of an optically accessible non-premixed rotating detonation engine, Combust. Flame. 176 (2017) 12–22.
[5] F.A. Bykovskii, S.A. Zhdan, E.F. Vedernikov, Continuous spin detonation of fuel-air mixtures, Combust. Explos. Shock Waves. 42 (2006) 463–471.
[6] I. Shen, T.C. Adamson Jr, Theoretical analysis of rotating two phase detonation in a rocket motor, 1973.
[7] F.A. Bykovskii, S.A. Zhdan, E.F. Vedernikov, Continuous spin detonation of a heterogeneous kerosene–air mixture with addition of hydrogen, Combust. Explos. Shock Waves. 52 (2016) 371–373.
[8] F.A. Bykovskii, S.A. Zhdan, E.F. Vedernikov, Continuous detonation of the liquid kerosene—air mixture with addition of hydrogen or syngas, Combust. Explos. Shock Waves. 55 (2019) 589–598.
[9] J. Kindracki, Experimental research on rotating detonation in liquid fuel–gaseous air mixtures, Aerosp. Sci. Technol. 43 (2015) 445–453.
[10] A.K. Hayashi, N. Tsuboi, E. Dzieminska, Numerical study on JP-10/air detonation and rotating detonation engine, AIAA J. (2020) 1–17.
[11] M. Zhao, J.-M. Li, C.J. Teo, B.C. Khoo, H. Zhang, Effects of variable total pressures on instability and extinction of rotating detonation combustion, Flow, Turbul. Combust. 104(1) (2020) 261-290.
[12] C.T. Crowe, M. Sommerfeld, Y. Tsuji, Multiphase flows with droplets and particles, CRC Press, London UK, 1998.
[13] B. Abramzon, W.A. Sirignano, Droplet vaporization model for spray combustion calculations, Int. J. Heat Mass Transf. 32 (1989) 1605–1618.
[14] H. Watanabe, A. Matsuo, K. Matsuoka, Numerical investigation on propagation behavior of gaseous detonation in water spray, Proc. Combust. Inst. 37 (2019) 3617–3626.
[15] T.E. Daubert, R.P. Danner, Data compilation tables of properties of pure compounds, Design Institute for Physical Property Data, American Institute of Chemical Engineers 1985.
[16] A.B. Liu, D. Mather, R.D. Reitz, Modeling the effects of drop drag and breakup on fuel sprays, SAE Tech. Pap. Ser. (2010) 1.
[17] Z. Naumann, L. Schiller, A drag coefficient correlation, Z Ver Deutsch Ing. 77 (1935) 318–323.
[18] W.E. Ranz, J. W. R. Marshall, Evaporation from drops, Part I., Chem. Eng. Prog. 48 (1952) 141–146.
[19] J. Fujii, Y. Kumazawa, A. Matsuo, S. Nakagami, K. Matsuoka, J. Kasahara, Numerical investigation on detonation velocity in rotating detonation engine chamber, Proc. Combust. Inst. 36 (2017) 2665–2672.
[20] M.D. Bohon, R. Bluemmer, C.O. Paschereit, E.J. Gutmark, Measuring rotating detonation combustion using cross-correlation, Flow, Turbul. Combust. 103 (2019) 271–292.
[21] C.J. Greenshields, H.G. Weller, L. Gasparini, J.M. Reese, Implementation of semi-discrete, non-staggered central schemes in a colocated, polyhedral, finite volume framework, for high-speed viscous flows. Int J Numer Methods Fluids 63 (2010) 1–21.
[22] H. Ghassemi, S.W. Baek, Q.S. Khan, Experimental study on binary droplet evaporation at elevated pressures and temperatures, Combust. Sci. Technol. 178 (2006) 1031–1053.
[23] M. Zhao, H. Zhang, Origin and chaotic propagation of multiple rotating detonation waves in hydrogen/air mixtures, Fuel. 275 (2020) 117986.
[24] M. Hishida, T. Fujiwara, P. Wolanski, Fundamentals of rotating detonations, Shock Waves. 19 (2009) 1–10.
[25] C.K. Westbrook, F.L. Dryer, Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames, Combust. Sci. Technol. 27 (1981) 31–43.
[26] 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.
[27] B. Imbert, L. Catoire, N. Chaumeix, G. Dupré, C. Paillard, Detonation properties of stoichiometric gaseous n-heptane/oxygen/argon mixtures, Proc. Combust. Inst. 30 (2005) 1925–1931.
[28] G.D. Roy, S.M. Frolov, A.A. Borisov, D.W. Netzer, Pulse detonation propulsion: challenges, current status, and future perspective, Prog. Energy Combust. Sci. 30 (2004) 545–672.
[29] S. Yao, J. Wang, Multiple ignitions and the stability of rotating detonation waves, Appl. Therm. Eng. 108 (2016) 927–936.
[30] J. Kindracki, Experimental research on rotating detonation in liquid fuel-gaseous air mixtures, Aerosp. Sci. Technol. 43 (2015) 445–453.
[31] H. Yamashita, M. Shimada, T. Takeno, A numerical study on flame stability at the transition point of jet diffusion flames, Symp. Combust. 26 (1996) 27–34.