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ABSTRACT
Two-dimensional numerical simulations on the two-phase rotating detonation wave of a stoichiometric ratio of the air-octane mixture by the discrete phase model are performed. The propagation process and stable flow field of the rotating detonation wave under nonpremixed and nonuniform injection conditions are analyzed. The effects of air injection total temperature and fuel injection inhomogeneity on the gas-liquid two-phase rotating detonation wave are investigated. The results show that under the same conditions, with the increase in the total temperature of air injection, the peak temperature, height, and propagation velocity of the detonation wave increase, but the peak pressure of the detonation wave decreases. The larger the jet spacing, the more pronounced the detonation wave is disturbed by the fuel jet. As the fuel jet spacing increases, the detonation wave propagation velocity decreases, but the peak temperature and peak pressure of the detonation wave increase. For the case of a jet spacing of 10 mm, the detonation wave cannot propagate when the air total temperature is 300 K, but the detonation wave can be stably propagated when the air total temperature is increased to 600 K. The stable propagation boundary of the rotating detonation wave with the combined action of the air total temperature and the jet spacing is obtained.

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I. INTRODUCTION
Detonation is a high efficient way of premixed combustion heat, which has the thermodynamic advantage of energetic and fast propagation, and has received much attention in the field of aerospace propulsion. At present, the propulsion system based on detonation includes three types: pulse detonation engine (PDE), oblique detonation wave engine (ODE), and rotating detonation engine (RDE). Compared to the conventional constant pressure combustion, detonation combustion has the advantages of lower entropy increase and higher thermal cycle efficiency.

The RDE uses the high temperature and high pressure gas produced by the rotating detonation wave to generate thrust. Reactants are introduced to the combustion chamber through an injection head at one end, and exhaust products are expelled through the open end of the annular combustor. Compared to the pulse detonation engine, RDE can continuously work and does not need repeated ignition naturally, which can solve the difficult problem of the high frequency repeating ignition of PDE. The RDE has a promising application in the field of aerospace, weaponry, navigation, and other thermal engineering areas, and they have attracted considerable attention in recent years. Some researchers from many countries, including Smirnov et al., Frolov et al., Hoke et al., Anand et al., Wolański et al., Gaillard et al., Ma et al., Nakagami et al., Li et al., and Bluemner et al., have carried out related investigations.

Many types of fuels for the RDE were investigated to obtain stable rotating detonation waves. The activity decreases successively in the order of acetylene, hydrogen, ethylene, methane, and kerosene, as found in previous publications. Accordingly, the difficulty in reaching a stable rotation detonation increases in the similar order. The research on rotating detonation fueled by hydrogen has obtained more results with better performances.

Liquid fuel is preferred to be applied in practice due to its high volume heat. Until now, few experiments on liquid fuel (including gas/liquid mixture fuel) RDE were conducted. Le et al. successfully obtained a detonation wave with liquid kerosene-hydrogen mixtures and attempted to perform the RDE tests with a prevaporized hydrocarbon fuel. Li et al. investigated the feasibility and operability of liquid-fuel RDE using a Jet A-1 fuel with premixed and...
nonpremixed injection strategies, with the supply air being heated up to 100 °C via an electronic heating device. The results showed that both the two strategies are able to obtain a rotating detonation wave. Frolov et al.27 carried out experiments on continuous detonation combustion of ternary hydrogen-liquid propane-air mixture in a large-scale annular combustor with 406 mm outer diameter and an annular gap of 25 mm, where the continuous detonation combustion of liquid propane was obtained for the first time by addition of hydrogen. Kindracki28 experimentally obtained the time/frequency-domain characteristics of ignition and propagation processes in the liquid kerosene RDE. For the RDE with the mixture of liquid kerosene and air in which the mass fraction of oxygen increased to 50%. Lin et al.30 also used the kerosene/H2 mixture as the fuel in the rotating detonation engine, and the experiments obtained a stable detonation wave with a velocity deficit of 20%–25%. Bykovskii31 obtained stable rotating detonation waves up to 100 m/s. 

In this paper, gas-liquid two phase RDE with octane (C8H18) as the fuel is simulated to obtain the rotating detonation wave propagation process and the flowfield in the nonpremixed conditions. The traces of octane droplets are computed by the Discrete Phase Model (DPM), and the influences of the total temperature and nonuniform fuel injection are investigated. This study is helpful for the further investigation on the gas-liquid two-phase RDE.

II. NUMERICAL METHOD AND PHYSICAL MODEL

A. Numerical method

Numerical simulations are performed to solve the coupled 2-D unsteady Reynolds time-averaged Navier-Stokes equations,

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \frac{\partial \mathbf{E}_x}{\partial x} + \frac{\partial \mathbf{F}_x}{\partial y} + S,$$

where \( \mathbf{Q} \) is the vector of the conservative variables and \( S \) is the vector of the source term caused by chemical reactions. \( E \) and \( F \) are the vectors of the convective flux. \( E_v \) and \( F_v \) are the vectors of the viscosity flux,

$$\begin{bmatrix} \rho_1 \\ \vdots \\ \rho_{ns-1} \\ \rho \\ \rho u \\ \rho v \\ \rho E \end{bmatrix} = \begin{bmatrix} \rho_1 u \\ \vdots \\ \rho_{ns-1} u \\ \rho u \\ \rho u^2 + p \\ \rho u v \\ (\rho E + p) u \end{bmatrix}, \quad (2)$$

$$\begin{bmatrix} D_1 \frac{\partial \rho_1}{\partial x} \\ \vdots \\ D_{ns-1} \frac{\partial \rho_{ns-1}}{\partial x} \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xx} u + \tau_{xy} v + q_x \end{bmatrix} = \begin{bmatrix} D_1 \frac{\partial \rho_1}{\partial y} \\ \vdots \\ D_{ns-1} \frac{\partial \rho_{ns-1}}{\partial y} \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yx} u + \tau_{yy} v + q_y \end{bmatrix}, \quad (3)$$

where \( \rho \) is the density, \( p \) is the pressure, \( \rho_i \) is the density of species \( i \), \( u \) and \( v \) are the velocity components of fluids, and \( D_i \) is the diffusion coefficient. The subscripts \( i = 1, 2, \ldots, N \), \( N - 1 \), \( N \) is the total number of species. \( \omega_i \) given by the chemical reaction kinetic model is the mass production rate of species \( i \),

$$\omega_i = M_i \sum_{j=1}^{neq} (\beta_{ij} - \alpha_{ij}) (R_{ij} - R_{ij^*}), \quad (4)$$

where \( M_i \) is the molar mass of species \( i \), \( R_{ij} \) and \( R_{ij^*} \) are the positive reaction rate and the reverse reaction rate of elementary reaction, respectively, \( \alpha_{ij} \) and \( \beta_{ij} \) are the stoichiometric coefficients of species \( i \) in the \( j \)th elementary reaction, and \( neq \) is the total number of elementary reaction.

The total energy \( E \) is defined as

$$E = ph - \frac{1}{2} \rho (u^2 + v^2), \quad (5)$$

where \( h \) is the specific enthalpy of the gas mixture.

The advective term is discretized by the 3rd-order MUSCL scheme which has a high resolution for catching the shock wave. Physical flux is decomposed by the AUSM vector flux splitting method. The time term is computed by the 2nd-order Runge-Kutta method, and the standard \( k-\varepsilon \) turbulence is used to model the turbulence. The fuel and the oxidizer are octane and air, respectively, whose reaction equation is used as Eq. (5). The coupled heat transfer and mass transfer are considered in the DPM model, and the Saffman lift, pressure gradient force, and the physical process of the droplet breakup and evaporation are also included. The octane droplet injection position is set as the group jet source,

$$C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 47N_2. \quad (6)$$

B. Model and boundary conditions

The RDE combustor is hollow cylindrical, and the height of the combustor is much less than its diameter; therefore, it is reasonable to convert the three dimensional annular combustor to two dimensional in order to decrease the computation demands. In this paper, the annular combustor is expanded to a 200 × 50 mm2 2D rectangular zone for the simulations, as shown in Fig. 1, where the boundary conditions are also labeled.

The air mass flux at the inlet boundary is 100 kg m−2 s−1, and the total temperature range is over 300 K–800 K, as shown in Table I. The lower boundary of the computational domain is the pressure-outlet with a back pressure of 0.1 MPa. Both right and left boundaries are set as the periodic boundary for data exchange. The octane droplet has a diameter of 20 μm, whose initial temperature is 300 K.
TABLE I. Computation conditions for the total temperature of air (octane jet spacing: 2 mm).

| Case no. | Temperature (K) |
|----------|-----------------|
| 1        | 300             |
| 2        | 400             |
| 3        | 500             |
| 4        | 600             |
| 5        | 700             |
| 6        | 800             |

TABLE II. Computation conditions for the octane jet spacing (total temperature of air: 300 K).

| Case no. | Distance (mm) |
|----------|---------------|
| 7        | 13.33         |
| 8        | 10            |
| 9        | 8             |
| 10       | 4             |
| 11       | 2.67          |
| 12       | 2             |
| 13       | 1.33          |
| 14       | 1             |
| 15       | 0             |

and injection speed is 20 m/s. The octane jet interval is shown in Table II, where the ideal uniform injection is used in case #15. The octane mass flux is 6.667 kg m$^{-2}$ s$^{-1}$ with the equivalent ratio of 1.0.

C. Numerical verification

1. Flowfield structure

   The temperature contours during the detonation wave propagating stably for case #5 are shown in Fig. 2, where A denotes the transverse detonation wave which propagates along the circumferential direction near the entrance, B is an oblique shock wave near the head of the detonation wave, C denotes a slip line which is a discontinuous surface between the new detonation products and the old products from the last cycle, D is the contact surface between the detonation products and the new reactants, and E represents the new reactants just injected. One can see that the detonation wave structures from the simulation and Bykovskii’s experiments are identical qualitatively.

2. Detonation wave parameters

   The histories of pressure and temperature at the monitor point M1 ($x = 100$ mm, $y = 49$ mm) for case #14 are shown in Fig. 3. One can see from this figure that the pressure increases sharply and reduces slowly when the detonation wave propagates through the monitor point. The pressure peak almost keeps constant for every period, which shows that the propagation of the detonation wave is stable. The pressure history agrees well with the temperature history, which proves that the shock wave and the chemical reaction coupled highly on the wave front. The peak pressure from the computation is 4.89 MPa, the peak temperature is 2898 K, and the averaged propagating velocity of the detonation wave is 1649 m/s. Compared to the C-J detonation wave theoretical results from CEA (Chemical Equilibrium with Application), the relative differences for the C-J pressure, temperature, and velocity are $-5.48\%$, $-0.67\%$, $-8.84\%$, respectively, which shows that the numerical method used in this paper has an acceptable accuracy.

III. RESULTS AND ANALYSIS

A. Analysis on detonation wave propagation process

   Taking case #1 as an example, the initiation and the propagation processes of the detonation wave are described in Fig. 4. One can see from this figure that after the initiation, a detonation wave and a deflagration wave are produced, and the propagation directions of these two waves are opposite. After they collide at $t = 154$ $\mu$s [Fig. 4(c)], these two waves continue to propagate along their original directions, and the detonation wave height grows quickly due to the existence of the triangle reactant mixing region [Fig. 4(e)]. A contact discontinuity surface is produced between the combustion products of the first cycle and that of the second cycle, and the contact surface tends to become stable with the propagation of the detonation wave [Fig. 4(f)], and at that time, the detonation state is transited from the initiation to the stable propagation.

   Figure 5(a) shows the mass fraction of vaporized octane at the state of stable propagation. One can see that the high fraction of vaporized octane is located in region D where there is a contact surface between the detonation products and the fresh reactants since the octane droplets are vaporized by the high temperature from the detonation products and then gather near the contact surface. It is obvious that the octane droplets are only found in region E [Fig. 5(b)] where the detonation wave can propagate stably. Only a small amount of vaporized octane can be found in region F, when the detonation wave sweeps through this region, the detonation wave cannot propagate in this region due to the low equivalence ratio.
FIG. 4. Temperature cloud diagram at different times in the combustion chamber: (a) $t = 70 \mu s$, (b) $t = 110 \mu s$, (c) $t = 154 \mu s$, (d) $t = 164 \mu s$, (e) $t = 172 \mu s$, and (f) $t = 210 \mu s$.

(about 0.11). Hence, the detonation wave can only propagate in region E.

Figure 6 shows the history of pressure, vaporized octane mass fraction, and octane droplet concentration. The mass fraction of the vaporized octane is low before the detonation wave arrives the monitor point since octane in the fresh reactant mixing region exists as the state of the droplet due to the low air total temperature of 300 K, as shown in Fig. 6 for the monitor points of M1 and M2 ($x = 100$, $y = 40$). When the detonation wave arrives at the monitor point, the vaporized octane increases immediately, since the octane droplet is broken and vaporized by the high temperature detonation wave, and then, vaporized octane reduces quickly due to the quick reaction with air.

B. The influence of air injection total temperature on detonation wave

Figure 7 shows the influence of the air total temperature on the detonation wave peak temperature and its temperature rise. One can see that the detonation wave peak temperature increases gradually with the increase in the air total temperature. The temperature rise of the detonation wave almost keeps constant, which means that the influence of the air total temperature on the detonation heat release of the octane droplet can be ignored.

Figure 8 shows the influence of the air total temperature on the detonation wave height and air injection velocity. One can see that the air injection velocity increases linearly with the air total temperature for the constant air mass flow rate. The detonation wave height is determined by the mixing zone height of the fresh reactants. The octane injection depth increases for increasing air injection velocity due to the following behavior of the droplet, which results in the increase in the detonation wave height.

Figure 9 shows the influence of the air total temperature on the detonation wave propagation velocity. One can see that the...
detonation wave propagation velocity increases linearly with increasing air total temperature. More octane droplets are vaporized for the higher air total temperature during the injection. For example, when the air total temperature is 800 K, the mass fraction of vaporized octane covers 12.2% when the detonation wave passes the monitor point (Fig. 10). From Fig. 9, one can see that the change trend of the detonation wave velocity is almost identical with that of the mass fraction of vaporized octane, and the high vaporization fraction is beneficial to the mixing of octane with air and to the steady propagation of the detonation wave. The vaporized octane participates in the reaction directly, which improves the reaction rate. Furthermore, high total temperature of air also raises the reactant activity. Figure 9 also shows that the C-J velocity at different air total temperatures. One can see that the difference between the C-J velocity and the detonation wave velocity reduces gradually as the air total temperature increases.

The influence of the air total temperature on the detonation peak pressure is shown in Fig. 11. The detonation peak pressure reduces monotonously for the increasing air total temperature. According to the C-J theory, the ratio of the peak pressure to the initial pressure grows as the detonation Mach number raises, and
the influence of the total temperature on the initial pressure is not obvious, while both the detonation Mach number and peak pressure reduce due to the increasing total temperature if other conditions keep constant.

C. The influence of nonuniform fuel injection on detonation wave

In order to investigate the influence of the fuel nonuniform injection on the detonation wave, the octane droplet injection position was set as the group jet source with a constant fuel mass flow rate to adjust the octane jet nonuniformity by changing the jet spacing; the detailed operations are shown in Table II.

1. The influence of nonuniform fuel injection on the flowfield

Figure 12 shows the pressure contours for the uniform injection and the injection with 4 mm jet spacing. The nonuniform injection with 4 mm spacing produces the more complicated flowfield than the uniform injection due to the interaction of the detonation wave and the octane jets, where there are many octane jets with a shape of vertical bar. The pressure and temperature at \( y = 45 \) mm in Fig. 12(a) are shown in Fig. 13 where the synchronous oscillation can be found in the pressure and temperature distributions, and the oscillation positions are identical with the octane injection position, as shown in Fig. 14.

The influence of the larger jet spacing on the detonation wave is more obvious. For the computation accuracy in this paper, the influence can be ignored when the octane jet spacing is less than 2 mm. The influence becomes stronger for the larger jet spacing although the disturbance frequency of the jet decreases, which can be observed in Fig. 15(a) for the jet spacing of 8 mm. When the jet spacing is increased to 13.3 mm, the detonation wave decouples quickly after the initiation [Fig. 15(b)], which means that the detonation wave cannot propagate stably at that situation.

2. The influence of nonuniform fuel injection on detonation wave propagation process

Figure 16 shows the influence of the octane jet spacing on the velocity, peak pressure, and temperature of the detonation wave.
Larger jet spacing tends to result in a higher peak pressure and temperature since it has the higher local equivalent ratio for the higher jet spacing. Larger jet spacing tends to reduce the propagation velocity of the detonation wave since the more nonuniform flowfield results in a higher velocity loss of the wave. When the jet spacing is around 1 mm, all three parameters of the detonation wave are close to the uniform injection.

D. The combined action of air total temperature and nonuniform fuel injection

In order to obtain the boundary for the stable propagation of the detonation wave, many simulations were conducted for the operations at different jet spacings and different air total temperatures. The results on whether the propagation is stable or not for all operations are shown in Fig. 17. One can see that the jet spacing of 10 mm is an obvious upper boundary for the stable propagation of the wave. With a jet spacing of 10 mm, the detonation wave cannot propagate when the air total temperature is lower than 300 K, but the detonation wave can be stably propagated when the air total temperature is increased to 600 K.

IV. CONCLUSIONS

In this paper, numerical simulations on liquid octane and air two-phase detonation are performed to study the influence of the air injection total temperature of 300–800 K and the fuel injection spacing of 0–14 mm. The simulation results show the following conclusions.

- With a constant air mass flow rate, higher air total temperature results in a higher peak temperature, a higher propagation velocity, and a larger height, but a lower peak pressure for the two-phase rotating detonation wave.
- With the decrease in the octane jet spacing, the detonation wave propagation velocity grows, while the peak pressure and peak temperature of the wave reduce. When the octane jet spacing is larger than 13.3 mm, the detonation wave cannot propagate stably.
- The octane jet spacing of 10 mm is an upper limitation for the stable propagation of the detonation wave. For the case of a jet spacing of 10 mm, the detonation wave cannot propagate when the air total temperature is lower than 300 K, but the detonation
wave can be stably propagated when the air total temperature is increased to 600 K.

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