

Influence of reactant spatial heterogeneity on propagation and performance of hydrogen-fueled rotating detonation waves

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ABSTRACT

Numerical simulations incorporating detailed chemistry are performed for two-dimensional rotating detonations subjected to reactant spatial heterogeneity. The objectives are to quantitatively evaluate how heterogeneity affects the detonation propagation, performance, and sustainability limit. An idealized heterogeneity model is adopted where a sinusoidal function parameterized by its amplitude A and non-dimensional wavelength λ is used to describe the local equivalence ratio. Results show that increasing heterogeneity promotes local quenching and re-initiation, generating strong transverse waves and enlarging cell size α . A parametric analysis shows that the cell size grows with A or λ , causing a reduced detonation height-to-cell-size ratio (H_{DW}/α). Excessive A or λ may cause detonation decoupling. The mean detonation velocity, specific impulse, and combustion efficiency decline monotonically with A or λ . A detonation limit boundary in A - λ space is identified. The critical λ decreases with A , and the detonation tends to fail when H_{DW}/α is too low.

1. Introduction

A detonation wave (DW) is a strong coupling between the shock and flame that propagates in a combustible gas mixture, wherein the flame is induced by adiabatic shock compression, and the shock becomes sustained due to support from combustion heat release. Compared with constant-pressure deflagrative combustion, DWs provide higher thermal efficiency and faster heat release rates due to its pressure-gain nature. Thermodynamics analysis has shown that detonation cycles provide around 20% higher efficiency compared with the Brayton cycle [1]. Utilizing an annular configuration that allows the DW to propagate continuously within the combustor, the rotating detonation engines (RDEs) [2–5] have promising applications in aerospace propulsion due to the aforementioned strengths of detonative combustion.

Ever since the first experimental demonstration in the 1950s by Voitsekhoyskii [6], RDEs have attracted vast research interests worldwide. In the past few decades, a substantial number of efforts have been paid to understand the detonation dynamics of RDEs through experimental [7–9], numerical [10–13] and analytical studies [14–16]. The performance of an RDE is found to be highly sensitive to the coupled dynamics of injection [17–19], plenum conditions [17,20,21], and

chamber geometry [22–25]. Specifically, many influencing parameters such as equivalence ratio, mass flow rate, and injection total pressure and temperature were also found to significantly alter the heat release and the fuel-refill process, affecting the propagation dynamics and velocity deficit characteristics of the DW [26–32].

Recently, nonidealities in RDEs have garnered increased attention. This interest arises because the expected efficiency gains of detonations are based on the assumption of DW propagation in homogeneous mixtures [33]. However, in practical applications, the wave always propagates in a heterogeneous environment [34,35]. Such heterogeneity is commonly a result of imperfect mixing of fuel and oxidant injected from separate injectors or slits [33–35]. Although premixed injections provide a homogeneous mixture and increase combustion efficiency, most practical engines adopt separate injections due to safety considerations [34]. Luan et al. [36] numerically showed that mixture inhomogeneity induces multi-wave modes with limited impact on global performance. Experimentally, Kou et al. [37] demonstrated that non-uniform injection narrows the detonability range and degrades stability, while Fan et al. [38] visualized the critical shock-reaction coupling mechanisms during non-premixed detonation initiation. Fujii et al. [39] found that the amount of incompletely consumed fuel is inversely proportional to DW

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velocity in an RDE, indicating that imperfect mixing can increase the detonation velocity deficit. Imperfect premixing also reduces peak pressure and leads to a complex flow field and wave instability in an RDE [40–42]. Variations in the local equivalence ratio have been shown to negatively impact the total pressure gain of the combustor [35]. Experimental results further demonstrate that variations in wave speeds and structures arise from imperfect premixing caused by different injection conditions [43]. In addition, the effects of periodic reactant concentration gradient on propagation of channelled DWs were numerically investigated by Wang et al. [44,45], showing that reactant heterogeneity significantly impacts the propagation of DW in a confined space [46]. Reactant concentration gradient has also been proved to significantly affect the detonation propagation in semi-confined reactive layers [47] and the deflagration to detonation transition process [48], causing complex combustion and shock systems. Hydrogen is a carbon-free fuel, and hence, increasing research interests have been garnered by the researchers on hydrogen-fueled RDEs, for instance, Refs. [12,29,32,46,47].

The interaction among numerous physical variables makes it challenging to isolate the effects of reactant heterogeneity and quantitatively assess its impact in most of the aforementioned studies. Consequently, the influence of reactant heterogeneity on the instability and cellular structure of DWs in RDEs is rarely investigated. Moreover, existing studies mainly focus on the propagation behaviors of sustained detonations through heterogeneous mixtures in RDEs, with little attention given to the detonability boundary. The detonation limit under the impact of reactant heterogeneity remains unclear, and the quantitative effects of perturbation amplitude and wavelength still need to be revealed. The current study models the reactant heterogeneity using an idealized model, which facilitates precise control of the pre-detonation heterogeneity. Since the reactant spatial heterogeneity is quantified by nondimensional parameters A and λ ($\lambda = L_\phi/\Delta_{\text{Ind}}$, where L_ϕ and Δ_{Ind} denote the dimensional perturbation wavelength and Zel'dovich-von Neumann-Döring induction length, respectively). It distinguishes the current study from previous studies [39] where the heterogeneity is generated by resolved mixing processes under case-specific conditions. Therefore, general trends of detonation dynamics under heterogeneity can be more systematically revealed in the current study using the idealized model.

Given the aforementioned considerations, the objectives of the current study are: 1) to evaluate the cellular structures and performance of the rotating detonations in the presence of reactant spatial heterogeneity, with a quantitative assessment of the effects of perturbation amplitude A and nondimensional wavelength λ ; and 2) to determine the detonation limit within the parameter space of A and λ . The remainder of this paper is structured as follows: Following this introduction, Section 2 describes the physical model and numerical methods. In Section 3, the numerical results are presented and analyzed. First, the propagation of heterogeneous DW is compared against its homogeneous counterpart to highlight the general flow features. Subsequently, the effects of perturbation amplitude and wavelength are assessed. Then, the detonation limit is determined and the correlation between the detonability boundary and perturbation is revealed. Finally, conclusions are drawn in Section 4.

2. Geometric configuration and numerical methods

The combustor of an RDE features a three-dimensional annular configuration. In cases where the annulus width is significantly smaller than the outer radius, the flow field can be effectively simplified into a 2D domain. Consequently, 2D simulations have been widely adopted and proven effective for capturing key detonation structures and widely adopted in previous studies [17,18,21,26,29]. The unrolled two-dimensional RDE computational domain is shown in Fig. 1. The circumferential and axial dimensions of the combustor are 30 cm and 10 cm respectively. These combustor scales are close to the experiments of

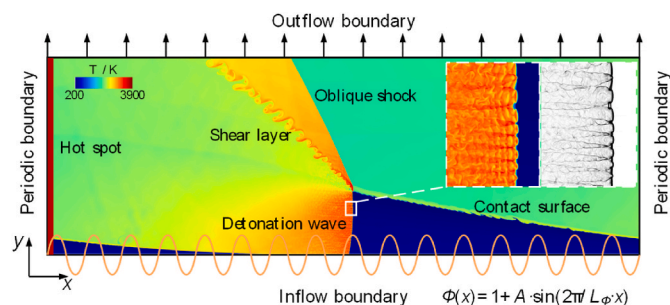


Fig. 1. Schematic diagram of the computational domain and boundary conditions.

Bluemner et al. [49], and those used in many previous numerical studies [18,21]. Premixed H_2/Air mixture is injected into the combustor through the inflow boundary at the bottom, where a Laval micro-nozzle assumption is adopted. Specifically, each cell on the inflow boundary is considered as an independent micro-Laval nozzle. The injection total pressure and total temperature are fixed as $p_t = 10$ atm and $T_t = 300$ K among all cases. The throat to exit area ratio of the micro-nozzles is fixed as $A_t/A_w = 0.2$. Working status of each micro nozzle depends on the pressure at the combustor head wall p_w , that is the pressure of the first layer of cells adjacent to the inflow boundary, and can be classified into four flow patterns:

- (a) If $p_t < p_w$, no injection can occur due to high back pressure at the nozzle exit;
- (b) If $p_{\text{cr1}} < p_w < p_t$, subsonic injection occurs;
- (c) If $p_{\text{cr2}} < p_w < p_{\text{cr1}}$, choking occurs at the nozzle throat, the injection remains subsonic;
- (d) If $p_w < p_{\text{cr2}}$, supersonic injection occurs and the injection process is free from p_w .

The calculation of the critical pressures (p_{cr1} and p_{cr2}) can be found in Ref. [50]. To model the idealized spatial heterogeneity of reactants, the inflow components are set as $2\phi\text{H}_2 + \text{O}_2 + 3.76\text{N}_2$, where ϕ denote the local equivalence ratio and varies spatially along the inflow boundary: $\Phi(x) = 1 + A\sin(2\pi/L_\phi \cdot x)$. Here, A and L_ϕ denote the perturbation amplitude and dimensional perturbation wavelength respectively. To make the L_ϕ more physically indicative, it is nondimensionalized using the 1-D Zel'dovich-von Neumann-Döring (ZND) induction length under stoichiometric condition: $\lambda = L_\phi/\Delta_{\text{Ind}}$. Since the pre-detonation state is fluctuating in the simulations, a representative pressure and temperature of $p = 1$ bar and $T = 293$ K are used when evaluating Δ_{Ind} . A Mach number-based hybrid outflow boundary condition is adopted at top boundary, where the first order extrapolation is adopted for supersonic zones, whereas a fixed backpressure of 1atm is used for subsonic zones [51]. Periodic boundary conditions are adopted at the left and right boundaries to guarantee that the DW can propagate continuously within the combustor. The DW is directly initiated by a hot spot ($p_h = 3.5$ MPa, $T_h = 2000$ K, $u_h = 1000$ m/s) as shown in Fig. 1 by the red rectangular on the left side of the domain. After initiation, each case is run to a steady state, which corresponds to a physical time of no less than 2 ms. Notably, this sinusoidal distribution of $\Phi(x)$ along the inlet resembles the heterogeneous pre-detonation mixture resulting from the imperfect mixing of fuel and oxidant from discrete injectors. It further benefits from the precise control of perturbation amplitude and wavelength, enabling a quantitative evaluation of its impacts on DW propagation. Consequently, results from the current study should be interpreted as conditional trends under an idealized heterogeneity model.

The simulations are performed using *PeleC* [52], an open-source adaptive-mesh compressible hydrodynamics code for reactive flows based on the AMReX framework [53]. *PeleC* has been successfully used in many previous studies pertinent to detonations, including RDEs [54,

55], detonation initiation by supersonic injection [56], oblique detonation waves [57,58] and deflagration to detonation transitions [59,60]. The governing equations are multi-component reactive Euler equations:

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = 0 \quad (2)$$

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho E \mathbf{u} + p \mathbf{u}) = 0 \quad (3)$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{u}) = \dot{\omega}_i \quad i = 1, 2, \dots, ns - 1 \quad (4)$$

where, ρ , $\mathbf{u}$, p , and E denote mixture density, velocity vector, pressure and total energy, respectively. Y_i and $\dot{\omega}_i$ represent the mass fraction and net production rate of i -th species. The equation system is closed by the ideal gas law. Burke's detailed hydrogen kinetics [61] is adopted for calculating $\dot{\omega}_i$, which is comprised of 21 elementary reactions among 9 species. A fourth-order piecewise linear method (PLM) is used for reconstruction of the convection term. This PLM is a modified version of the piecewise parabolic method (PPM) proposed by Colella and Woodward [62]. An iterative scheme based on a spectral deferred correction approach (SDC) [63] is adopted for time-stepping. The stiff-chemistry terms are integrated using ARKODE [64] via the SUNDIALS library [65,66].

Block structured adaptive mesh refinement (AMR) is adopted to better resolve the key flow and combustion structures. The detailed AMR refinement strategy is shown in Table 1. Here, the density difference is for identifying shocks. The species HO_2 is used as a flame tracer for recognizing the flame fronts. Temperature difference and vorticity are used to capture the shear layers. Four levels of AMR are adopted for the heterogeneous cases while five levels are adopted for the homogeneous baseline case ($A = 0, \lambda = 0$). The base mesh (level 0) is 480×160 ($\Delta x = \Delta y = 0.625$ mm). Such AMR strategy results in a finest grid of $\Delta x = \Delta y = 39$ μm and $\Delta x = \Delta y = 19.5$ μm under four and five levels of AMR, respectively. Finer grids are used in the homogeneous case due to the smaller induction length and cell size, ensuring sufficient computational grids within the induction zone compared to heterogeneous (off-stoichiometric) flows. Fig. 2 shows the 1-D ZND induction length Δ_{Ind} and Chapman-Jouguet (CJ) velocity D_{CJ} as a function of equivalence ratio. One can readily found that, Δ_{Ind} is drastically increased by multiple orders of magnitude when the reactants are off-stoichiometric. Especially in the fuel-lean region, Δ_{Ind} can increase by over 200 times when the equivalence ratio is below 0.4, which corresponds to a perturbation amplitude of $A = 0.6$. Specifically, Δ_{Ind} at $\phi = 0.4$ is 4.627 mm compared to 0.176 mm at $\phi = 1.0$. Such drastic jump in Δ_{Ind} makes it improper to use the same cell size for homogeneous and heterogeneous flows. To guarantee the results are grid independent, a resolution study is conducted for both heterogeneous and homogeneous cases, which can be found in Appendix A to this paper. Apart from the cases for grid independence test, a total of 24 cases were performed to cover a wide range of perturbation amplitude and wavelength ($A \in [0, 1.0]$, $\lambda \in [0, 214]$). All simulations are performed on a high-end workstation running with dual EPYC 7542 processors (64 cores), and each heterogeneous

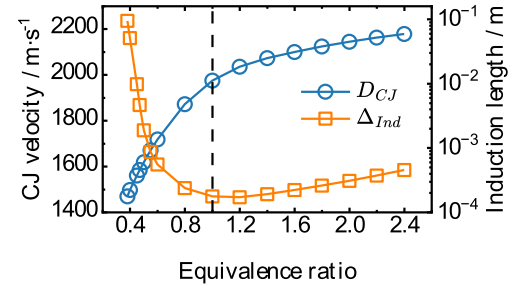


Fig. 2. CJ detonation velocity D_{CJ} , and corresponding 1-D ZND induction length Δ_{Ind} of a H_2/Air mixture with varying equivalence ratios. The vertical dashed line indicates the stoichiometric line.

case takes around 96 h. Although large gradients in temperature and reactant concentration exist within the combustor, transport phenomena are proven negligible based on comparisons with viscous simulation results, as detailed in Appendix B.

3. Results and discussion

3.1. Detonation structures in homogeneous flow

We first examine the flow and combustion structures of the baseline case where the equivalence ratio is spatially uniform along the inflow boundary ($A = 0, \lambda = 0$). This baseline case serves as a reference for other cases with perturbations of different amplitude and wavelength. Unless otherwise specified, the flow features to be discussed are captured during the steady state (i.e., the DW has crossed the periodic boundaries more than 6 times). The temperature contour of this baseline case is already shown in Fig. 1. It is observed that the key flow features, including the DW, contact surface, oblique shock and shear layer are all well resolved in Fig. 1. To better demonstrate the AMR hierarchy and grid distributions, an outline of the grid blocks as well as the distribution of AMR level are shown in Fig. 3. As seen, regions of all the key flow features are all well refined with higher AMR level, validating the effectiveness of the refinement criteria adopted in this study as listed in Table 1.

To show the detailed detonation structures, zoomed-in views of this homogeneous case near the DW front are plotted in Fig. 4, by contours of temperature, pressure, heat release rate (HRR) and numerical soot foil, respectively. Fine structures due to wave front instability are observed. The incident shocks, transverse waves (TWs) and Mach stems are clearly visible in Fig. 4(b). Despite these fine structures on the wave front, the macroscopic properties of the DW show a relative stable propagation mode. As shown in Fig. 4(c), the DW height is around $H_{\text{DW}} = 3.17$ cm, which is significantly greater than the cell size α in Fig. 4(d). The DW height is extracted based on the distribution of HRR, the point with the largest y-coordinate where $\text{HRR} > 10^{13} \text{ J/m}^3/\text{s}$ inside the computational domain is extracted as the DW height. It is clear in Fig. 4(d) that H_{DW} , characterized by the height of the cellular band, only shows very slight oscillation, evidencing a stable propagation mode. Here, $H_{\text{DW}}/\alpha \approx 31$, which means that the fuel-refill zone ahead of the DW is sufficiently thick for a stable propagation of the DW under the current homogeneous inflow conditions.

We then examine the unsteady detonation propagation process for the homogeneous case. Time-series of the DW position X_{DW} is shown in Fig. 5(a). Here, X_{DW} is obtained by tracking the x-coordinate of shock front on the inflow boundary. X_{DW} undergoes cyclic sudden drops, which are denoted with open circles in Fig. 5(a) and corresponds to the instants when the DW passes through the periodic boundaries. The wave velocity can be obtained by differentiating X_{DW} with respect to time. It is also nondimensionalized by the CJ velocity ($p = 1$ bar, $T = 293$ K, $\phi = 1$) to show the velocity deficit characteristics in Fig. 5(b). Upon direct initiation by the hotspot at $t = 0$ ms, D/D_{CJ} initially shows a chaotic

Table 1

Mesh refinement criteria.

Refinement variable	Threshold value
Density difference: $\max(\frac{\partial \rho}{\partial x} dx, \frac{\partial \rho}{\partial y} dy)$	0.1 kg/m ³
Flame tracer magnitude: (Y_{HO_2})	150×10^{-6}
Temperature difference: $\max(\frac{\partial T}{\partial x} dx, \frac{\partial T}{\partial y} dy)$	50 K
Vorticity magnitude	10^6 s^{-1}

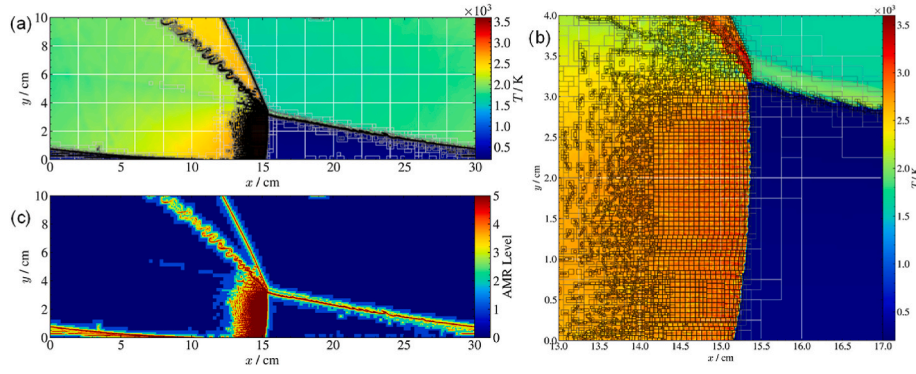


Fig. 3. (a) Distribution of AMR blocks superimposed on the temperature field, (b) zoomed-in view of the DW front, and (c) distribution of AMR level. Each block in (a) and (b) represents a 32×32 grid cluster.

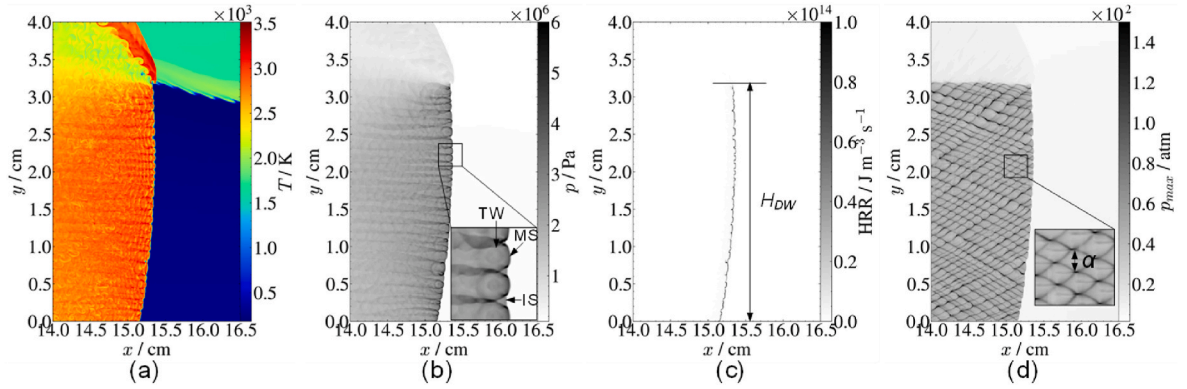


Fig. 4. Detonation structure of the baseline case with homogeneous inflow ($A = 0, \lambda = 0$): (a) temperature, (b) pressure, (c) heat release rate, and (d) numerical soot foil. IS: incident shock, MS: Mach stem, TW: Transverse wave.

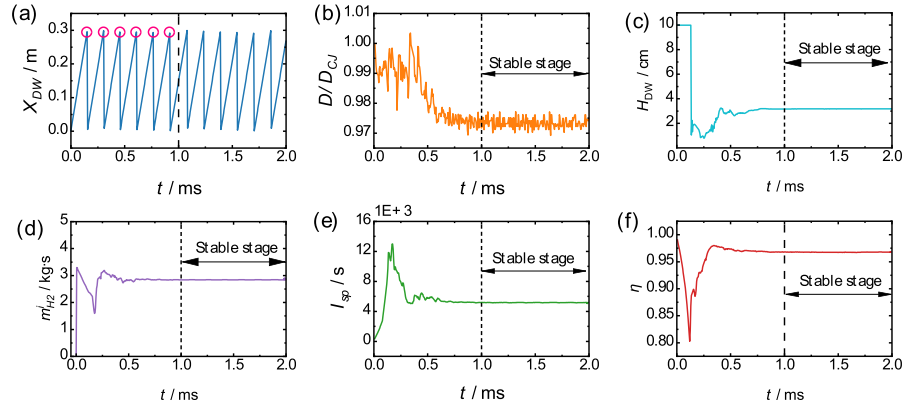


Fig. 5. Instantaneous evolution process of (a) DW location X_{DW} and (b) nondimensionalized wave velocity D/D_{CJ} , (c) DW height, (d) H_2 inflow mass flow rate, (e) specific impulse I_{sp} , and (f) combustion efficiency η .

mode with drastic oscillations. After $t = 1$ ms, the DW has crossed the periodic boundary 6 times and enters a stable stage. In this stage, D/D_{CJ} only demonstrates slight fluctuations, and the velocity deficit is only around $D_f = (D_{CJ} - D)/D_{CJ} \approx 2.3\%$. This further proves that a stable stage is already reached after $t = 1$ ms, and the simulated physical time (2 ms) in the current study is sufficient for steady state analyses. The time series of the DW height, inflow H_2 mass flow rate, specific impulse and combustion efficiency (η) are shown in Fig. 5(c), (d), 5(e) and 5(f) respectively. The specific impulse is calculated as $I_{sp} = \int_{A_o} [\rho v^2 + (p - p_b)] dA_o / g \dot{m}_{H_2}^i$, where the hydrogen inflow mass flow rate is computed

as $\dot{m}_{H_2}^i = \int_{A_i} Y_{H_2} \rho v dA_i$. The combustion efficiency is essentially a measurement of the fraction of hydrogen consumed within the combustor computed as $\eta = (\dot{m}_{H_2}^i - \dot{m}_{H_2}^o) / \dot{m}_{H_2}^i$, where $\dot{m}_{H_2}^i$ and $\dot{m}_{H_2}^o$ denote the mass flow rates of hydrogen along the inlet and outlet of the combustor. Similar to D/D_{CJ} in Fig. 5(b), I_{sp} and η gradually enter a stable stage after some large initial oscillations. Statistics are then performed within the stable stage to obtain the average specific impulse and combustion efficiency. The time-averaged specific impulse is $\bar{I}_{sp} = 5184$ s, which is comparable to many previous studies on H_2 /Air RDEs [21,29,67]. The time-averaged combustion efficiency is $\bar{\eta} = 96.7\%$, meaning that almost

all fuel injected is consumed.

3.2. Detonation structures in heterogeneous flow

3.2.1. Transition from homogeneous to heterogeneous detonation

In this subsection, the detonation structures in heterogeneous flow will be assessed. We first run the simulation in homogeneous flow to a stable stage (e.g. the stable stage detonated in Fig. 5). Starting from that point (denoted by $t = t_0$), we impose the perturbations onto the inflow boundary and continue the simulation until another stable stage is reached in heterogeneous flow. This implementation minimizes the

influence of the hot-spot-induced initiation process on the transient flow fields of different heterogeneous cases. The unsteady transition process from homogeneous to heterogeneous flow is illustrated in Fig. 6 by contours of temperature, pressure and H_2 mass fraction. Here, the perturbation amplitude and wavelength are selected as ($A = 0.5$, $\lambda = 53$).

Initially, at $t = t_0 + 0.005$ ms (the first column), the detonation front in homogeneous flow shows a weak instability characterized by small-scale transverse waves. When the heterogeneous mixture is progressively introduced from the inflow boundary, the lower portion of the reactant layer becomes heterogeneous. Local fuel-lean and -rich strips

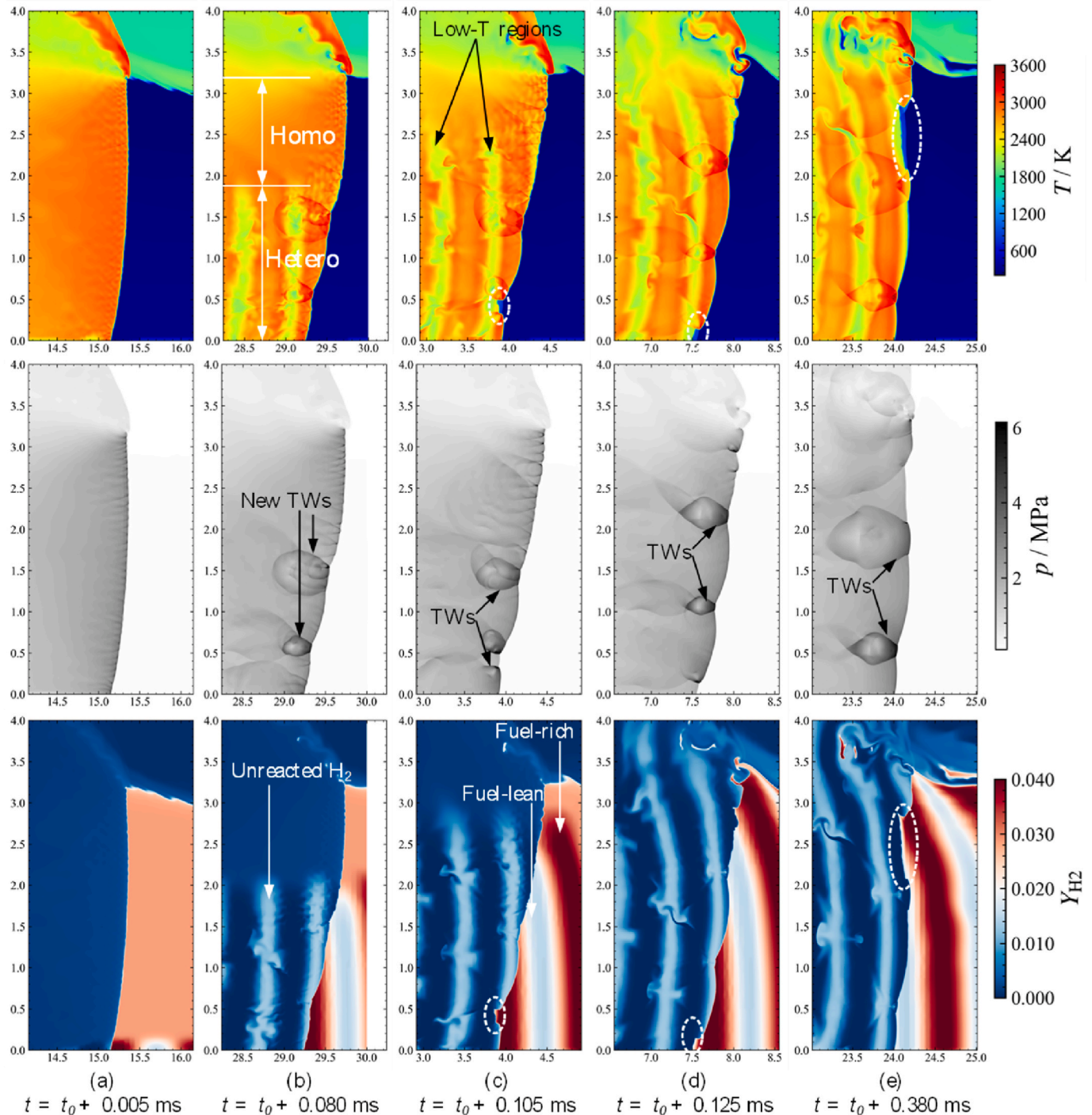


Fig. 6. Transition from homogeneous to heterogeneous detonation. (a) $t = t_0 + 0.005$ ms, (b) $t = t_0 + 0.080$ ms, (c) $t = t_0 + 0.105$ ms, (d) $t = t_0 + 0.125$ ms, (e) $t = t_0 + 0.380$ ms. Upper row: temperature; middle row: pressure; bottom row: H_2 mass fraction. TW: Transverse Waves.

appear alternately along the longitudinal direction. Several local quenches are observed as the DW passes through the fuel-lean strips, which are marked with dashed ellipses in Fig. 6. Consequently, the reinitiation after these local quenches results in the strong and large-scale transverse waves (labeled TWs). It can also be observed in Fig. 6 (b) and (c) that the DW becomes tilted due to enhanced velocity deficit in the heterogeneous portion. Moreover, a substantial amount of H_2 within the fuel-rich strip remains unreacted behind the DW. The low-temperature regions, which correspond to the fuel-lean strips with low heat release, are also observed behind the DW. All local quenches are observed within the fuel-lean strips, whereas the flame front always keeps coupled to the leading shock when it traverses the fuel-rich strips. This is because Δ_{ind} grows significantly faster on the low equivalence ratio side of Fig. 2. Comparing Fig. 6(a) and (e), it is found that the cellular structures become distorted in the heterogeneous flow. This is consistent with the experimental observations of Rankin et al. [43], where a distorted cellular pattern due to locally varying fuel concentrations is observed in a non-premixed RDE through chemiluminescence imaging. Rankin's experiments [43] also indicated that detonation occasionally exists under fuel-lean conditions while persisting consistently under stoichiometric conditions. This is also qualitatively consistent with the current observations that the local quenching is more likely to occur in the fuel lean regions.

To better illustrate the highly unsteady DW front structure and triple-point trajectories during the transition process, the numerical soot foil is shown in Fig. 7. It is clearly observed that the cell size is drastically increased when the pre-detonation mixture gradually becomes heterogeneous. The forced growth in cell size by reactant heterogeneity was also observed previously in simulations of channeled detonations [44, 45]. The increase in cell size evidence a stronger front instability and a lower detonability in heterogeneous mixtures compared to the homogeneous ones. The non-dimensional DW height drops markedly from around $H_{DW}/\alpha \approx 31$ to $H_{DW}/\alpha \approx 3$, which indicates a higher tendency of detonation failure due to short reactant layer height. The correlation between the detonability and H_{DW}/α will be discussed later in Section 3.3. As depicted in Fig. 2, the ZND induction length Δ_{ind} always increases when the mixture equivalence ratio deviates from unity. Due to the scaling relationship between the induction length and cell size, the larger Δ_{ind} in the fuel-rich and fuel-lean regions leads to the larger cell size.

The time-averaged D/D_{CJ} , I_{sp} , and η in the stable stage of both the homogeneous and heterogeneous cases are tabulated in Table 2 for comparison. The above three quantities decline slightly when the mixture becomes heterogeneous. As already plotted in Fig. 2, D_{CJ} increases monotonically with equivalence ratio. The smaller D_{CJ} at lower equivalence ratio is simply a result of lower heat release under fuel-lean conditions. Noticeably, the slope is much steeper in the fuel-lean side. This means that the large velocity reduction in the fuel-lean region dominates the wave velocity in heterogeneous flow and explains the decrease in D/D_{CJ} compared to homogeneous ones. In addition, η drops from 96.7% to 89.4%, suggesting a larger fraction of H_2 remains unreacted behind the DW and escapes from the combustor eventually.

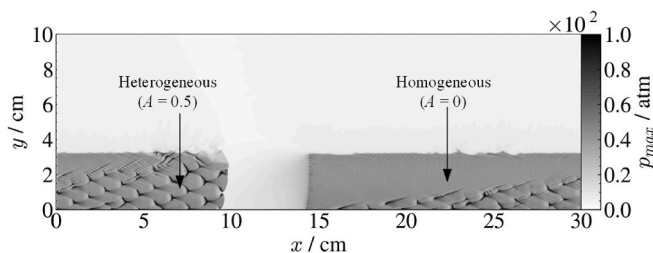


Fig. 7. Numerical soot foil during the transition from homogeneous to heterogeneous detonation.

Table 2

Time-averaged statistics of homogeneous and heterogeneous detonation in the stable stage.

	D/D_{CJ}	I_{sp}/s	η
Homogeneous ($A = 0.0$)	0.978	5184	96.7%
Heterogeneous ($A = 0.5$)	0.936	4975	89.4%

This decline in η is simply a result of un-reacted H_2 strip as shown in Fig. 6(b). The drop in η , eventually leads to the decline in specific impulse. These findings imply that reactant heterogeneity could affect the stability and performance of the DW and may need to be considered when designing the injection strategies of an RDE.

3.2.2. Effects of perturbation amplitude A

In this subsection, the effects of perturbation amplitude A are assessed. To this end, we fix the perturbation wavelength as $\lambda = 53$, while incrementally increasing the amplitude from $A = 0.25$ to 1.0 in consecutive cases. The results in terms of stable stage temperature and H_2 mass fraction are illustrated in Fig. 8. It is observed that as A gradually increases, both the temperature and H_2 distribution becomes increasingly heterogeneous. Specifically, the post-detonation low-temperature and unreacted H_2 strips become more pronounced. This implies that an increased amount of H_2 remains unreacted behind the DW. Note that the DW remains self-sustained even when the perturbation amplitude is pushed to the upper limit of $A = 1.0$ in Fig. 8 (d), where the leanest region has an equivalence ratio of 0. This suggests that when λ is sufficiently short (e.g. $\lambda = 53$ for all cases in Fig. 8), the DW can always keep sustained under the impact of reactant heterogeneity.

To quantitatively evaluate the unreacted H_2 observed in Fig. 8 and its effect on combustion characteristics, the spatial- and time-averaged mean of H_2 mass fraction (Y_{H_2}), mean of HRR (HRR_{Avg}), and standard deviation of HRR (HRR_{SD}) are shown in Fig. 9. The statistics are performed by first calculating the volume-weighted mean along the x -direction for each fixed y , followed by a temporal average among different time instants during the stable stage. The horizontal dashed lines indicate the time-averaged DW height in different cases. The DW height increases slightly with A . In Fig. 9(a), Y_{H_2} drops markedly in the detonative zone (i.e., $y < H_{DW}$) for all cases, evidencing the majority of the injected H_2 is consumed by the DWs. Consequently, as shown in Fig. 9 (b), almost all the heat release is clustered inside the detonative zone. However, Y_{H_2} increases monotonically as A increases, confirming more H_2 remain unburnt behind the DW. Therefore, HRR_{Avg} inside the detonative zone decreases as A increases due to more H_2 remain unreacted. The standard deviation of HRR increases with A , as shown in Fig. 9(c). Specifically, HRR_{SD} increases slightly as A increases from 0 to 0.25, but rises drastically when A further increases from 0.25 to 0.5, suggesting that DW instability is intensified at larger A .

To better demonstrate the effects of A on the DW propagation and instabilities, the numerical soot foils of a complete rotating cycle recorded during the stable stage are shown in Fig. 10. It is observed that the cell size increases gradually as A increases. When the amplitude is small (see $A = 0.25$, Fig. 10(a)), the cell size is almost unchanged ($H_{DW}/\alpha \approx 32$) compared to homogeneous ones depicted in Fig. 4(d) ($H_{DW}/\alpha \approx 31$). This is consistent with the observations in Fig. 9(c), where only minor oscillations of HRR are observed as A increases from 0 to 0.25. When the amplitude is increased to $A = 0.5$ in Fig. 10(b), the cell size increases drastically ($H_{DW}/\alpha \approx 3$). Quantitatively, the average cell size grows dramatically from $\alpha \approx 0.1$ cm at $A = 0.25$ to 1.1 cm at $A = 0.5$. Nevertheless, as the amplitude is further increased to $A = 0.75$ and 1.0 , the cell size only shows a minor increase (reaching $\alpha \approx 1.6$ cm at $A = 1.0$). This means that impact of amplitude is limited by the current short wavelength of $\lambda = 53$. The irregularity of the cells is also noticeably increased due to increase A . The DW height also demonstrates larger oscillations due to the increased cell irregularity at larger A .

We then performed time-based statistics for all cases shown in Fig. 10

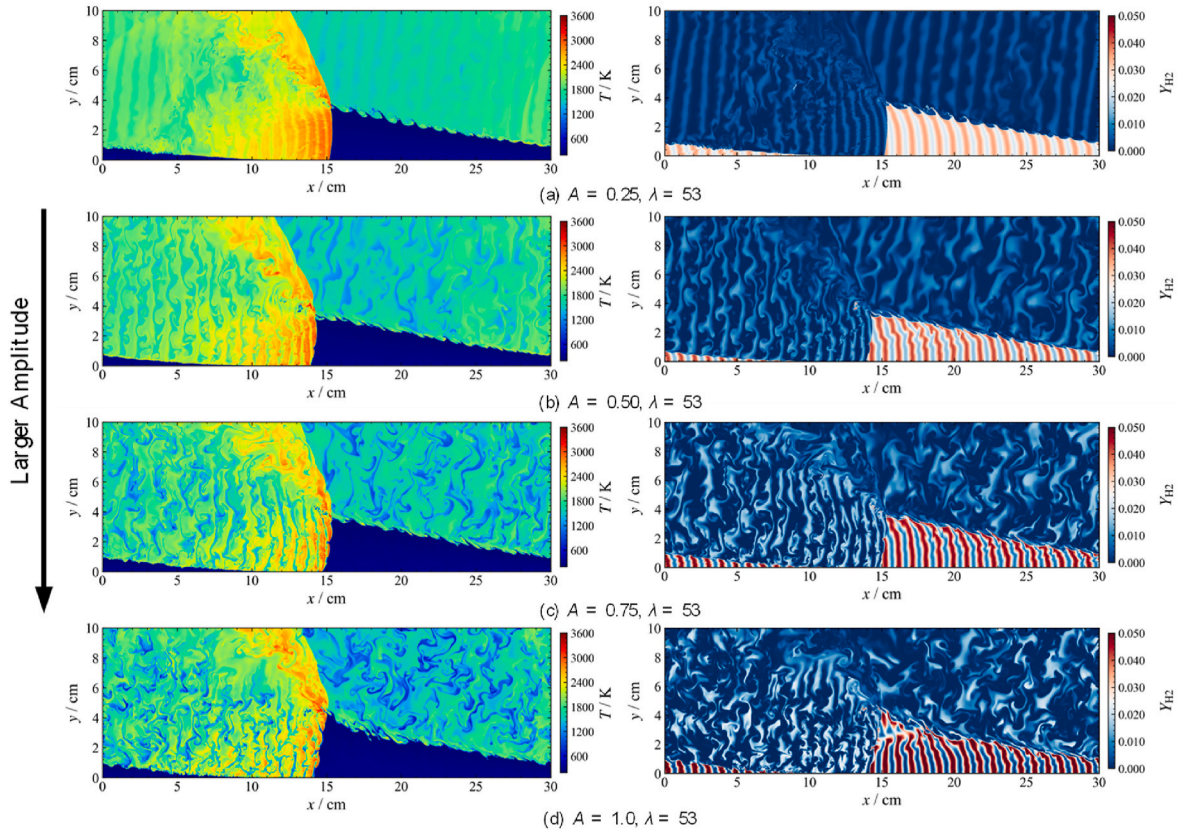


Fig. 8. Detonation structures with varying perturbation amplitude A . (a) $A = 0.25$, (b) $A = 0.5$, (c) $A = 0.75$, (d) $A = 1.0$. The perturbation wavelength is fixed as $\lambda = 53$. Left column: temperatures, right column: H_2 mass fractions.

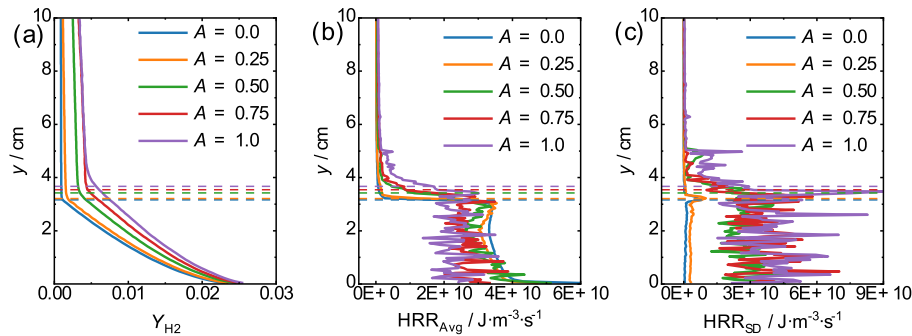


Fig. 9. Distributions of (a) mean of H_2 mass fraction, (b) mean of HRR, and (c) standard deviations of HRR along the y -direction under varying perturbation amplitude A . The perturbation wavelength is fixed as $\lambda = 53$. The horizontal dashed lines indicate the time-averaged DW height.

to evaluate the properties of DWs during the stable stage. The emphasis is laid on the effects of A on both the mean and standard deviations of D/D_{CJ} , I_{sp} , η , and H_{DW} . The average wave velocity in Fig. 11(a) shows a monotonical decline as A increases. Specifically, D/D_{CJ} declines from 97.8% at $A = 0$ to 82.5% at $A = 1.0$, meaning that the velocity deficit is considerably enhanced by increased A . As discussed previously, such increased velocity deficit is simply a result of lower D_{CJ} in the fuel-lean regions where the heat release is low (see Fig. 2). The decreased D/D_{CJ} also means a longer time is required for the DW to complete a rotating cycle and explains the slight increase of H_{DW} as observed in Fig. 11(d). The standard deviation of wave speed increases by several orders of magnitude as the amplitude increases to $A = 1.0$. This increased fluctuation in wave velocity is a result of increased DW instability as discussed in Figs. 6, 9 and 10. Additionally, the mean and standard deviations of I_{sp} and η show similar trends with respect to A . Both the

mean of I_{sp} and η decrease monotonically, whereas their standard deviations increase gradually as A increases. The decline in means of I_{sp} and η is a result of unreacted H_2 that eventually escapes the combustor while the increase of their standard deviations is caused by intensified DW instabilities characterized by larger cell size and oscillations in heat release as discussed previously.

Since the perturbation wavelength is fixed as a relatively small value of $\lambda = 53$ in Fig. 10 and, the DW remains self-sustained even at the largest amplitude of $A = 1.0$, we then increase and fix the perturbation wavelength to a larger value of $\lambda = 71$, while progressively increase A to re-evaluate its effects. The results in terms of numerical soot foil under varying A are shown in Fig. 12. As A is gradually increased, similar trends are observed as those in Fig. 10. The cell size in Fig. 12 increases gradually as the amplitude increases from $A = 0.0$ to $A = 0.75$. Nevertheless, the DW eventually decouples when the amplitude is excessively

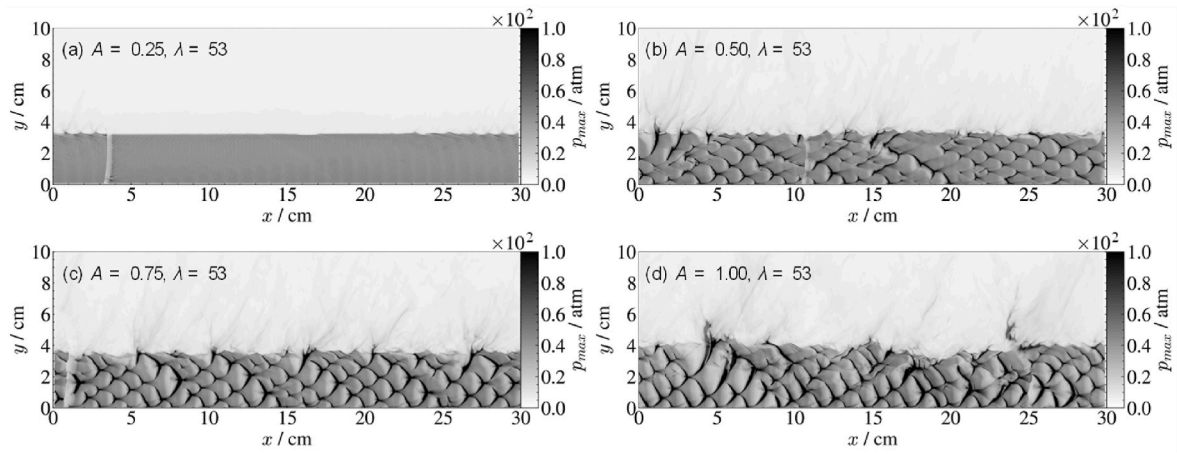


Fig. 10. Numerical soot foils with varying perturbation amplitude A . (a) $A = 0.25$, (b) $A = 0.50$, (c) $A = 0.75$, (d) $A = 1.0$. The perturbation wavelength is fixed as $\lambda = 53$.

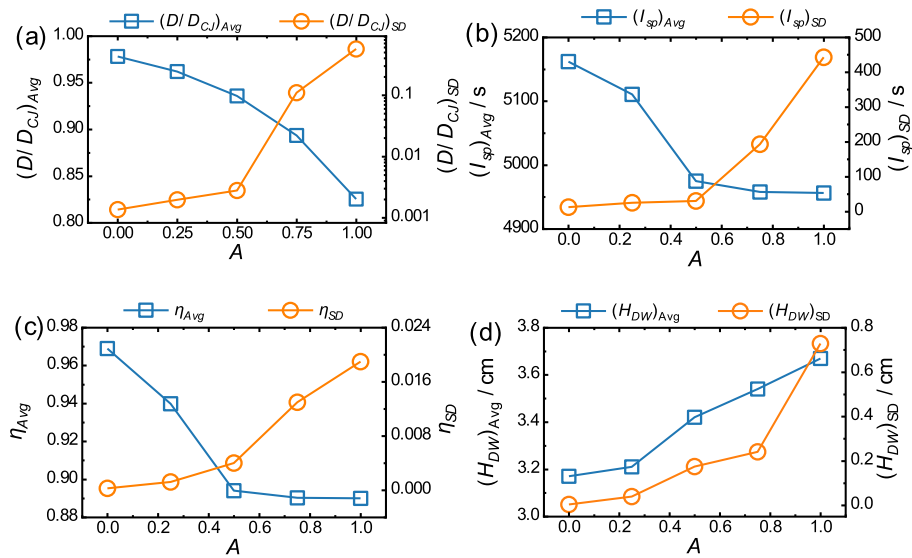


Fig. 11. Time-averaged mean and standard deviation of (a) DW speed, (b) specific impulse, (c) combustion efficiency, and (d) DW height under varying perturbation amplitude A . The perturbation wavelength is fixed as $\lambda = 53$.

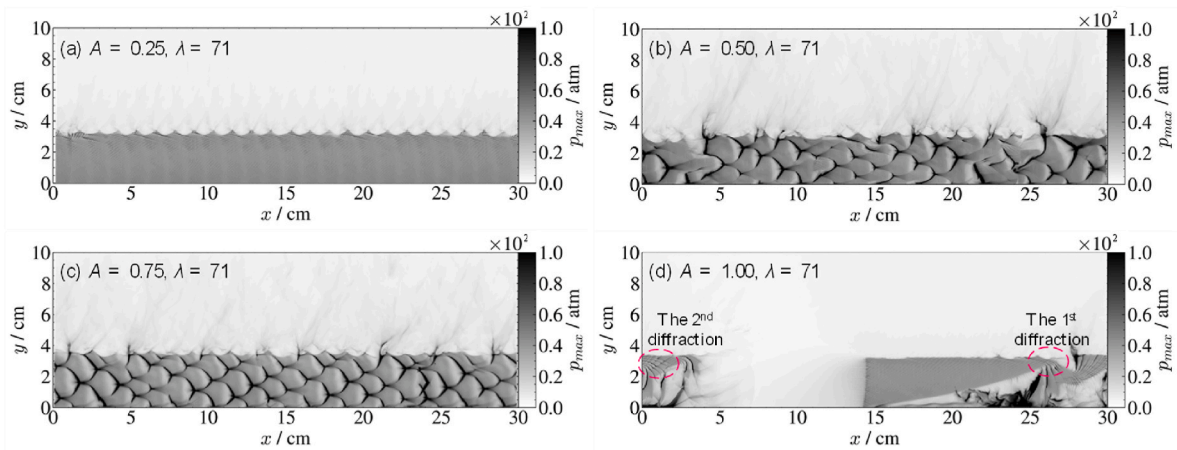


Fig. 12. Numerical soot foil with varying perturbation amplitude A . (a) $A = 0.25$, (b) $A = 0.50$, (c) $A = 0.75$, (d) $A = 1.0$. The perturbation wavelength is fixed as $\lambda = 71$.

large ($A = 1.0$) in Fig. 12(d). This means that under the current fixed wavelength ($\lambda = 71$), the DW may fail if the amplitude surpasses some critical value, confirming the negative impact of A on detonability of the mixture. Comparing Figs. 10(d) and 12(d), one can readily found that the DW is sustained in the former ($A = 1.0, \lambda = 53$) while decouples in the latter ($A = 1.0, \lambda = 71$). This evidences that λ also has a significant impact on the detonability of the mixture, which will be discussed later in Section 3.2.3.

To show the details during the detonation failure process due to large A in Fig. 12(d), the transient flow fields are shown in Fig. 13 by contours of temperature and H_2 mass fraction superimposed on nondimensional density gradient magnitude. At $t = t_0 + 0.005$ ms in Fig. 13(a), the mixture inside the fuel-refill zone is mostly homogeneous and the DW propagates stably. At $t = t_0 + 0.05$ ms in Fig. 13(b), the lower portion of the fuel-refill zone gradually becomes heterogeneous because of perturbations imposed on the inflow boundary. Unlike the case illustrated in Fig. 6 where the DW remain coupled in the heterogeneous portion, the DW decouples locally in this case on the lower portion to form an oblique shock. The survived DW on the upper portion of the fuel-refill zone then diffracts at $t = t_0 + 0.065$ ms in Fig. 13(c) due to the formation of strong transverse wave caused by local explosions. This diffraction is denoted as the 1st diffraction in Fig. 12(d). The diffracted DW only survived on the upper homogeneous portion while quenches on the lower heterogeneous portion. The survived DW then undergoes another diffraction (see the 2nd diffraction in Fig. 12(d)). As the fuel-refill zone has become completely heterogeneous during the 2nd diffraction, the diffracted DW cannot survive in this completely heterogeneous mixture with extremely low detonability, hence the DW fully decouples

eventually. Since no re-initiations are observed after the two diffractions, it is confirmed that the mixture with extremely high perturbation amplitude ($A = 1.0, \lambda = 71$) is not suitable for DW propagation. The critical perturbation amplitude for sustained DW propagation under the current wavelength ($\lambda = 71$) is between $A = 0.75$ and $A = 1.0$. Note that this critical amplitude may vary with the wavelength and will be assessed later in Section 3.3.

3.2.3. Effects of perturbation wavelength λ

In this subsection, we assess the effects of perturbation wavelength λ on DW propagation and performance. To this end, the perturbation amplitude is fixed as $A = 0.5$ while the wavelength is increased gradually from $\lambda = 53$ to 214. The results in terms of temperature and H_2 mass fraction contours are shown in Fig. 14. Generally, unreacted H_2 strips widely exist behind DW among all cases. As λ increases, both the fuel-rich and fuel-lean strip grows wider. As a result, both the temperature and reactant distribution become more heterogeneous.

Fig. 15 presents the spatial- and time-averaged mean of H_2 mass fraction (Y_{H_2}), HRR (HRR_{Avg}), and standard deviation of HRR (HRR_{SD}) to highlight the effects of λ on combustion characteristics, with time-averaged H_{DW} indicated by horizontal dashed lines. The DW height shows a slight increase as λ increases. Similar to Fig. 9, the consumption of H_2 and heat release is clustered in the detonative zone for all cases. Nonetheless, the effect of λ on the amount of unreacted H_2 is limited. As shown in Fig. 15(a) and (b), marginal influence of λ on the mean of Y_{H_2} and HRR are observed for all heterogeneous cases ($A \neq 0$). This is a result of the nature of the sinusoidal function, where the wavelength λ only stretches or compresses this distribution spatially but does not alter the

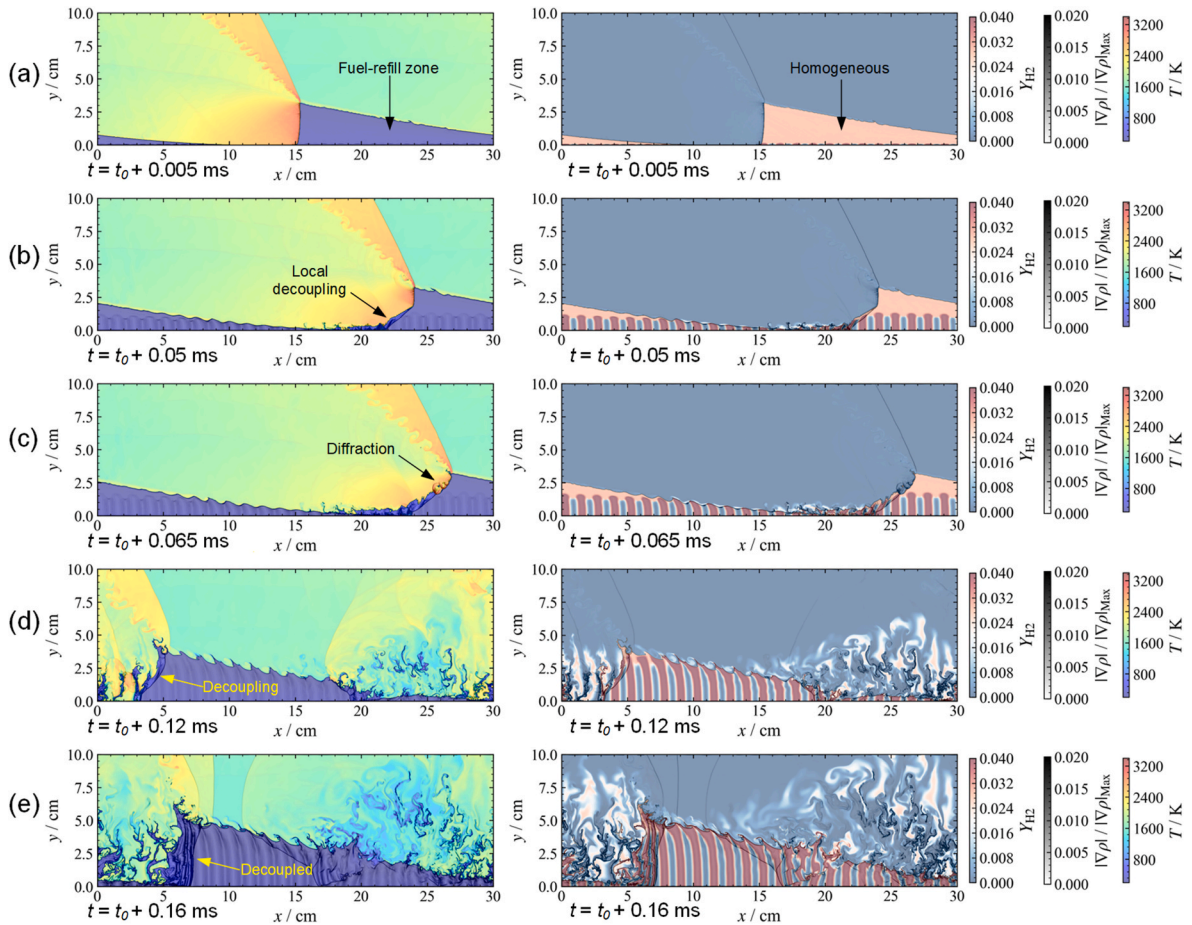


Fig. 13. Transient evolution process ($A = 1.0, \lambda = 71$) of detonation decoupling due to excessive perturbation amplitude. (a) $t = t_0 + 0.005$ ms, (b) $t = t_0 + 0.05$ ms, (c) $t = t_0 + 0.065$ ms, (d) $t = t_0 + 0.12$ ms, (e) $t = t_0 + 0.16$ ms. Left column: semi-transparent temperature contour superimposed on nondimensional density gradient magnitude. Right column: semi-transparent H_2 mass fraction contour superimposed on nondimensional density gradient magnitude.

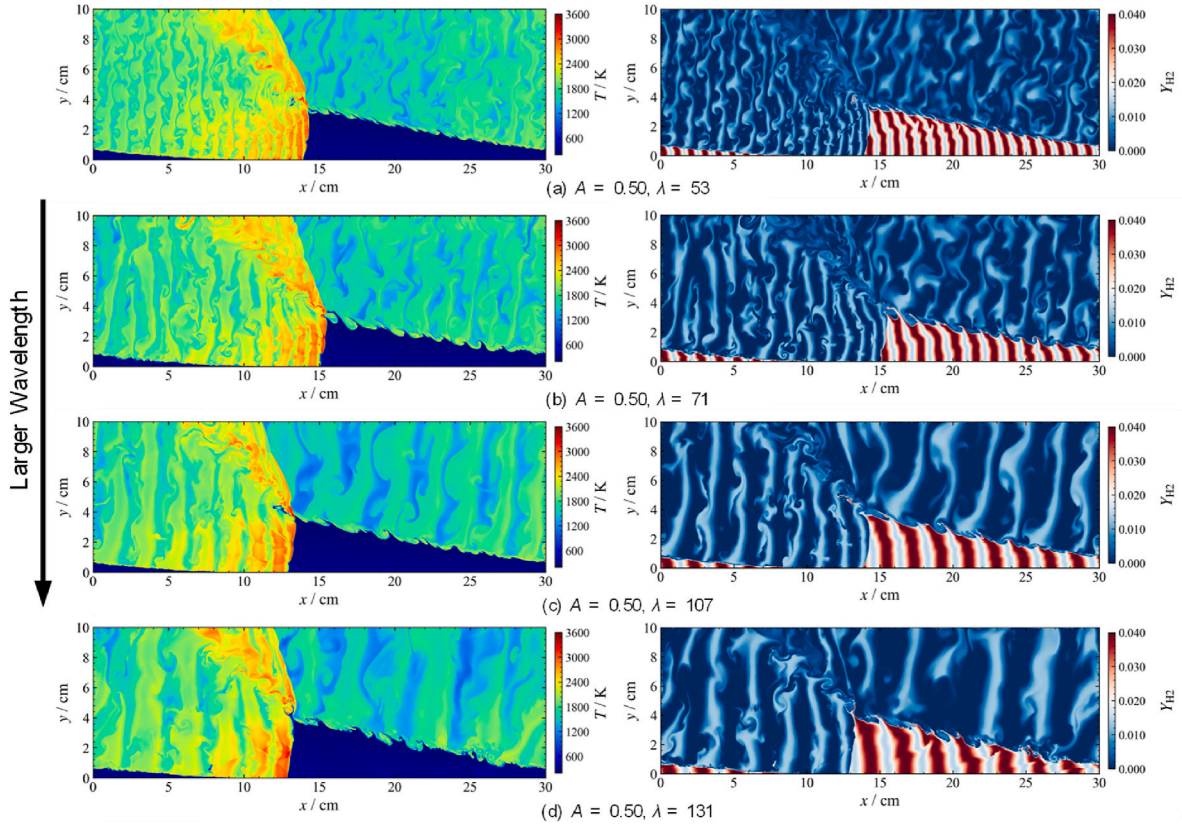


Fig. 14. Detonation structures with varying perturbation wavelength λ . (a) $\lambda = 53$, (b) $\lambda = 71$, (c) $\lambda = 107$, (d) $\lambda = 131$. The perturbation amplitude is fixed as $A = 0.5$.

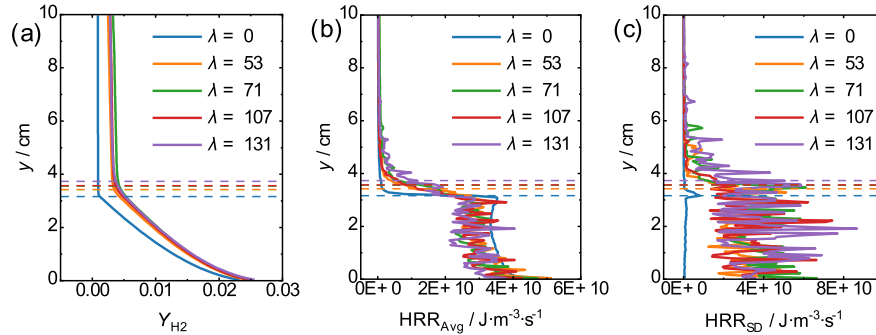


Fig. 15. Distributions of (a) mean of H_2 mass fraction, (b) mean of HRR, and (c) standard deviations of HRR along the y -direction. The perturbation amplitude is fixed as $A = 0.5$. The horizontal dashed lines indicate the time-averaged DW height.

overall mixture composition. The total proportion of the mixture that exists in fuel-rich or fuel-lean states is fixed under different λ . Larger oscillations are observed as λ increases in Fig. 15(c), which implies that the DW instability is significantly intensified by λ , confirming the negative impact of increasing λ on DW stability.

The numerical soot foils recorded during the stable stage are shown in Fig. 16. Generally, it is readily observed that both the cell size and irregularity increase noticeably as λ increases. Although the DW height also increases slightly with larger λ , the significant increase in cell size dominates the nondimensional DW height. It decreases from around $H_{DW}/\alpha \approx 3$ to 1 as wavelength increases from $\lambda = 53$ in Fig. 16(a) to $\lambda = 131$ in Fig. 16(d). Specifically, as λ increases from 53 to 131 at a fixed amplitude of $A = 0.5$, the average cell size α grows from approximately 1.1 cm to 3.6 cm. The larger cell size at longer λ indicates that, similar to the perturbation amplitude A discussed previously in Section 3.2.2,

increasing λ also has a considerably negative impact on the DW stability. This is consistent with the observations in Fig. 15. Note that although the instability of the DW front is intensified by large λ , the DW remains sustained for all cases shown in Fig. 16. However, if λ is further increased to some larger value such that the cell size exceeds the DW height, the DW may decouple. This will be discussed later in this section.

The effects of λ on properties and performance of the DWs are then assessed through time-based statistics during the stable stage. As shown in Fig. 17(a), the mean of D/D_{CJ} only decreases mildly while its standard deviation increases significantly with λ . Specifically, the mean of D/D_{CJ} only slightly decrease from 0.935 to 0.90 as λ is increased by around 3 times (from $\lambda = 53$ to 131), suggesting a minor effect of λ on velocity deficit of the DW. This is because the amount of unreacted H_2 , and hence the overall heat release, is almost independent of λ (see Fig. 15(a) and (b)). The increase in standard deviation of D/D_{CJ} is caused by the

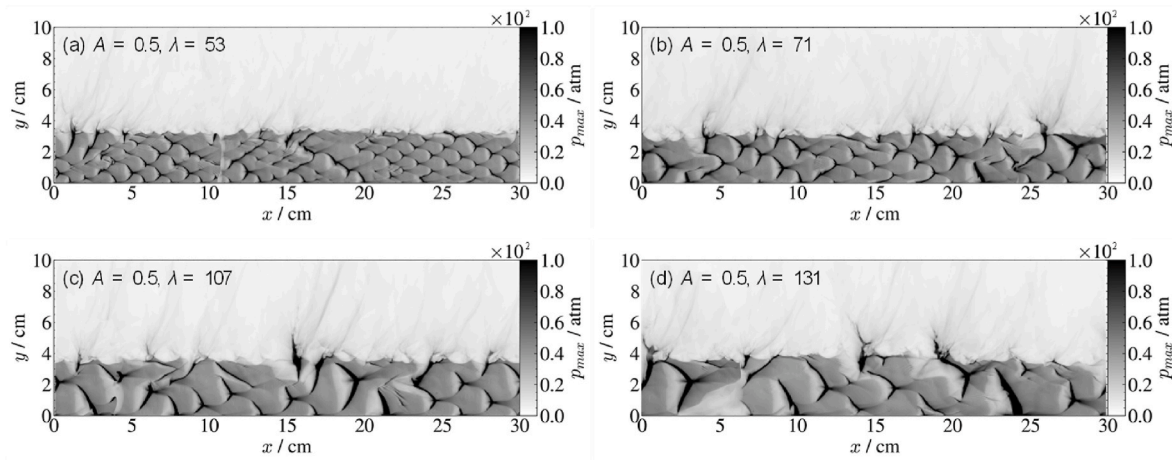


Fig. 16. Numerical soot foils with varying perturbation wavelength λ . (a) $\lambda = 53$, (b) $\lambda = 71$, (c) $\lambda = 107$, (d) $\lambda = 131$. The perturbation amplitude is fixed as $A = 0.5$.

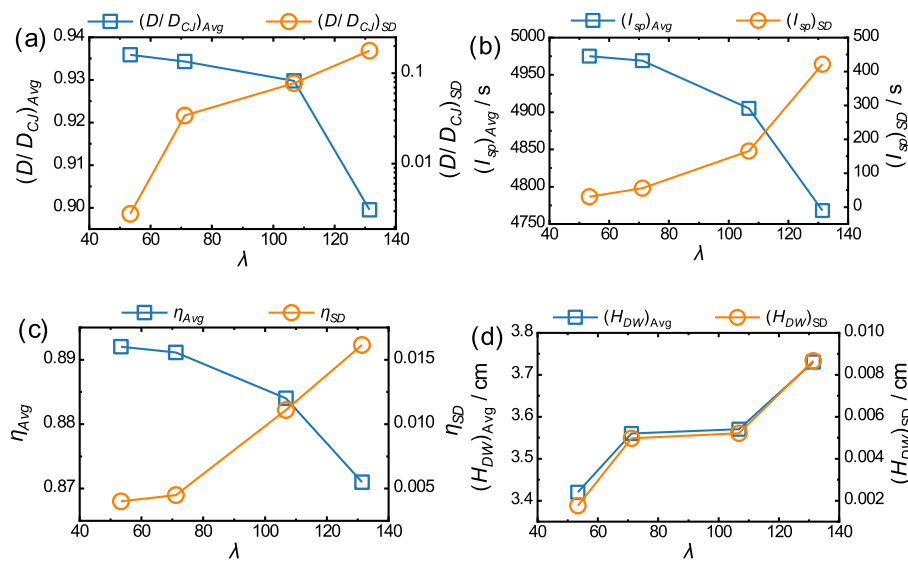


Fig. 17. Time-averaged mean and standard deviation of (a) wave speed, (b) specific impulse, and (c) combustion efficiency and (d) DW height under varying perturbation wavelength λ . The perturbation amplitude is fixed as $A = 0.5$.

increased DW instability as depicted in Figs. 15 and 16. Likewise, the mean of η only decreases very slightly from around 0.89 to 0.87, while its standard deviation increases mildly. Similarly, the mean of the specific impulse also drops slightly with increasing λ for the same reason. In Fig. 17(d), the time-averaged H_{DW} and its standard deviation increases mildly due to the decrease in D/D_{CJ} and intensified instability.

Since the DWs of all the cases in Fig. 14 remain sustained under the impact of heterogeneity with different wavelength, we now retain the amplitude as $A = 0.5$ while further pushing the wavelength to a larger value of $\lambda = 214$ to test the detonation limit. The resultant transient flow fields are shown in Fig. 18 by contours of temperature and H_2 mass fraction overlaid on nondimensional density gradient magnitude. Generally, the DW is gradually decoupled in this case. At $t = t_0 + 0.002$ ms, the DW in homogeneous flow is propagating stably. When the heterogeneous flow is gradually introduced from the inflow boundary (Fig. 18 (b)), local quenching is observed on the lower portion of the DW. Similar to the observations in Fig. 6, this local quenching occurs as the DW is passing through a fuel-lean strip. Local re-initiation then occurs upon the arrival of transverse waves from the upper portion of the DW. As time proceeds to $t = t_0 + 0.137$ ms in Fig. 18 (c), the mixture within the entire fuel-refill zone becomes heterogeneous and another

local quenching occurs on the upper portion. Before re-initiation can occur on the upper portion of the DW, another local quenching is formed on the lower portion in Fig. 18(d) as the DW transmits a new fuel-lean strip. Eventually, the DW is fully decoupled after the frequently occurred local quenches. From a macroscopic perspective, based on the trends of cell size observed in Fig. 16, the detonation failure in this case may be due to the nondimensional DW height H_{DW}/a being smaller than unity. This DW failure also confirms that, similar to the perturbation amplitude discussed previously in Section 3.2.2, the detonability of the mixture is also significantly influenced by the perturbation wavelength. Generally, the DW irregularity is enhanced while the performance is slightly deteriorated as the perturbation wavelength is increased. The critical perturbation wavelength for sustained DW propagation under the current amplitude ($A = 0.50$) is between $\lambda = 131$ and $\lambda = 214$.

3.3. Detonation limits

In preceding sections, the detonation structures in heterogeneous flow are revealed, and the emphasis is laid on the effects of perturbation amplitude A and wavelength λ . It was found that both factors have negative impacts on the DW stability and performance. The flame front

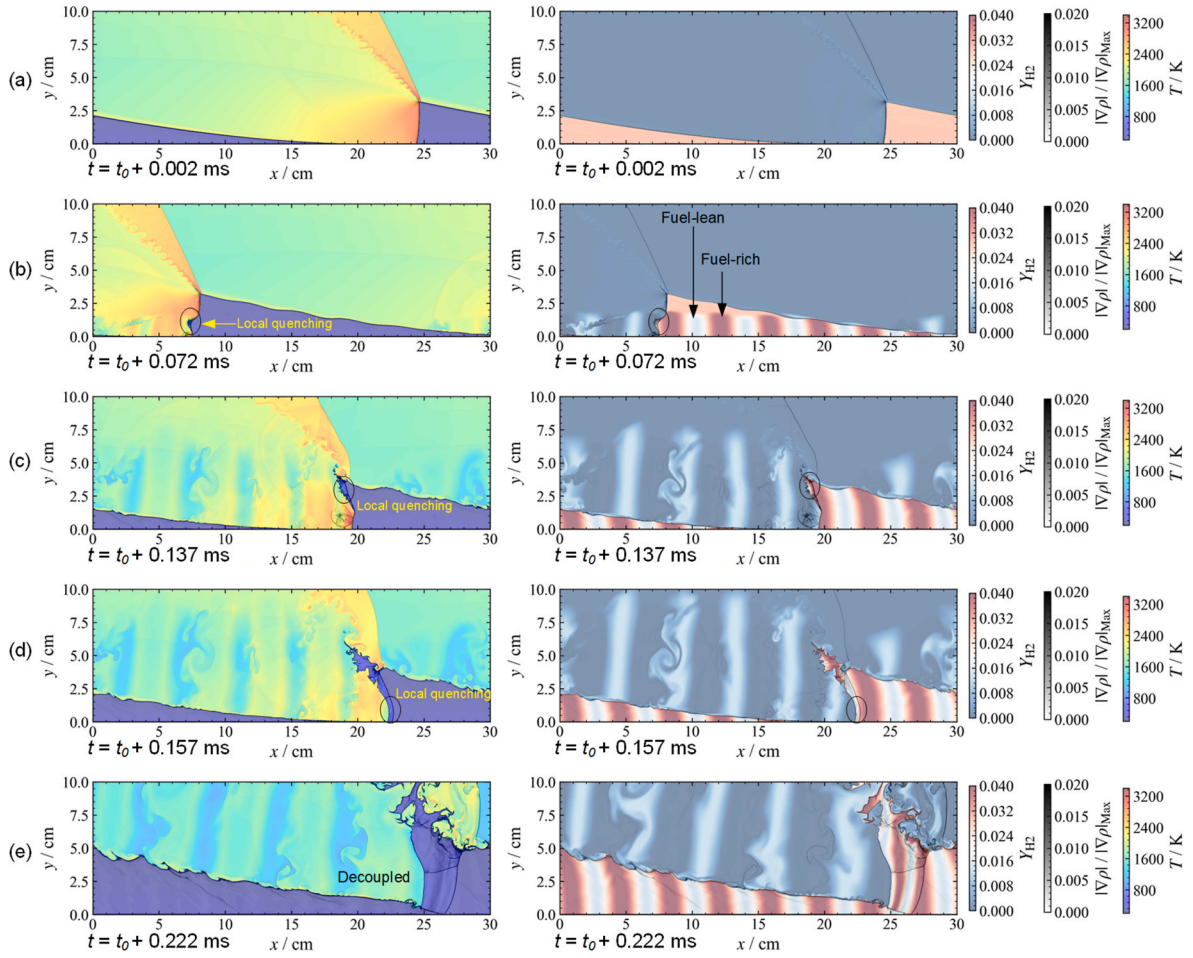


Fig. 18. Transient evolution process ($A = 0.5$, $\lambda = 214$) of detonation decoupling due to excessively large perturbation wavelength λ . (a) $t = t_0 + 0.002$ ms, (b) $t = t_0 + 0.072$ ms, (c) $t = t_0 + 0.137$ ms, (d) $t = t_0 + 0.157$ ms, (e) $t = t_0 + 0.222$ ms. Left column: semi-translucent temperature contour superimposed on nondimensional density gradient magnitude. Right column: semi-translucent H_2 mass fraction contour superimposed on nondimensional density gradient magnitude.

may decouple with the precursor shock due to local quenches, causing detonation failure at excessively large A and λ . To reveal the critical conditions for detonation sustainability, more cases among varying A and λ are performed. The resultant detonability and time-averaged wave velocity are summarized in Fig. 19(a) and (b).

As depicted in Fig. 19(a), the detonability of the cases is governed jointly by A and λ . The DW tends to decouple at large A and λ . The critical perturbation wavelength (indicated by the dashed lines in Fig. 19(a)), above which the DW decouples, decreases as A increases. The background contour in Fig. 19(a) indicates the standard deviation of HRR in the detonative zone (see Figs. 9(c) and 15(c)). A qualitative rule can be found in Fig. 19(a). Despite the variation in either A or λ , the

detonability of the heterogeneous mixture seems to be positively correlated to the nondimensional DW height (H_{DW}/α). Due to the high irregularity of cells at large values of A and λ , it is challenging to obtain an accurate threshold value. Qualitatively speaking, however, the DW decouples when H_{DW}/α falls below some critical value. This is further evidenced by the contour of HRR_{SD} , which serves as another measurement of DW instability in addition to H_{DW}/α . Generally, HRR_{SD} increases with A and λ . The DW tends to decouple when HRR_{SD} is excessively large. Both H_{DW} and α increases with A and λ . The former is due to enhanced DW velocity deficit at larger A or λ (see Fig. 19(b)) that produces a longer rotating-cycle time of the DW. The latter is caused by the significant increase of induction length in off-stoichiometric conditions

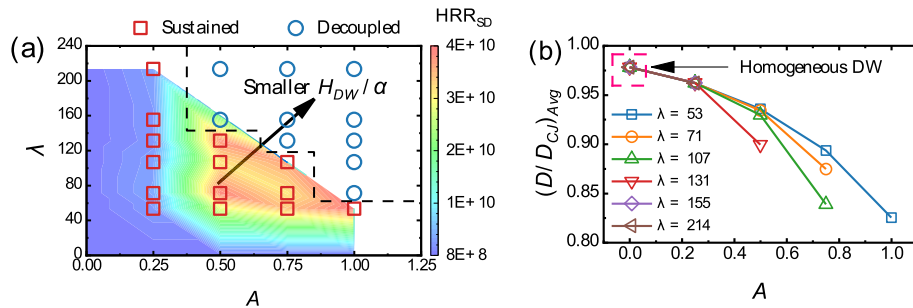


Fig. 19. (a) Detonation limit within the parameter space of perturbation amplitude A and wavelength λ and, (b) Time-averaged detonation velocity under different wavelengths as a function of perturbation amplitude A . HRR_{SD} indicates the fluctuation of HRR in the detonative zone.

(see Fig. 2). As discussed previously, the increase of α is more drastic than that of H_{DW} . Consequently, the value of H_{DW}/α tends to fall as either A or λ increases. At larger amplitude, a shorter λ is required to increase the H_{DW}/α , such that the DW can be sustained. This explains the reduction of critical perturbation wavelength as A increases.

4. Conclusions

Due to the imperfect mixing of fuel and oxidant, DWs commonly propagate through heterogeneous flows in practical engines, making the impact of such heterogeneity inevitable. In this study, we conducted two-dimensional simulations incorporating detailed hydrogen kinetics to model hydrogen-fueled rotating detonations with idealized inflow perturbations in equivalence ratio, characterized by prescribed amplitude (A) and nondimensional wavelength (λ). The objective is to identify general trends of detonation dynamics in heterogeneous flows, with particular emphasis on the effects of A and λ .

The rotating detonation structures in homogeneous flows are analyzed first to set the baseline. Results show that the DW can propagate stably through the homogeneous flow with a non-dimensional DW height of around $H_{DW}/\alpha \approx 31$. As the pre-detonation mixture gradually becomes heterogeneous, both the cell size (α) and its irregularity increase drastically. The transition from homogeneous to heterogeneous detonation is characterized by the emergence of stronger transverse waves due to re-initiations following local quenches and unreacted H_2 strips behind the DW.

A parametric study is then carried out to quantitatively assess the effects of A and λ and determine the detonation limit. It is found that, as either A or λ increases, the cell size grows monotonically, resulting in a decreased H_{DW}/α . This drastic rise of cell size is dominated by the remarkably increased induction length in the fuel-lean region. The DW tends to decouple when A and λ are excessively large. Statistics show that the mean of (D/D_{CJ}) declines monotonically as A or λ increases. Such velocity deficit is dominated by the decrease of D_{CJ} in the fuel-lean region with low heat release. As for performance, it is found that both the mean of specific impulse (I_{sp}) and combustion efficiency (η) slightly decrease as A increases. This mildly deteriorated performance is found to be caused by the increase of the amount of unreacted H_2 strip behind the DW that escape the combustor. The effects of λ on the DW performance is limited since the amount of unreacted H_2 is rarely affected by λ . Due to enhanced DW front instability at larger A and λ , the standard deviations of I_{sp} and η increase considerably as A or λ increases. These results confirm that reactant heterogeneity has negative impact on both the DW stability and performance.

Finally, the detonation limit is determined within the parameter space of A and λ . A distinct boundary is identified between the

detonatable and decoupled regions. It is found that the critical perturbation wavelength, above which the DW decouples, decreases monotonically with A . The detonability of the heterogeneous mixture shows a positive correlation to the nondimensional DW height (H_{DW}/α). Qualitatively speaking, the DW tends to decouple when H_{DW}/α is excessively low. Here, H_{DW}/α only serves as a qualitative detonation instability indicator. Further studies are still required to quantitatively determine the critical value of H_{DW}/α . This trend is quantitatively evidenced by the fluctuations in HRR of the detonative zone. In practical applications, the perturbation wavelength can be reduced by adding a sufficient number of injectors, while the amplitude can be minimized by optimizing the injectors to achieve a higher degree of fuel/oxidant premixing. As an initial attempt to determine the detonation limit of heterogeneous flows in an RDE, this study is limited to two-dimensional DWs subjected to idealized heterogeneity. Consequently, the three-dimensional curvature effect [68] of a practical annular combustor is neglected, which may also impact the detonability of heterogeneous mixtures. Such 3-D curvature effects will be considered and studied in detail in future studies. It's also worth mentioning that multi-wave effects may also affect the sustainability of the DW through wave interactions. It would be interesting to conduct further studies by considering the multi-wave effects.

CRedit authorship contribution statement

Xinke Shao: Writing – original draft, Software, Resources, Investigation, Conceptualization. **Qingyang Meng:** Writing – review & editing, Investigation, Funding acquisition. **Ken Chun Kit Uy:** Writing – review & editing, Investigation. **E Fan:** Writing – review & editing, Software, Investigation. **Lisong Shi:** Writing – review & editing, Software, Investigation. **Chih-Yung Wen:** Writing – review & editing, Supervision, Project administration, Investigation, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix. A. Resolution study

A.1 DW in heterogeneous flow

The case of $A = 0.75$, $\lambda = 53$ is used for grid independence validation of detonation in heterogeneous flows. Temperature contours and numerical soot foils recorded during the stable stage are shown in Fig. A1. Both the wave and cellular structures are hardly affected by the AMR levels, indicating the current mesh strategy (4 levels of AMR) for heterogeneity detonations is adequate. The time-averaged D/D_{CJ} and I_{sp} during the stable stage for different levels of AMR are also compared in Table. A1. Evidently, very minor discrepancies are observed, justifying the reasonability of the current mesh used.

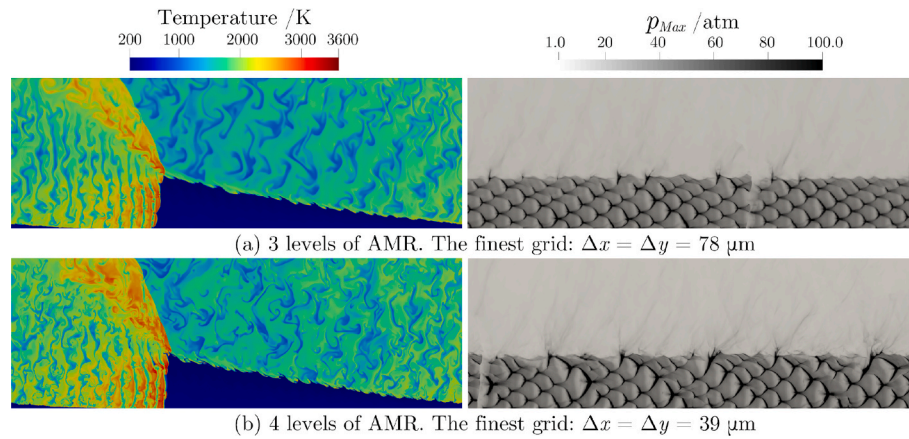


Fig. A1. Temperature and numerical soot foil in the heterogeneous flow ($A = 0.75, \lambda = 53$). (a) 3 levels, (b) 4 levels. $N = 43$ Mean = 5123.

Table.A1 Time-averaged mean and standard deviation of D/D_{CJ} and I_{sp} during the stable stage for different levels of AMR ($A = 0.75, \lambda = 53$)

AMR levels	$(D/D_{CJ})_{Avg}$	$(D/D_{CJ})_{SD}$	$(I_{sp})_{Avg}/s$	$(I_{sp})_{SD}/s$
3	0.89340	0.10956	4957.86267	192.93592
4	0.88876	0.12546	5023.66299	181.96301

A.2 DW in homogeneous flow

The temperature contours for the base line case $A = 0, \lambda = 0$ under different levels of AMR is illustrated in Fig. A2. The pressure and temperature distributions along the inflow boundary are also plotted in Fig. A3 for quantitative comparison. Despite some fine structures at higher levels of AMR, the flow structures are almost unchanged under different AMR levels. The time-averaged D/D_{CJ} and I_{sp} during the stable stage for different levels of AMR are also compared in Table. A2. Obviously, the results are insensitive to the grid change, evidencing the current mesh to be adequate.

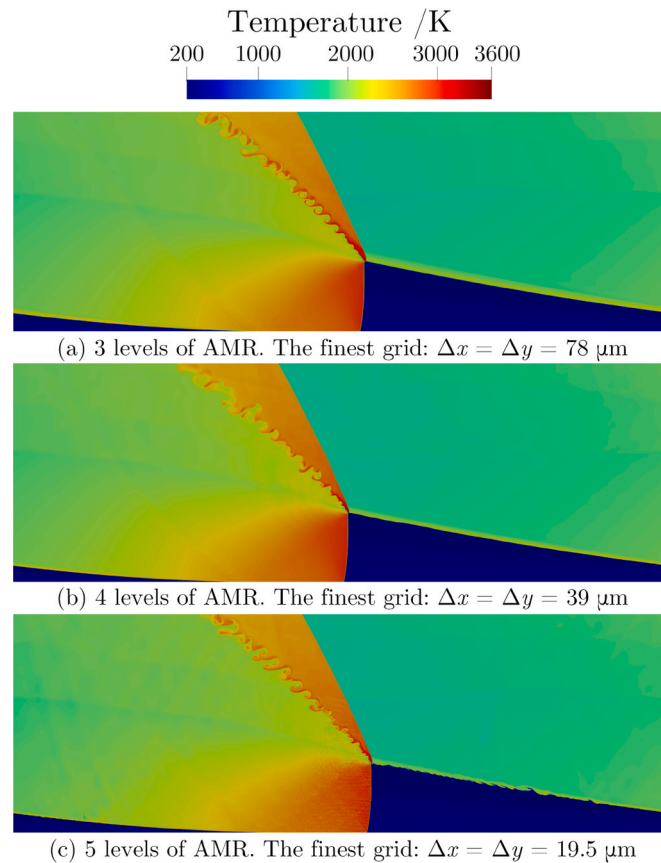


Fig. A2. Temperature contours with varying levels of AMR: (a) 3 levels, (b) 4 levels, (c) 5 levels.

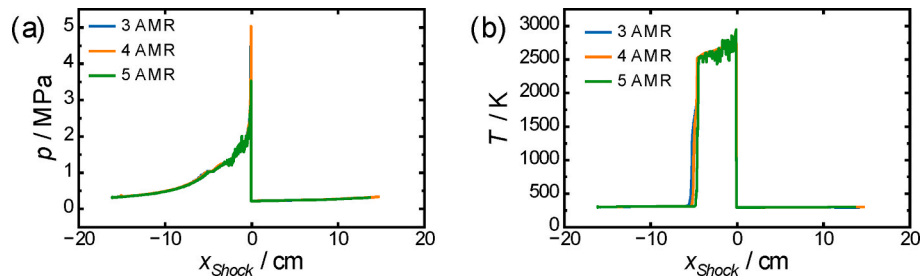


Fig. A3. Distributions of (a) pressure and (b) temperature along the inflow boundary in shock-frame with different levels of AMR.

Table A2

Time-averaged mean and standard deviation of D/D_{CJ} and I_{sp} during the stable stage for different levels of AMR ($A = 0, \lambda = 0$)

AMR levels	$(D/D_{CJ})_{Avg}$	$(D/D_{CJ})_{SD}$	$(I_{sp})_{Avg/s}$	$(I_{sp})_{SD/s}$
3	0.97818	0.00136	5163.24735	12.97345
4	0.97324	0.00161	5161.32125	11.78206
5	0.97487	0.00713	5184.10845	43.88035

Appendix. B. Effect of transport phenomena

To validate the inviscid assumption adopted in the current study, we conducted additional simulations incorporating transport phenomena by solving the time-accurate, multi-component reactive Navier-Stokes equations. These results are compared with the inviscid cases in Fig. A4. As shown, transport phenomena demonstrate minimal influence on the detonation structures. Even under the largest fuel concentration gradient considered in this study ($A = 1.00, \lambda = 53$), their effects remain negligible. Furthermore, when transport phenomena are included, cell size and irregularity increase with perturbation amplitude, aligning with trends observed in the current inviscid simulations. The reasonability of inviscid assumption is thus verified.

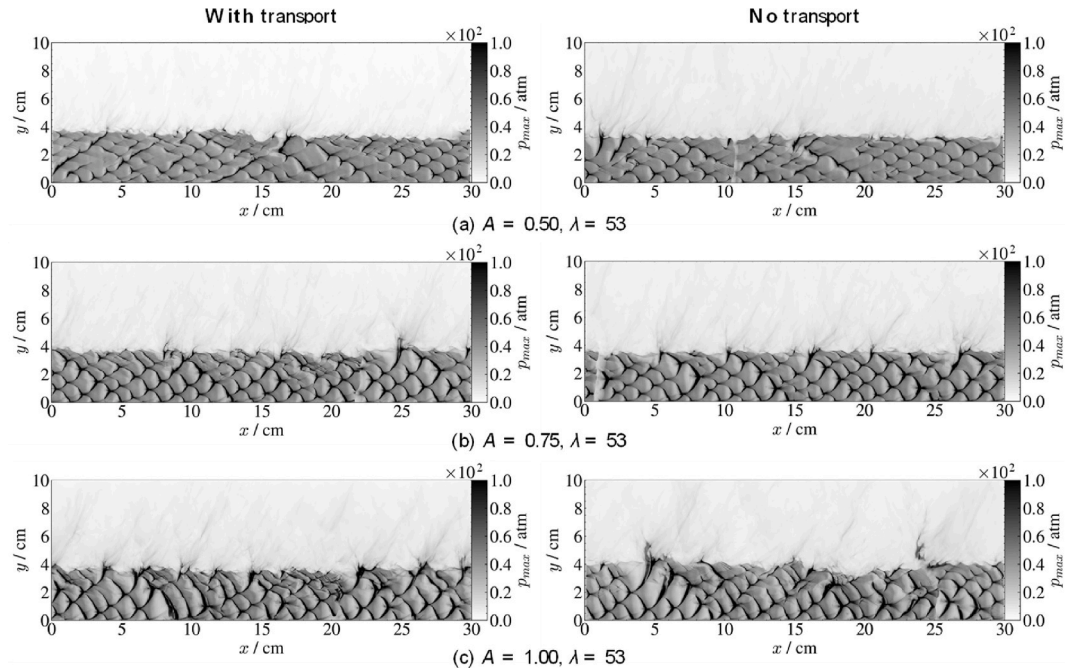


Fig. A4. Numerical soot foil with varying perturbation amplitude A . Left column: with transport; right column: no transport. (a) $A = 0.50, \lambda = 53$, (b) $A = 0.75, \lambda = 53$, (c) $A = 1.00, \lambda = 53$.

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