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Different modes of reaction front propagation in *n*-heptane/air mixture with concentration non-uniformity

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Abstract

According to the reactivity gradient theory of Zel'dovich, the non-uniformity in temperature or concentration can lead to detonation development under certain conditions. In the literature, there are many studies on detonation development caused by temperature gradient or hot spot. However, the modes of supersonic reaction front propagation and detonation development regime caused by concentration non-uniformity have not been investigated previously. In this study, one-dimensional simulations were conducted to investigate the transient autoignition and reaction front propagation processes in *n*-heptane/air mixture with concentration non-uniformity. With the increase of equivalence ratio gradient, three modes (supersonic autoignitive reaction front, developing detonation and subsonic reaction front) of reaction front propagation induced by concentration non-uniformity were identified. The effects of heat conduction and mass diffusion on these three modes were examined and it was demonstrated that molecular diffusion has little influence on the first two modes. The detonation development regime caused by concentration non-uniformity was reported in this paper. This regime was found to be similar to the one caused by temperature gradient. A non-dimensional parameter was proposed to characterize the lower limit of the detonation regime. Furthermore, the effects of initial temperature on the detonation development regime were examined. It was found that the detonation development regime becomes wider as the initial temperature decreases. The initial temperature was shown to only have great impact on the upper limit of the detonation development regime while it has little influence on the lower limit. The influence of initial temperature was explained using the volumetric energy density of the mixture.

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Keywords: Autoignition modes; Detonation development; Concentration non-uniformity; n-Heptane

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1. Introduction

In spark ignition engines (SIEs), the thermal efficiency can be improved through increasing the compression ratio. However, high compression

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Fig. 1. Change of ignition delay time, excitation time and critical equivalence ratio gradient with equivalence ratio for *n*-heptane/air mixture at 1000 K and 40 atm.

ratio also helps to induce engine knock, which causes severe engine damage. According to the theory of Zel'dovich [1] on reactivity gradient-induced combustion modes, the non-uniformity in temperature or concentration can lead to detonation development under certain conditions, which has direct relevance to engine knock. As reviewed by Bartenev and Gelfand [2], many studies were conducted to verify and extend the theory of Zel'dovich. For examples, Bradley and coworkers [3,4] identified different modes of reaction front propagation and proposed an operational peninsula within which detonation can develop from a hot spot; Bradley and Kalghatgi [5] further extended their theory of detonation peninsula to the study of knocking in spark ignition engines; Kurtz and Regele [6] analyzed different time scales involved in detonation development from a hot spot; and Dai et al. [7,8,22] demonstrated that low-temperature chemistry has great impact on detonation development induced by temperature gradient. In these studies, the hot or cool spot model with linear temperature distribution was used and detonation mode was indeed observed at certain temperature gradient.

However, most of the previous studies focused on temperature gradient. There are only a few studies concerning concentration gradient. For examples, El-Asrag and Ju [9] investigated the autoignition of DME/air mixture with both temperature and mixture stratification; Sun et al. [10] studied the ignition to flame transition in stratified *n*-heptane and toluene mixtures; and Bansal et al. [11], Luong et al. [12] and Bhagatwala et al. [13] conducted direct numerical simulations of autoignition in several fuel/air mixtures with composition inhomogeneity. Unfortunately, in these studies detonation development was not observed and little attention was paid to the modes of supersonic reaction front propagation induced by concentration non-uniformity (except the very recent study by Zhang et al. [23] who studied detonation formation with concentration gradient in *n*-heptane/air). It is not clear whether similar modes of reaction front propagation can be induced by concentration and temperature gradients. Moreover, it is not clear whether there is a detonation development regime induced by concentration gradient.

The above-mentioned considerations constituted the motivation for the present study. The objectives were to identify possible modes of reaction front propagation induced by fuel concentration non-uniformity and to find the corresponding critical conditions for detonation development. Unlike previous studies, this study reported, possibly for the first time, the regime for detonation development induced by concentration non-uniformity. Moreover, the effects of initial temperature on the detonation development regime were examined.

2. Numerical model and specifications

One-dimensional numerical simulation was conducted to investigate different modes of reaction front propagation induced by fuel concentration non-uniformity. As one of the main component of Primary Reference Fuel (PRF) for gasoline, *n*-heptane was considered here. It is noted that *n*-heptane is different from gasoline fuel used in SIEs in terms of the octane number. The skeletal mechanism for *n*-heptane [14] was used due to its small size and accurate prediction of *n*-heptane/air ignition at a broad range of temperature and pressure.

Figure 1 shows the ignition delay time τ_i and excitation time τ_e (defined as the time interval between 5% and maximum heat release rate) as a function of equivalence ratio ϕ for *n*-heptane/air at 1000 K and 40 atm. It is seen that τ_i decreases monotonically with ϕ . Therefore, spatial equivalence ratio non-uniformity causes a distribution of local ignition delay time, and it can induce sequential autoignition events.



Fig. 2. The initial conditions used in the simulation of reaction front propagation in a 1D closed chamber with the length of L.

According to the reactivity gradient theory of Zel'dovich [1], different modes of reaction front propagation can be observed depending on the value of equivalence ratio gradient. The reaction front propagation speed u_a caused by equivalence ratio gradient is

$$u_a = \left(\frac{d\tau_i}{dx}\right)^{-1} = \left(\frac{d\tau_i}{d\phi} \cdot \frac{d\phi}{dx}\right)^{-1} \tag{1}$$

It is noted that here "front propagation" was used to describe the sequential ignition rather than flame, and thereby it is equivalent to "ignition locus displacement". When the reaction front speed u_a is close to local sound speed, a, the chemical reaction and pressure wave induced by heat release can be coherently coupled and their mutual reinforcement lead to detonation development [1]. Similar to the critical temperature gradient [3,4], we introduced a critical equivalence ratio gradient determined by the condition of $u_a = a$:

$$\left(\frac{d\phi}{dx}\right)_c = \left(a\frac{d\tau_i}{d\phi}\right)^{-1} \tag{2}$$

Figure 1 also plots the critical equivalence ratio gradient $(d\phi/dx)_c$. Since τ_i decreases with ϕ (i.e., $d\tau_i/d\phi < 0$), we have $(d\phi/dx)_c < 0$ according to Eq. (2). The magnitude of the $(d\phi/dx)_c$ is shown to increase with ϕ . This is because that τ_i of richer mixture becomes less sensitive to ϕ .

Since the ignition delay time is shorter at fuelrich mixture, autoignition reaction front propagation can be induced by a negative equivalence ratio gradient. We considered the transient autoignition process induced by fuel concentration nonuniformity in a 1D closed planar chamber. As shown in Fig. 2, the initiation zone located near the left boundary was modeled by a linear distribution of equivalence ratio with negative gradient. The initial equivalence ratio distribution is:

$$\phi(x, t = 0) = \begin{cases} 1.0 + (x - x_s) \frac{d\phi}{dx} & \text{for } 0 \le x \le x_s \\ 1.0 & \text{for } x_s \le x \le L \end{cases}$$
(3)

where x_s is the size of initiation zone; L = 5 cm is the 1D chamber size; and $d\phi/dx$ is the equivalence ratio gradient (it is a negative constant to be specified). Therefore, everywhere outside of the initiation zone is filled with stoichiometric *n*-heptane/air mixture. The mixture is initially static ($u_0 = 0$ m/s) with $T_0 = 1000$ K and $P_0 = 40$ atm, as depicted in Fig. 2. Adiabatic, nonpenetrative, reflective boundary conditions were adopted for both boundaries at x = 0 and x = L.

Similar to our previous studies [7,8], we simulated the autoignitive reaction front propagation process using the in-house code A-SURF. The conservation equations for 1D, compressible, reactive flow were solved using the finite volume method. The details on governing equations, numerical methods, and code validation for A-SURF can be found in Refs. [7,8,15,16] and were provided in the Supplementary material. Dynamically adaptive mesh was used to efficiently and accurately resolve the propagation of reaction front, shock wave and detonation [7,17]. The skeletal mechanism of *n*-heptane [14] was considered in simulation and CHEMKIN packages [18] were incorporated into A-SURF to calculate the thermodynamic and transport properties as well as the reaction rates. We used the finest mesh size of $\Delta x = 2 \,\mu m$ and time step size of $\Delta t = 0.4 \, \text{ns.}$ As shown by Fig. S3 in the Supplementary material, numerical convergence was ensured by further decreasing the time step and mesh size in simulation.

3. Results and discussion

3.1. Different modes of reaction front propagation

In previous studies (e.g., [3,7]) on reaction front propagation induced by hot/cool spots, a non-dimensional temperature gradient was introduced based on the critical temperature gradient. Similarly, here we introduced the following



Fig. 3. Temporal evolution of temperature, pressure and heat release rate distributions for $T_0 = 1000$ K, $P_0 = 40$ atm, $x_s = 2$ mm: (a) $\xi = 1.0$, the time sequence is 0: 0.0 µs, 1: 620.7 µs, 2: 628.9 µs, 3: 629.1 µs, 4: 629.3 µs, 5: 629.7 µs, 6: 629.9 µs, 7: 630.1 µs; (b) $\xi = 5.0$, the time sequence is 0: 0.0 µs, 1: 625.0 µs, 2: 625.8 µs, 3: 626.4 µs, 4: 627.0 µs, 5: 628.9 µs, 6: 629.5 µs, 7: 630.2 µs.

non-dimensional equivalence ratio gradient:

$$\xi = \frac{d\phi}{dx} \bigg/ \bigg(\frac{d\phi}{dx} \bigg)_c = \frac{a}{u_a} = a \frac{d\tau_i}{d\phi} \cdot \frac{d\phi}{dx}$$
(4)

in which the last two equations is obtained by using Eqs. (1) and (2). Equation (4) indicates that ξ represents the ratio between local sound speed and autoignition front speed. Therefore, ξ determines the coupling between local autoignition and pressure wave generated by heat release [3,4]. It is noted that a detonation does not develop exactly at $\xi = 1$. This will be demonstrated by Fig. 3(a) and discussed in Section 3.2.

Simulations were conducted for different values of initiation zone size x_s and initial temperature T_0 . Due to space limit, only the results for $x_s = 2 \text{ mm}$ and $T_0 = 1000 \text{ K}$ were presented here. The pressure was fixed to be $P_0 = 40 \text{ atm}$. Different values of $0 \le \xi \le 100$ were considered. The critical gradient $(d\phi/dx)_c$ used to determine ξ was calculated using the mean equivalence ratio in the initiation zone.

The temporal evolution of temperature, pressure and heat release rate distributions for $\xi = 1$ and $\xi = 5$ are shown in Fig. 3. A supersonic autoignitive reaction front is observed in Fig. 3(a) for $\xi = 1$. The initiation zone size is $x_s = 2$ mm and the corresponding $\Delta \phi$ is only 0.0078. At the end of combustion, the temperature and pressure are close to their equilibrium values, $T_{eq} = 3103$ K and $P_{eq} = 134$ atm. The reaction front propagation speed, u_a , is shown as line #1 in Fig. 4, which also



Fig. 4. Reaction front propagation speed as a function of its location for different values of ξ . The *CJ* detonation speed ($D_{CJ} = 1860 \text{ m/s}$) and sound speed (a = 590 m/s) are denoted by two horizontal dashed lines.

presents the results for other values of ξ . Besides, in Fig. 4 two horizontal dashed lines denote two speeds: the Chapman–Jouguet detonation speed, $D_{CJ} = 1860 \text{ m/s}$, and sound speed, a = 590 m/s (both are evaluated at $T_0 = 1000 \text{ K}$ and $P_0 = 40 \text{ atm}$ for stoichiometric *n*-heptane/air). At $\xi = 1$, the propagation speed is always above 2400 m/s and it eventually becomes extremely large (above 10^5 m/s). Since u_a is much larger than the local



Fig. 5. Temporal evolution of temperature, pressure and heat release rate distributions for $T_0 = 1000$ K, $P_0 = 40$ atm, $x_s = 2$ mm and $\xi = 17.2$. The time sequence is 0: 0.0 µs, 1: 605.8 µs, 2: 613.6 µs, 3: 618.9 µs, 4: 620.4 µs, 5: 622.5 µs, 6: 623.6 µs, 7: 625.5 µs, 8: 628.8 µs.

sound speed *a*, the autoignition front and the pressure wave cannot be coherently coupled and thereby no detonation is developed at $\xi = 1$. Similar phenomenon was observed for temperature gradient induced reaction front propagation in [3,7].

When the normalized equivalence ratio gradient is increased from $\xi = 1$ to $\xi = 5$, the reaction front propagation speed is greatly reduced according to Eq. (4). Consequently, detonation is developed as shown in Fig. 3(b). Detonation first develops (line #2 in Fig. 3b) within the initiation zone 0 $\leq x \leq 2$ mm and then it propagates to the right until thermal explosion occurs in the unburned mixture around $t = 629.5 \,\mu s$ (line #6). Once all the mixture is consumed, the detonation degenerates into a shock wave (line #7) propagating to the right. For $\xi = 5$, the reaction front propagation speed (line #2) in Fig. 4) is very close to the CJ detonation speed when it is located within 1.2 < x < 7.5 mm. When the reaction front passes x = 7.5 mm, autoignition occurs in the undetonated mixture and then the reaction front propagates at extremely high speed, which is similar to the case of $\xi = 1$.

Figure 5 shows the results for $\xi = 17.2$. It is observed that a foregoing shock is formed in front of the reaction front. At $t = 618.9 \,\mu\text{s}$ (line #3), local explosion due to autoignition occurs around x = 0.4 cm (see the local peak pressure on line #3) and it triggers two pressure waves propagating in the opposite directions (line #4). The pressure wave propagating to the right induces successive autoigni-



Fig. 6. Temporal evolution of the location and speed of the shock wave and reaction front for $\xi = 17.2$. The *CJ* detonation speed and sound speed are denoted by two horizontal lines.

tion since the mixture there is already close to autoignition after it is compressed by the foregoing shock. The heat release from local autoignition further strengths the pressure wave. Consequently, the pressure wave is coherently coupled with heat release and it evolves to a shock-reaction complex (line #6), which can be explained by the SWACER (shock wave amplification by coherent energy release) mechanism [19]. At $t = 625.5 \,\mu s$ (line #7), this shock-reaction complex becomes a detonation.

Figure 6 shows the location and speed of the foregoing shock wave and the reaction front for ξ = 17.2. The whole process consists of four stages as marked in Fig. 6. The shock wave propagates (at nearly constant speed around 900 m/s) in front of the reaction front during the first two stages. During stage 1, the reaction front propagates at the speed around 200 m/s, which is below the sound speed. During stage 2, local explosion mentioned above occurs ($t = 618.9 \,\mu$ s, line #3 in Fig. 5) and it induces abrupt acceleration of reaction front propagation. Eventually, in stage 3 the reaction front catches up the shock wave and a self-sustaining detonation is formed which propagates to the right at D_{CI} . Finally in stage 4, thermal explosion occurs throughout the mixture in front of the detonation and then the reaction is completed (line #8 in Fig. 5). Similar results were observed for reaction front propagation caused by temperature gradient in [7].

At higher value of $\xi = 39.4$ shown in Fig. 7, there is no foregoing shock wave as observed for $\xi = 17.2$. From $t = 542.8 \,\mu s$ (line #1) to $t = 605.3 \,\mu s$ (line #2), the reaction front propagates at subsonic speed below 100 m/s (see the line #6 for $\xi = 39.4$ in Fig. 4). At $t = 613.5 \,\mu s$ (line #3), local autoignition occurs around the reaction front, which generates a shock-reaction complex. It is noted that detonation is not developed since the mixture on the right has reacted to such an extent that there is not



Fig. 7. Temporal evolution of temperature, pressure and heat release rate distributions for $T_0 = 1000$ K, $P_0 = 40$ atm, $\xi = 39.4$ and $x_s = 2$ mm. The time sequence is 0: 0.00 µs, 1: 542.8 µs, 2: 605.3 µs, 3: 613.5 µs, 4: 614.3 µs, 5: 614.7 µs, 6: 615.4 µs, 7: 616.1 µs.

enough chemical energy to support a detonation. At $t = 615.4 \,\mu s$ (line #6), all the mixture is burned and thereby the reaction-shock complex becomes a shock wave propagating to the right (line #7). In Fig. 4, line #6 depicts the reaction front speed for $\xi = 39.4$. Two stages can be identified: in the first stage the reaction front propagates at subsonic speed; and in the second stage the reaction front becomes supersonic and its speed reaches extremely high value above the *CJ* detonation speed due to the autoignition of unburned mixture on the right. Line #6 in Fig. 4 indicates that, for $\xi = 39.4$ the reaction front does not propagate at *CJ* denotation speed. This also indicates that detonation is not developed for $\xi = 39.4$.

With further increase in the normalized equivalence ratio gradient to $\xi = 100$, the reaction front propagates much slower than the pressure wave (i.e., $u_a < a$) and denotation cannot be developed as indicated by Fig. 8. Figure 8 shows that from $t = 470.8 \,\mu\text{s}$ (line #1) to $t = 586.6 \,\mu\text{s}$ (line #3), the reaction front propagates smoothly. Around t = $611.6 \,\mu\text{s}$ (line #4) on, global thermal explosion occurs throughout the unburned mixture in front of the reaction front. Therefore, line #7 in Fig. 4 indicates that for $\xi = 100$, the reaction front first propagates very slowly; then there is an abrupt increase in propagation speed, which is caused by global thermal explosion throughout the unburned mixture in front of the reaction front.



Fig. 8. Temporal evolution of temperature, pressure and heat release rate distributions for $T_0 = 1000$ K, $P_0 = 40$ atm, $\xi = 100$ and $x_s = 1$ mm, the time sequence is 0: 0.0 µs, 1: 470.8 µs, 2: 524.1 µs, 3: 586.6 µs, 4: 611.6 µs.

In summary, similar to temperature gradient (e.g., [3,7]), equivalence ratio gradient can induce different modes of reaction front propagation. Three modes were identified, namely the supersonic autoignitive reaction front ($\xi = 1$), the developing detonation ($\xi = 5$ and $\xi = 17.2$), and the subsonic reaction front ($\xi = 39.4$ and $\xi = 100$). Besides, the effects of heat conduction and mass diffusion on these three modes were examined in simulation (not shown due to space limit). As demonstrated by Fig. S4 in the Supplementary material, molecular diffusion has little influence on the first two modes and it only affects the propagation speed of the subsonic reaction front.

3.2. Detonation development regime

Following Gu et al. [3], the detonation development regime is characterized by two non-dimensional parameters: one is the nondimensional gradient of equivalence ratio (or temperature [3,7]), ξ , which represents the ratio between local sound speed and reaction front propagation speed according to Eq. (4); and the other is the non-dimensional time, ε , which is the ratio of acoustic time (x_s/a) to excitation time τ_e , i.e., $\varepsilon = x_s/(a\tau_e)$. For ε , a and τ_e were calculated using the mean equivalence ratio in the initiation zone. In our simulation, different initiation zone sizes, $x_s = 0.3, 0.5, 1, 2$ and 3 mm, were considered so that different values of ε were reached.



Fig. 9. Maximum pressure and detonation regime in the $\xi - \varepsilon$ diagram for stoichiometric *n*-heptane/air at $T_0 = 1000$ K and $P_0 = 40$ atm.

Figure 9 plots the maximum pressure for 34 sets of (ξ, ε) considered in our simulation. At the same size of initiation zone, the maximum pressure first increases and then decreases as ξ increases. The detonation development regime was identified in the ξ - ε diagram: concentration non-uniformity induced detonation develops only for $\xi_l < \xi < \xi_u$, i.e., in the regime on the right side of the C-shaped curve in Fig. 9. At small ξ below the lower branch of the C-shaped curve (i.e., $\xi < \xi_l$), supersonic autoignitive reaction front occurs (e.g., $\xi = 1$ shown in Fig. 3a). At large ξ above the upper branch of the Cshaped curve ($\xi > \xi_u$), subsonic reaction front appears (e.g., $\xi = 39.4$ shown in Fig. 7). When ε is too small (e.g., $\varepsilon < 1.5$), there is no detonation development. Similar detonation development regime was identified for temperature gradient induced reaction front propagation in [3,7].

Figure 9 indicates that no detonation is developed for ξ close to unity (see Fig. 3a). However, Eq. (4), $\xi = alu_a$, indicates that for $\xi \approx 1$ there should be coherent coupling between the reaction front and pressure wave since their speeds are close. According to Gu et al. [3], this is because during the induction period, heat conduction and species diffusion change the value of ξ evaluated based on the initial equivalence ratio or temperature distribution. However, as demonstrated by Fig. S4 in the Supplementary material, diffusion has little influence on the supersonic reaction front propagation. Therefore, the explanation of Gu et al. [3] seems needing improvement.

We found that successful detonation development also depends on the third non-dimensional parameter defined as $\eta = \Delta \tau_i / \tau_e$, where $\Delta \tau_i = \tau_i (x = x_s) - \tau_i (x = 0)$ is the ignition delay time difference within the initiation zone and τ_e denotes the mean excitation time. Since $u_a \approx x_s / \Delta \tau_i$, $\xi = a/u_a$ and ε $= x_s / (a \tau_e)$, we have $\eta = \xi \varepsilon$. The non-dimensional parameter η represents the ratio of the heat release



Fig. 10. Effect of the initial temperature on detonation regime in the $\xi - \varepsilon$ diagram: square, $T_0 = 1000$ K; triangle, $T_0 = 900$ K; circle, $T_0 = 750$ K. Closed symbols denote that detonation is developed while open symbols denote that no detonation is developed. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

rate and the speed of reaction front propagation in a given length x_s . At small value of η , the reaction front propagates outside the initiation zone before all heat in the initiation zone is released. Therefore, there is not enough energy to trigger detonation development. Besides, small value of η means that the ignition delay time difference between mixtures inside and outside the initiation zone is small. Therefore, all the mixture ignites at nearly the same time and thus there is no detonation development. According to above discussion, there must be a lower limit, η_c for the value of η , namely ($\xi \varepsilon$) > η_c . This is a necessary condition for detonation development and it explains why the lower limit, ξ_l , decreases as ε increases. Based on the present simulations for *n*heptane, the value of η_c is around 20. Therefore, detonation development occurs only for $\xi \varepsilon > 20$. In Fig. 9, the lower boundary of the detonation development regime overlaps with the curve $\xi \varepsilon = 20$.

We also studied the influence of initial temperature on the detonation development regime. The results for three initial temperatures of $T_0 = 750,900$ and 1000 K were plotted in Fig. 10. The detonation regimes for different initial temperatures are quite different: the detonation regime for $T_0=1000$ K is "C-shaped", while it is a "peninsula-like" structure for $T_0 = 900$ K and $T_0 = 750$ K, which are similar to the results of Gu et al. [3]. The lower limits are nearly the same and are well described by the red curve of $\xi \varepsilon = 20$. However, the upper limits are quite different: when the initial temperature decreases from $T_0 = 1000$ K to $T_0 = 750$ K, the upper limit moves up and thereby the detonation development regime becomes wider. The broadening of the detonation regime with decreasing initial temperature can be explained by the amount of heat release in the mixture. At fixed initial pressure, when

the initial temperature decreases, the volumetric energy density of the mixture increases, resulting in more heat release which promotes detonation development.

Therefore, Fig. 10 indicates that the detonation regime cannot be completely determined by the non-dimensional parameter, ξ and ε . Factors that affect the volumetric energy density of the mixture, for examples the initial temperature and equivalence ratio, must also be taken into consideration. Different fuels may have different detonation regimes due to different energy densities. This is different from the opinion of Bates et al. [20], who proposed that the detonation regime is nearly universal for different fuels.

4. Conclusions

Transient autoignition and reaction front propagation processes in *n*-heptane/air mixture were simulated to investigate the modes of reaction front propagation and detonation development regime caused by concentration non-uniformity. It was found that similar to temperature gradient, equivalence ratio gradient can also induce different modes of reaction front propagation. With the increase of equivalence ratio gradient, three modes, supersonic autoignitive reaction front, developing detonation and subsonic reaction front, were identified. Heat conduction and mass diffusion were shown to have little influence on the first two modes. Since equivalence ratio gradient can lead to detonation development, similar to temperature non-uniformity, concentration non-uniformity also plays an important role in engine knock.

The detonation development regime caused by concentration non-uniformity was identified in the plot of two non-dimensional parameters, namely the normalized temperature gradient, ξ , and the ratio of acoustic time to excitation time, ε . The lower limit of the detonation regime, ξ_l , was found to be determined by the condition of $(\xi \varepsilon) > \eta_c = 20$. Therefore, ξ_l decreases as ε increases. Besides, it was shown that the initial temperature has great impact on the upper limit of the detonation development regime, ξ_u . At lower initial temperature, the volumetric energy density of the mixture becomes higher and thus the detonation development regime becomes broader (i.e., ξ_u becomes larger). However, the lower limit is nearly independent of the initial temperature and it is determined by the condition of $(\xi \varepsilon) > \eta_c = 20$.

It is noted that this paper focused on stoichiometric *n*-heptane/air mixture. Fuel-lean mixture will be considered in future study since lean *n*-heptane/air is used in HCCI engine. Since the excitation time increases dramatically as the equivalence decreases (see Fig. 1), detonation development regime is expected to be narrower at lower value of equivalence ratio. Besides, only 1D simulations were conducted here and thereby many effects in real 3D turbulent flow were ignored, including turbulence, complex shock–shock or shock– boundary layer interaction, and so on. Nevertheless, the stochastic temperature/concentration gradients in 3D turbulent flow in engines can be estimated [21] and the 1D model can be used to determine whether detonation development appears in 3D combustion in engines [20].

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi: 10.1016/j.proci.2016.06.086.

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