

Numerical study on detonation initiation by multiple hot spots

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Abstract

Detonation initiation is important not only for the development of advanced detonation engines and but also for the control of accidental explosion. There are mainly two types of detonation initiation, i.e., direct initiation and indirect initiation. This work focuses on direct detonation initiation which has a short initiation distance but requires large amount of energy deposition. Specially, we investigate the reduction in the critical initiation energy through replacing the single hot spot by multiple hot spots. The transient detonation initiation process in a stoichiometric $H_2/O_2/Ar$ mixture is examined through two-dimensional simulations considering detailed chemistry. It is found that under the same initiation energy, detonation initiation fails for a single large hot spot while successful detonation initiation can be achieved by employing six small hot spots. The collisions among adjacent transverse detonation waves induce new local explosions, which play a pivotal role in detonation initiation. To further assess the impact of wave collision, we change the hot spot energy used in the multiple hot spot configuration. For relatively low initiation energy, the blast wave quickly decays and decouples with the reaction zone. Consequently, the collision among transverse shock waves cannot induce new local explosion and detonation initiation fails. Increasing the initiation energy can enhance the blast wave and is favorable to the formation of local explosion, facilitating the rapid detonation initiation. Furthermore, the influence of hot spot number on detonation initiation is assessed. Interestingly the hot spot number is found to have non-monotonic effect on detonation initiation. Splitting a single hot spot into multiple hot spots enhances detonation initiation since the wave collision helps to induce local explosion. However, as the hot spot number increases, the energy of each hot spot is decreased and becomes excessively dispersed, which results in relatively weak blast wave and thereby weak wave interaction. Consequently, local explosion cannot be triggered and detonation initiation fails for relatively large hot spot numbers. This study provides insights on promoting detonation initiation through multiple hot spots.

Keywords: Detonation initiation; Critical initiation energy; Multiple hot spots; Shock wave collision

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Information for Colloquium Chairs and Cochairs, Editors, and Reviewers

1) Novelty and Significance Statement

The novelty of this work is that the transient detonation initiation process induced by multiple hot spots is investigated for the first time by simulations considering detailed chemistry. It is found that multiple hot spot helps to promote detonation initiation and thereby reduces the critical initiation energy. The underlying mechanisms are interpreted. Moreover, the effects of the initial initiation energy and hot spot number on detonation initiation processes are assessed and interpreted.

It is significant because this work demonstrates the feasibility of reducing the detonation initiation energy by using multiple hot spots. The collisions among adjacent transverse detonation waves are found to induce new local explosions and play a pivotal role in detonation initiation. It is shown that there is an optimum hot spot number for detonation initiation. Therefore, this study provides insights on promoting detonation initiation and reducing initiation energy through multiple hot spots.

2) Author Contributions

- Jie Sun: performed the research, analyzed the data, and drafted the manuscript.
- Pengfei Yang: aided in interpreting the results and revised the manuscript.
- Yiqing Wang: aided in interpreting the results and helped to design some figures.
- Zheng Chen: conceived the original idea, designed the research, and supervised the project.
- All authors discussed the results and contributed to the final manuscript.

3) Authors' Preference and Justification for Mode of Presentation at the Symposium

The authors prefer **OPP** presentation at the Symposium, for the following reasons:

- The novelty and significance of this work can be readily understood by the audience during oral presentation.
- The complicated wave interactions and local explosions can be more clearly illustrated by oral presentation.
- The transient detonation initiation process and the underlying mechanisms can be well presented by PPT.

1. Introduction

Detonation is a supersonic mode of combustion consisting of a shock wave coupled with a reaction zone [1]. Recently, detonation has received increasing attentions and has promising applications in advanced propulsion systems since it helps to achieve higher thermal efficiency and faster burning rate than deflagration [2]. Meanwhile, it is imperative to mitigate the occurrence of detonation in accident explosions since detonation has high overpressure and is extremely destructive [3]. Understanding detonation initiation is important not only for the development of advanced detonation engines and but also for the control of accident explosion.

Detonation initiation can be primarily categorized into indirect initiation and direct initiation [1]. Indirect initiation usually refers to the deflagration-to-detonation transition (DDT), which requires relatively low initiation energy but long initiation distance [4]. Direct initiation requires large amount of energy deposition so that detonation can be quickly formed [5]. One of the key parameters for direct detonation initiation is the critical initiation energy, E_C , which is an intrinsic property of a combustible mixture and depends on the mixture composition as well as the thermal conditions [1]. Successful direct detonation initiation is achieved only when sufficient energy is deposited, i.e., $E \geq E_C$.

In the literature, there are many studies on the measurement and prediction of critical initiation energy (see [6] and references therein). Here we focus on the endeavors to reduce the critical initiation energy and to promote detonation initiation. For example, it has been demonstrated that plasma discharge can be used to facilitate detonation initiation in pulsed detonation engines [7-9]. Plasma helps to produce active radicals and species (e.g., ozone) which can reduce the ignition delay time and thereby promote detonation initiation. Our previous work [10] examined how ozone addition affects detonation initiation, and showed that both ozonolysis reaction and ozone decomposition reaction help to reduce the critical initiation energy. The focusing effects of reflected shock waves can also help to initiate the detonation with lower initiation energy, which was demonstrated by simulations [11, 12] and experiments [13, 14].

Besides, spatial redistribution of the ignition is another effective way to reduce the critical energy for detonation initiation. Vasilev [15] reviewed the optimum ways for the detonation initiation process in terms of the spatial distribution of the input energy and proposed that multiple hot spots can promote detonation initiation. Guo et al. [16] simulated detonation initiation through dual-hot spot ignition and found that the collisions among adjacent shock waves induced by each hot spot can reduce the required initiation energy. Vasilev [17] measured the triple-point trajectory in a cylindrical detonation wave initiated by six hot spots. He found that detonation can

initiated at lower initial pressure than the critical value by using the multiple hot spots. However, due to the limitation in experimental measurement, there is no detailed information on the characteristics of flow, reaction and wave interaction during the detonation initiation by multiple hot spots. Consequently, the underlying mechanisms of detonation initiation by multiple hot spots are not well understood. Besides, the influence of hot spot number and energy on detonation initiation have not been assessed. This motivates the present study.

This work aims to simulate and interpret the transient detonation initiation induced by multiple hot spots in a $H_2/O_2/Ar$ mixture. Specifically, we first compare the detonation initiation processes induced by a single hot spot and multiple hot spots, and assess the impact of multiple hot spots on the critical initiation energy. Then, the impact of the initial initiation energy on detonation initiation processes induced by multiple hot spots is examined. Finally, we assess the influence of hot spot number on detonation initiation. The remainder of the paper is organized as follows. The model and numerical methods are introduced in Section 2. After that the results are presented and discussed in Section 3. Conclusions are summarized in Section 4.

2. Model and numerical methods

We conduct two-dimensional simulations for the transient detonation initiation induced by different numbers of hot spot as depicted in Fig. 1. Since the present simulations are performed in 2D configuration, the initial hot spots can be identified as uniform line ignition sources perpendicular to the x - y plane.

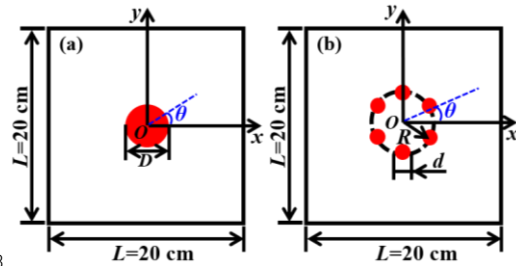


Fig. 1. Schematic of initial hot spot settings for (a) single hot spot and (b) multiple hot spots.

The computational domain is filled with static $H_2/O_2/Ar$ mixture ($X_{H_2}:X_{O_2}:X_{Ar} = 2:1:7$) of 300 K and 0.6 atm. Ar is used as the dilution gas to enhance the stability of the cellular detonation wave. The hot spot has the same $H_2/O_2/Ar$ mixture but has much higher temperature, $T_h = 3000$ K, and pressure denoted as P_h . We fix the total area of the hot spots, S_h ,

$$S_h = \frac{\pi D^2}{4} = \frac{N\pi d^2}{4} = 6\pi \text{ (mm}^2\text{)} \quad (1)$$

where $D = 4.899$ mm is the diameter of the single hot spot, and d and N are respectively the diameter and

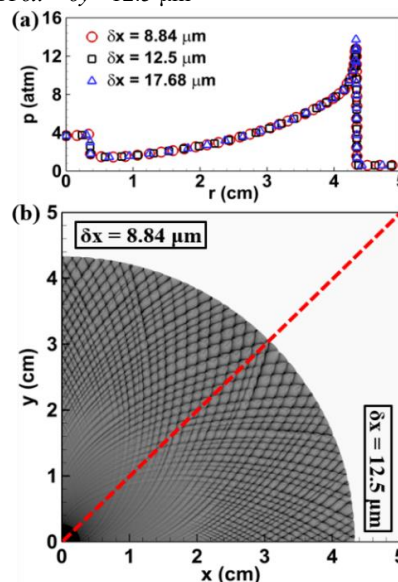
1 number of hot spots in Fig. 1(b). Besides, the
 2 circumference radius of the hot spot center is fixed to
 3 be $R = 3$ mm for multiple hot spot configuration,
 4 which is closed to the hot spot radius for the single hot
 5 spot configuration (~ 2.45 mm). Note that this value
 6 may affect the detonation initiation process, which
 7 needs to be explored in future studies.

8 Due to symmetry, a quarter of the whole domain,
 9 i.e., $0 \leq x \leq 10$ cm and $0 \leq y \leq 10$ cm, is considered in
 10 simulations. Symmetric conditions are used at the
 11 boundaries of $x = 0$ and $y = 0$. The outflow conditions
 12 are used at boundaries of $x = 10$ cm and $y = 10$ cm. In
 13 simulations we consider the detailed hydrogen
 14 chemistry by Conaire et al. [18] which consists of 10
 15 species and 21 elementary reactions. The transient
 16 detonation initiation process is simulated using the in-
 17 house code detonationFoam [19], which is developed
 18 based on OpenFOAM [20] and has been thoroughly
 19 validated for gaseous detonation simulation [19]. It
 20 has been successfully used in our previous studies on
 21 oblique detonation waves [21, 22]. The details on
 22 governing equations, numerical methods and code
 23 validation can be found in Ref. [19] and thereby are
 24 only briefly described below.

25 In detonationFoam, the finite volume method is
 26 used to solve the Euler equations for fully-
 27 compressible, multi-component reactive flows. The
 28 second-order MUSCL scheme with the pressure-
 29 corrected approximate Riemann solver, HLLC-P [23],
 30 is used to calculate the convective flux. The operator
 31 splitting approach is used so that the flow and
 32 chemical reaction processes are solved separately. The
 33 first-order Euler scheme is adopted for time
 34 advancement. The stiff ordinary differential equation
 35 solver, *seulex*, which employs an extrapolation
 36 algorithm based on the linearly implicit Euler method
 37 with step size control and order selection, is used to
 38 handle the chemical reaction [24]. Moreover, adaptive
 39 mesh refinement [25] and dynamic load balancing [26]
 40 are used to improve the computational efficiency.

41 To ensure grid convergence, we compare the results
 42 for detonation initiation by single hot spot predicted
 43 by simulations using three different grid sizes. For the
 44 cases shown in Fig. 2, the coarse grid sizes are 70.7
 45 μm , 100 μm and 141.4 μm , respectively. All the cases
 46 use 3-level refinement mesh and the corresponding
 47 minimum grid size is 8.84 μm , 12.5 μm and 17.68 μm .
 48 For the simulation results, pressure distributions along
 49 the lines of $\theta = 0^\circ$, 0.1° , ..., and 90° are extracted,
 50 where θ is shown in Fig. 1. Then the average value of
 51 these pressure distributions is calculated to get the
 52 circumferentially-averaged pressure profile. Figure 2
 53 shows that the circumferentially-averaged pressure
 54 profiles and triple-point trajectories predicted by
 55 different grid sizes are almost the same. Therefore, in
 56 all simulations we use the minimum grid size of 12.5
 57 μm with the coarse grid size of 100 μm . The induction
 58 length for the $\text{H}_2/\text{O}_2/\text{Ar}$ mixture at 0.6 atm and 300 K
 59 is calculated to be 123.9 μm . Therefore, there are

60 about 10 points within the induction zone for the grid
 61 size of $\delta x = \delta y = 12.5$ μm

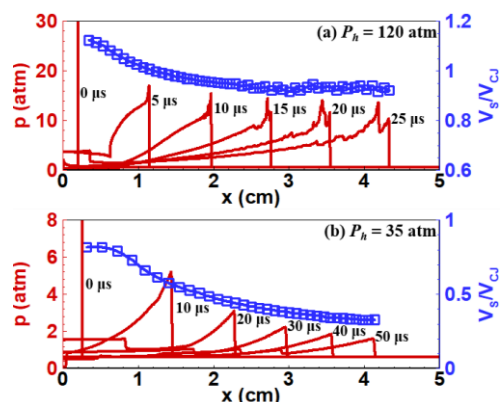


62
 63 Fig. 2. (a) Distribution of the circumferentially-averaged
 64 pressure and (b) triple-point trajectories predicted by
 65 different grid sizes for single hot spot with $P_h = 120$ atm.

66 3. Results and discussion

67 3.1 Detonation initiation by a single hot spot

68
 69 First, we simulate detonation initiation induced by
 70 a single hot spot with different initiation energies
 71 (which depends on the pressure of the hot spot, P_h).
 72 The temporal evolution of the pressure profiles, and
 73 normalized propagation speed of the leading shock
 74 wave along x -axis are shown in Fig. 3 for $P_h = 120$
 75 atm and $P_h = 35$ atm.
 76
 77
 78



79
 80 Fig. 3. The temporal evolution of the pressure profiles along
 81 x -axis and the change of normalized propagation speed of the
 82 shock wave with its position, V_s/V_{CJ} , for (a) $P_h = 120$ atm
 83 and (b) $P_h = 35$ atm. The Chapman-Jouguet (CJ) detonation
 84 speed for the $\text{H}_2/\text{O}_2/\text{Ar}$ mixture is $V_{CJ} = 1686$ m/s.

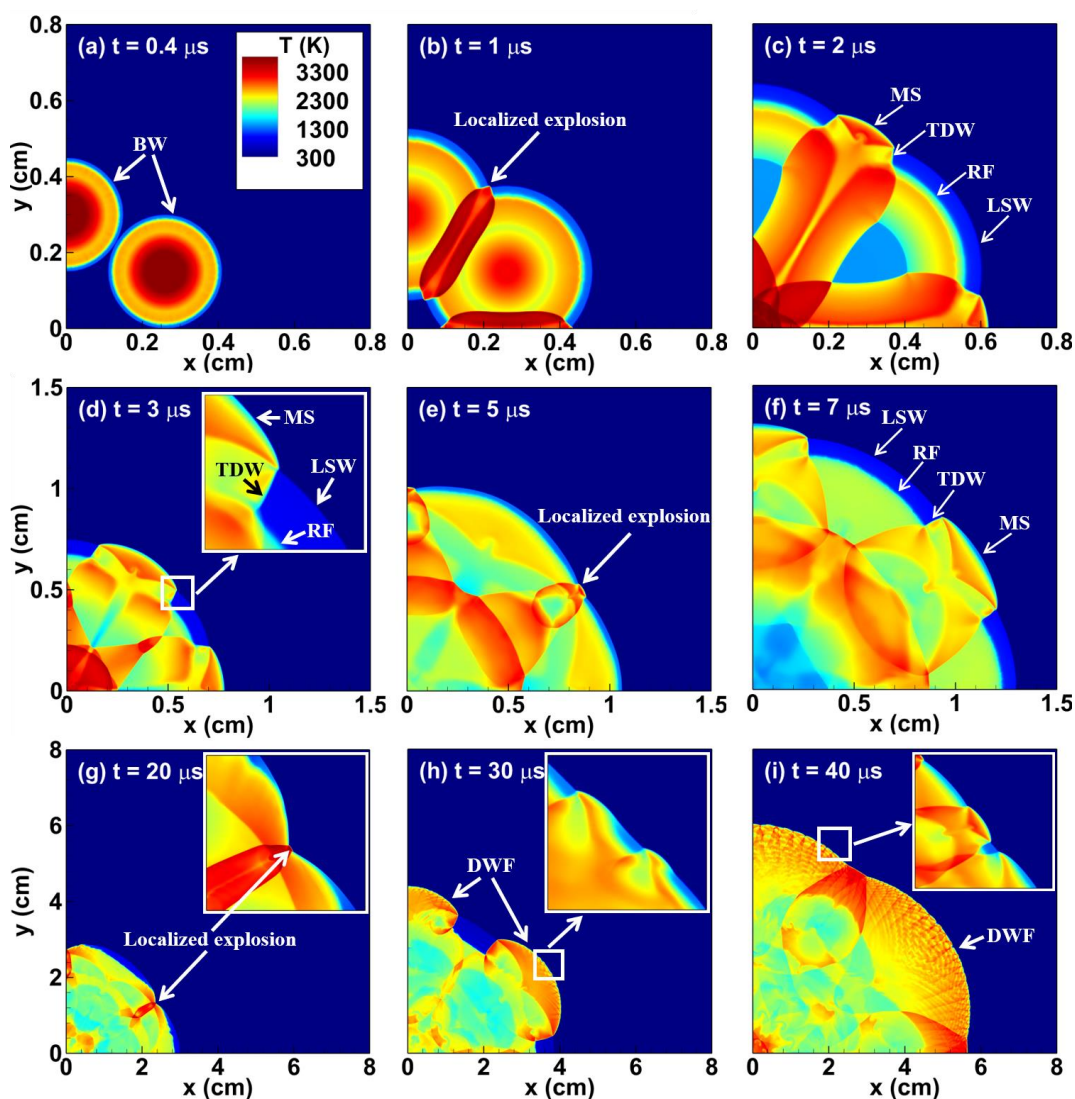
1 Successful detonation initiation is achieved for P_h
 2 = 120 atm and Fig. 3(a) shows that the shock speed
 3 gradually attenuates from the initial overdriven state
 4 to the steady-propagation state. Note that due to wave
 5 front curvature, the shock speed is slightly lower than
 6 Chapman-Jouguet (CJ) detonation speed. Besides,
 7 Figure 3(a) shows double-peak structures for the
 8 pressure profiles at $t = 15, 20$ and $25 \mu\text{s}$. The first peak
 9 corresponds to pressure rise caused by the leading
 10 shock wave, while the second peak is caused by
 11 transverse wave. When the initial hot spot pressure is
 12 reduced to $P_h = 35$ atm, Fig. 3(b) shows that both the
 13 peak pressure and shock speed gradually decrease. At
 14 around $t = 100 \mu\text{s}$, the shock speed is only one-third
 15 of the CJ detonation speed (i.e., $V_s/V_{CJ} = 0.33$),
 31

16 indicating that the detonation initiation fails.

17 The above results show that failed detonation
 18 initiation occurs for a single hot spot with $P_h = 35$ atm.
 19 This will be used as a reference case for comparison
 20 with detonation initiation induced by multiple hot
 21 spots in the following subsection.

22 3.2 Detonation initiation by multiple hot spots

23 Here we use six hot spots ($N = 6, d = 2$ mm), as
 24 illustrated in Fig. 1(b), to initiate the detonation.
 25 According to Eq. (1), the amount of total initiation
 26 energy of the single hot spot (i.e., Fig. 1a, $d = 4.9$ mm)
 27 is equal to that of six hot spots (i.e., Fig. 1b) for the
 28 same $P_h = 35$ atm.
 30



32
 33 Fig. 4. The temporal evolution of temperature contour during detonation initiation induced by multiple hot spots with $P_h = 35$
 34 atm. BW: blast wave; MS: Mach stem; TDW: transverse detonation wave; LSW: leading shock wave; RF: reaction front; DWF:
 35 detonation wave front. An animation of the whole detonation initiation process is shown in the Supplementary Material.
 36

1 The detonation initiation process induced by six
 2 hot spots is shown Fig. 4. Due to symmetry only one
 3 and a half hot spots are shown. The whole initiation
 4 process can be divided into three stages. The first-
 5 stage evolutions are depicted in Figs. 4 (a-c). At $t =$
 6 $0.4 \mu\text{s}$, Fig. 4(a) shows that the hot spots trigger rapid
 7 local autoignition, leading to the formation of
 8 diverging cylindrical blast waves (BW). The
 9 diverging BWs collide with each other, resulting in
 10 highly compressed regions with high pressure and
 11 temperature. This induces local explosion as shown in
 12 Fig. 4(b). The strong pressure waves induced by these
 13 local explosions further interact with arc shock waves
 14 originating from the initial hot spots, forming triple-
 15 wave structures consisting of Mach stem (MS),
 16 transverse detonation wave (TDW) and
 17 leading/incident shock wave (LSW), propagating
 18 outward as shown in Fig. 4(c). This first stage is
 19 mainly determined by hot spot autoignition and
 20 thereby it is referred to as the hot spot initiation stage.

21 The second stage evolutions are depicted in Figs.
 22 4(d-f). Since the MS corresponds to relatively strong
 23 shock, chemical reactions immediately happen after
 24 the MS, and the distance between MS and the
 25 following reaction front (RF) is very small. On the
 26 contrary, the LSW has relatively low intensity and
 27 thereby there is a huge gap between the LSW and the
 28 RF (see Fig. 4d). As the triple-wave structures
 29 propagate, the transverse detonation waves spread
 30 towards both sides of the MS, consuming the mixture
 31 between the LSW and the RF (see Fig. 4d). Figures
 32 4(c-e) shows that the width of the MS gradually
 33 increases and the MS evolves into a new LSW. The
 34 collision between two transverse detonation waves
 35 induces newly localized explosion as shown in Fig.
 36 4(e), which then produces a new MS and a pair of
 37 TDWs propagating in the opposite directions as
 38 shown in Fig. 4(f). The next transition between MS
 39 and LSW, and the collision and reflection between a
 40 pair of TDWs continue during the propagating of the
 41 triple-wave structure. This is similar to the wave
 42 structure evolution occurring in cellular detonation.
 43 However, during this stage, the formation and
 44 evolution of the triple-wave structure is still
 45 determined by the initial hot spots. Therefore, this
 46 stage ($3 \mu\text{s} < t < 20 \mu\text{s}$) is referred to as the transition
 47 stage.

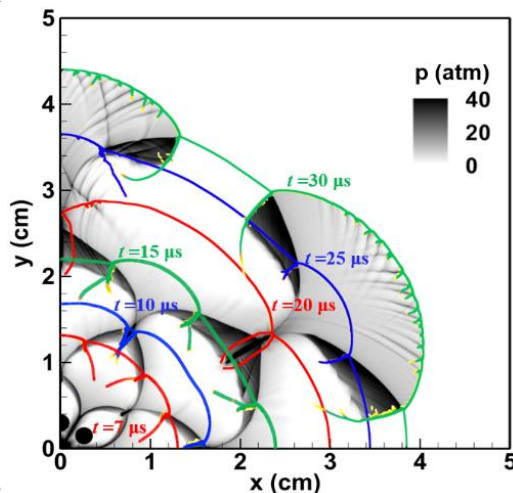
48 The third stage corresponds to the development and
 49 quasi-steady propagation of a circular expanding
 50 detonation as shown in Figs. 4(g-i). At $t = 20 \mu\text{s}$, Fig.
 51 4(g) shows that the collision between a pair of TDWs
 52 induces local explosion. Figure 4(h) shows micro sub-
 53 structures appearing on the MS, indicating that the
 54 MS evolves into a typical circular diverging
 55 detonation wave front (DWF). At $t = 40 \mu\text{s}$, Fig. 4(i)
 56 shows that there are many micro triple-wave
 57 structures on the detonation wave front, indicating the
 58 formation of cellular detonation. Similar observations
 59 were reported and interpreted by Jiang et al. [27] and
 60 Shen et al. [28]. As the DWF propagates outwardly,
 61 its curvature decreases and thereby cellular instability

62 develops, resulting in the generation of new transverse
 63 detonation waves [28].

64 Compared with the failed detonation initiation
 65 induced by a single hot spot shown in Fig. 3(b),
 66 successful detonation initiation is achieved by using
 67 multiple hot spots with the same total initiation energy
 68 as shown in Fig. 4. This shows that the multiple hot
 69 spots can effectively reduce the critical initiation
 70 energy. For the initiation process induced by a single
 71 hot spot, the cylindrical blast wave induced by the hot
 72 spot gradually attenuates due to the expansion effect,
 73 resulting in the decoupling between the leading shock
 74 wave and the reaction front, i.e., detonation initiation
 75 failure. However, for the initiation process by multiple
 76 hot spots, multiple blast waves are generated by the
 77 local autoignition triggered by each hot spot and the
 78 collisions between these blast waves induce local
 79 explosions, which play an important role in the
 80 achievement of successful detonation initiation.

81 Figure 5 shows the temporal evolution of wave
 82 front and the numerical soot foil during the successful
 83 detonation initiation by multiple hot spots. During the
 84 transition stage, it is seen that transverse detonation
 85 waves correspond to the high-pressure regions. In fact,
 86 the numerical soot foil records the transverse
 87 detonation wave trajectories, manifesting as fish-
 88 scale-like cell structure [29]. At $t = 30 \mu\text{s}$, cellular
 89 detonation wave has formed and small-scale
 90 detonation cells on DWF are clearly observed.

91



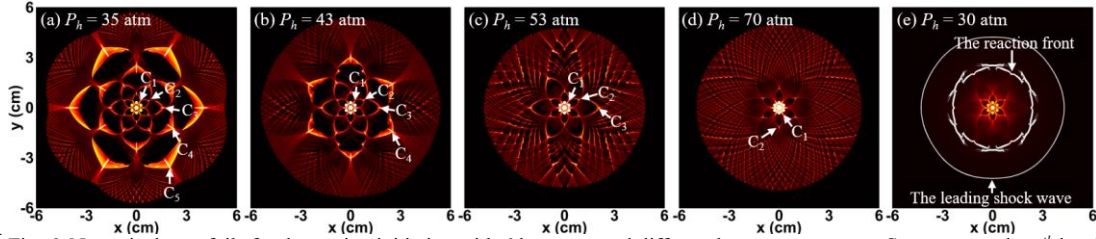
92
 93 Fig. 5. Numerical soot foil for the case with 6 hot spots and
 94 $P_h = 35 \text{ atm}$. The wave fronts at different times, $t = 7, 10, 15,$
 95 $20, 25$ and $30 \mu\text{s}$, are superimposed.

96

97 3.3 Effects of initiation energy

98

99 In the above two subsections, the hot spot pressure
 100 is fixed to be $P_h = 35 \text{ atm}$. Here different hot spot
 101 pressures (i.e., different initiation energies) are
 102 considered and the detonation initiation processes are
 103 recorded in Fig. 6. Note that we still consider 6 hot
 104 spots with $d = 2 \text{ mm}$ as depicted in Fig. 1(b).



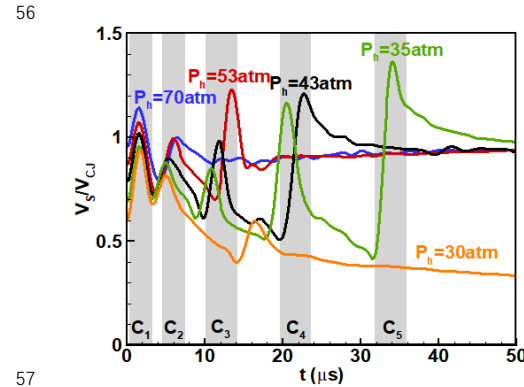
1
2 Fig. 6. Numerical soot foils for detonation initiation with 6 hot spots and different hot spot pressures. C_n represents the n^{th} local
3 explosion caused by the collisions between adjacent blast waves. The animations of these detonation initiation processes are
4 shown in the Supplementary Material.

5
6 Figure 6 shows the numerical soot foils for
7 successful (Figs. 6a-d) and failed (Fig. 6e) detonation
8 initiations. The results for $P_h = 35$ atm discussed in the
9 previous subsection are plotted in Fig. 6(a). In Fig. 6,
10 C_n represents the n^{th} local explosion caused by the
11 collisions between adjacent blast waves. For an
12 example, for $P_h = 35$ atm C_1 in Fig. 6(a) corresponds
13 the collision and local explosion shown in Fig. 4(b).

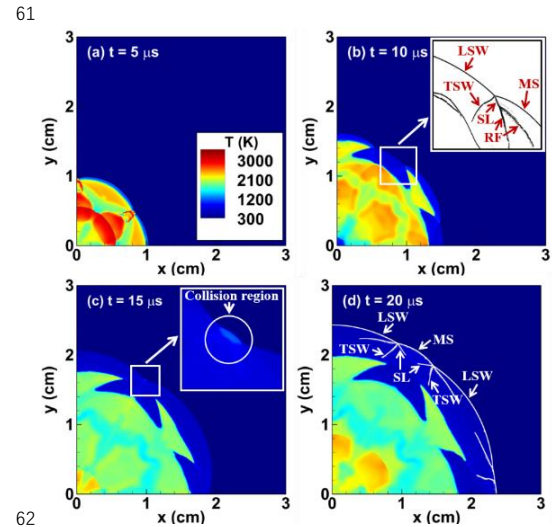
14 With the increase of initiation energy or hot spot
15 pressure, Figs. 6(a-d) shows that the cycle number of
16 local explosion-blast wave decreases for the
17 successful detonation initiation cases. Specifically,
18 five, four, three and two cycle are respectively
19 observed for $P_h = 35, 43, 53$ and 70 atm (Figs. 6 a-d).
20 This is expected since the higher the hot spot pressure
21 results in the stronger the blast waves and more
22 intense collisions, which induce stronger local
23 explosion and accelerate successful detonation
24 initiation. Consequently, high initiation energy (or
25 high hot spot pressure) facilitates the development of
26 numerical disturbances between the leading shock
27 wave and the reaction front, inducing transverse
28 detonation waves and shortening the initiation
29 distance, i.e., reducing the number of localized
30 explosion-blast wave propagation cycles. As shown in
31 the Supplementary Material, the numerical soot foil
32 shown in Fig. 6(d) agrees qualitatively with the
33 experimental results reported by Vasilev [15, 17]. In
34 Fig. 6(e), detonation initiation fails for $P_h = 30$ atm. It
35 is observed that the leading shock wave finally
36 decouples with the reaction front.

37 In Fig. 7, we compare the evolution of
38 circumferentially-averaged normalized shock wave
39 speed V_s/V_{CJ} for different hot spot pressures. For
40 successful detonation initiation, quasi-steady
41 propagation is finally reached when V_s/V_{CJ} is slightly
42 below, yet close to, unity. It is seen that before the
43 quasi-steady propagation, there are several abrupt
44 acceleration-deceleration processes, which
45 correspond to the local explosions, $C_1 \sim C_5$, as shown
46 in Fig. 6. For an example of $P_h = 35$ atm, the sudden
47 increase of V_s at $t = 10.8 \mu\text{s}$ is due to C_3 local
48 explosion shown in Fig. 6(a). Figure 7 also shows that
49 the peak value of V_s caused by the same C_n local
50 explosion increases with the hot spot pressure. This is
51 mainly because higher initiation energy can induce
52 stronger collisions and localized explosions. Note that
53 the wave speed is calculated from the

54 circumferentially-averaged value and that high wave
55 speed can be achieved due to wave collision.



56
57
58 Fig. 7. The normalized propagation speed of the wave front,
59 V_s/V_{CJ} , for different hot spot pressures. The local explosions,
60 $C_1 \sim C_5$ represent the local explosions depicted in Fig. 6.



61
62
63 Fig. 8. Temperature contour for the failed detonation
64 initiation with $P_h = 30$ atm. The wave structures are
65 superimposed on (b) and (d). LSW: leading shock wave; MS:
66 Mach stem; TSW: transverse shock wave; SL: slip line; RF:
67 reaction front.

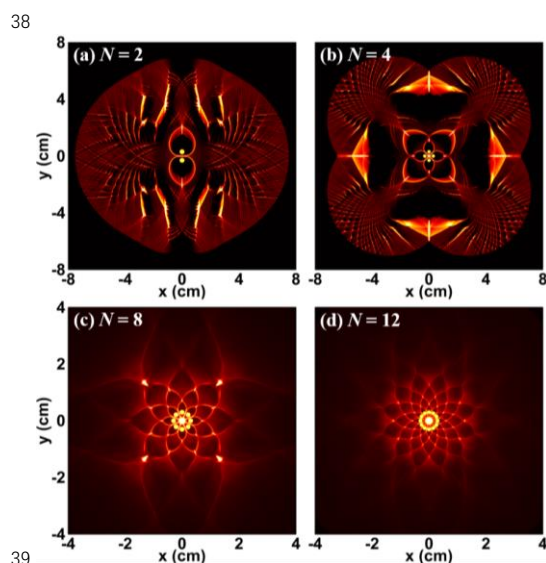
68
69 For case of $P_h = 30$ atm, Fig. 7 also shows that V_s
70 decreases to $0.34V_{CJ}$ at $t = 50 \mu\text{s}$, indicating that

1 detonation initiation fails. For this case, the
 2 temperature contours and wave structures are shown
 3 in Fig. 8. At $t = 5 \mu\text{s}$, local explosion occurs. However,
 4 at $t = 10 \mu\text{s}$, the transverse shock wave (TSW) is
 5 shown to decouple with the RF. Subsequently, Fig. 8(c)
 6 shows that the collision between a pair of TSWs is not
 7 strong enough to induce new local explosion.
 8 Consequently, Fig. 8(d) shows that the distance
 9 between the leading shock waves and reaction zone
 10 further increases, resulting in the failure of detonation
 11 initiation.

13 3.4 Effects of initial hot spot number

15 In previous subsections, the hot spot number is
 16 fixed to be either $N = 6$ or $N = 1$. Here we assess the
 17 effect of hot spot number on detonation initiation with
 18 fixed total hot spot area of $S_h = 6\pi \text{ mm}^2$ and fixed hot
 19 spot pressure of $P_h = 35 \text{ atm}$, i.e., the total initiation
 20 energy is unchanged.

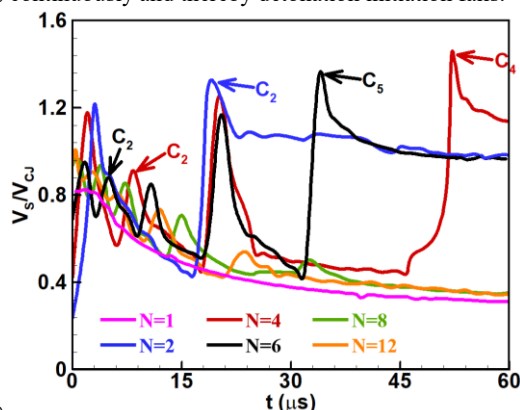
21 Simulations for different hot spot numbers have
 22 been conducted. The results for hot spot number of N
 23 $= 2, 4, 8,$ and 12 are present in Fig. 9. For $N = 2$ and 4 ,
 24 Figs. 9(a) and 9(b) show that fine cellular structures
 25 develop on the wave fronts. The propagation of triple-
 26 wave structures consisting of MS, TDW and LSW are
 27 clearly shown in the animation provided in the
 28 Supplementary Material. The wave fronts are found to
 29 tightly couple with the reaction fronts. Therefore,
 30 successful detonation initiation is achieved for $N = 2$
 31 and 4 . However, for $N = 8$ and 12 Figs. 9(c) and 9(d)
 32 show that the numerical soot foils decays significantly
 33 and are almost invisible in the region of $(x^2 + y^2)^{1/2} > 3$
 34 cm. Similar to results shown in Fig. 6(e) and Fig. 8(d),
 35 the reaction zone is found to decouple with the leading
 36 shock waves. Therefore, detonation initiation fails for
 37 $N = 8$ and 12 .



40 Fig. 9. Numerical soot foils for different hot spot numbers.

41 P_h is fixed to 35 atm. The animations of these detonation
 42 initiation processes are shown in the Supplementary Material.
 43

44 Figure 10 compares the circumferentially-averaged
 45 normalized propagation speed of the wave front,
 46 V_s/V_{CJ} , for $N = 1, 2, 4, 6, 8$ and 12 . Similar to Fig. 7,
 47 Fig. 10 shows there are abrupt-acceleration-
 48 deceleration processes, in which the peak speed
 49 corresponds to the local explosion induced by wave
 50 collision ($C_1 \sim C_2$ for $N = 2$, $C_1 \sim C_4$ for $N = 4$ and C_1
 51 $\sim C_5$ for $N = 6$). It is noticed that the time taken to
 52 reach the quasi-steady detonation propagation stage
 53 changes non-monotonically with the hot spot number:
 54 the shortest time is taken for $N = 2$ while the time for
 55 $N = 6$ is shorter than that for $N = 4$. Therefore, there is
 56 an optimum hot spot number for detonation initiation.
 57 For $N = 8$ and 12 , Fig. 10 shows that V_s/V_{CJ} decreases
 58 continuously and thereby detonation initiation fails.



59 Fig. 10. The normalized propagation speed of the wave front,
 60 V_s/V_{CJ} , for different hot spot numbers. P_h is fixed to 35 atm.
 61

62
 63 The above results show that detonation initiation
 64 fails for $N = 1, 8$ and 12 but succeeds for $N = 2, 4$ and
 65 6 . Therefore, for the same initiation energy, the hot
 66 spot number N has a non-monotonic effect on
 67 detonation initiation. This can be explained as follows.
 68 As discussed in subsection 3.2, the local explosion
 69 induced by wave collision play an important role in
 70 detonation initiation by multiple hot spots. Increasing
 71 the hot spot number from $N = 1$ to $N = 2$ introduces
 72 wave collisions and localized explosions, which
 73 promotes the detonation initiation. However, for fixed
 74 total initiation energy, the strength each hot spot
 75 decreases with the increase of hot spot number.
 76 Consequently, wave collision and local explosion
 77 become weaker for larger hot spot number. This can
 78 be quantitatively elucidated by the decreasing local
 79 peak wave speed caused by C_2 collision, $V_s/V_{CJ} = 1.33$,
 80 0.91 and 0.88 for $N = 2, 4,$ and 6 , respectively, as
 81 shown in Fig. 10. For relatively large hot spot number,
 82 $N = 8$ and 12 , the strength of individual hot spot is not
 83 enough to induce strong local explosion, resulting in
 84 detonation initiation failure.
 85

1 4. Conclusions

2
3 In this study, we conduct 2D simulations of
4 detonation initiation by single hot spot and multiple
5 hot spots in a stoichiometric $H_2/O_2/Ar$ mixture. First,
6 we compare the detonation initiation induced by a
7 single hot spot and by six hot spots with the same
8 initiation energy. The detonation initiation process
9 induced by multiple hot spots mainly consists of three
10 stages: the hot spot initiation stage, the transition stage,
11 and the detonation development and quasi-steady
12 propagation stage. It is found that detonation initiation
13 fails for the single hot spot but succeeds for six hot
14 spots, demonstrating that multiple hot spot helps to
15 promote detonation initiation and thereby reduces the
16 critical initiation energy. This is due to the facts that
17 the collisions among waves induced by multiple hot
18 spots periodically introduce new local explosions, and
19 these local explosions further enhance the wave
20 intensity and accelerate chemical reaction and local
21 autoignition. The coherent coupling between pressure
22 waves and chemical reactions eventually induces self-
23 sustained, circular detonation propagation with
24 cellular structure on its front.

25 Then we assess the effects of initiation energy on
26 detonation initiation by multiple hot spots. For fixed
27 hot spot number of $N = 6$, increasing the initiation
28 energy (hot spot pressure) can greatly reduce the
29 number of cycles for local explosion occurring in the
30 transition stage and thereby accelerate detonation
31 initiation. This is because the higher the hot spot
32 pressure, the stronger the blast waves and their
33 collisions, which induce stronger local explosion and
34 accelerate successful detonation initiation.

35 Finally, we examine the effect of hot spot number
36 on detonation initiation under the same total initiation
37 energy. Although splitting a single hot spot into 2, 4
38 and 6 smaller hot spots leads to a transition from the
39 failed to successful detonation initiation, detonation
40 initiation fails again when the hot spot number is
41 increased to 8 and 12, indicating the effects of hot spot
42 number on detonation initiation are non-monotonic.
43 This is because for fixed total initiation energy, the
44 strength of each hot spot decreases with the increase
45 of hot spot number. Consequently, wave collision and
46 local explosion becomes weaker for larger hot spot
47 number and thereby detonation initiation fails for
48 relatively large hot spot numbers.

49 This work helps to understand detonation initiation
50 by multiple hot spots. In this work, we adopt uniform
51 hot spots to initiate detonation and the initiation
52 energy is determined by initial hot spot pressure. This
53 setting is different from the practical applications. In
54 future studies, it would be interesting to evaluate the
55 detonation initiation process for multiple hot spot
56 configurations considering more practical initiation
57 methods. Besides, 2D simulations are conducted here
58 while more complicated and stronger wave
59 interactions are expected in 3D case, which need to be
60 explored in future studies.

61

62 Supplementary materials

63
64 The animations of different detonation initiation
65 processes are provided.

66 References

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68
69 [1] J.H.S. Lee, *The detonation phenomenon*, Cambridge
70 University Press, Cambridge, 2008.
71 [2] P. Wolański, Detonative propulsion, *Proc. Combust. Inst.*
72 34 (2013) 125-158.
73 [3] G. Ciccarelli, S. Dorofeev, Flame acceleration and
74 transition to detonation in ducts, *Prog. Energy Combust.*
75 *Sci.* 34 (2008) 499-550.
76 [4] E.S. Oran, V.N. Gamezo, Origins of the deflagration-to-
77 detonation transition in gas-phase combustion, *Combust.*
78 *Flame* 148 (2007) 4-47.
79 [5] L. He, P. Clavin, On the direct initiation of gaseous
80 detonations by an energy source, *J. Fluid Mech.* 277 (2006)
81 227-248.
82 [6] B. Zhang, C. Bai, Methods to predict the critical energy
83 of direct detonation initiation in gaseous hydrocarbon
84 fuels – An overview, *Fuel* 117 (2014) 294-308.
85 [7] C. Cathey, F. Wang, T. Tang, A. Kuthi, M. Gundersen, J.
86 Sinibaldi, C. Brophy, E. Barbour, R. Hanson, J. Hoke, F.
87 Schauer, J. Corrigan, J. Yu, Transient plasma ignition for
88 delay reduction in pulse detonation engines, *AIAA-Paper*
89 2007-443.
90 [8] J.K. Lefkowitz, Y. Ju, C.A. Stevens, T. Ombrello, F.
91 Schauer, J. Hoke, The effects of repetitively pulsed
92 nanosecond discharges on ignition time in a pulsed
93 detonation engine, *AIAA-Paper* 2013-3719.
94 [9] D. Zheng, B. Wang, Acceleration of DDT by non-thermal
95 plasma in a single-trial detonation tube, *Chin. J. Aeronaut.*
96 31 (2018) 1012-1019.
97 [10] J. Sun, B. Tian, Z. Chen, Effect of ozone addition and
98 ozonolysis reaction on the detonation properties of
99 $C_2H_4/O_2/Ar$ mixtures, *Proc. Combust. Inst.* 39 (2023)
100 2797-2806.
101 [11] N.N. Smirnov, O.G. Penyazkov, K.L. Sevrouk, V.F.
102 Nikitin, L.I. Stamov, V.V. Tyurenkova, Detonation onset
103 following shock wave focusing, *Acta Astronaut.* 135
104 (2017) 114-130.
105 [12] P.S. Utkin, A.I. Lopato, A.A. Vasil'ev, Mechanisms of
106 detonation initiation in multi-focusing systems, *Shock*
107 *Waves* 30 (2020) 741-753.
108 [13] Y. Li, B. Zhang, Visualization of ignition modes in
109 methane-based mixture induced by shock wave focusing,
110 *Combust. Flame* 247 (2023) 112491.
111 [14] Z. Yang, B. Zhang, Numerical and experimental
112 analysis of detonation induced by shock wave focusing,
113 *Combust. Flame* 251 (2023) 112691.
114 [15] A.A. Vasil'ev, Cellular structures of a multifront
115 detonation wave and initiation, *Combust. Explos. Shock*
116 *Waves* 51 (2015) 1-20.
117 [16] H. Guo, N. Zhao, H. Zheng, C. Sun, J. Yang, Numerical
118 simulation of the direct initiation by double-point laser
119 ignition, *J. Combust. Sci. Technol.* 01 (2021) 43-51.
120 [17] A.A. Vasil'ev, *Dynamic Parameters of Detonation*, in: F.
121 Zhang (Ed.), *Shock waves science and technology library*,
122 Vol. 6, Springer-Verlag Berlin, Heidelberg, 2012.
123 [18] M. O'Conaire, H.J. Curran, J.M. Simmie, W.J. Pitz, C.K.
124 Westbrook, A comprehensive modeling study of hydrogen
125 oxidation, *Int. J. Chem. Kinet.* 36 (2004) 603-622.
126 [19] J. Sun, Y. Wang, B. Tian, Z. Chen, detonationFoam: An

- 1 open-source solver for simulation of gaseous detonation
2 based on OpenFOAM, *Comput. Phys. Commun.* 292
3 (2023) 108859.
- 4 [20] OpenFOAM, <https://openfoam.org>.
- 5 [21] J. Sun, P. Yang, B. Tian, Z. Chen, Effects of wedge-
6 angle change on the evolution of oblique detonation wave
7 structure, *Phys. Fluids* 34 (2022) 096112.
- 8 [22] J. Sun, P. Yang, B. Tian, Z. Chen, Evolution and Control
9 of Oblique Detonation Wave Structure in Unsteady Inflow,
10 *AIAA J.* 61 (2023) 11.
- 11 [23] W. Xie, R. Zhang, J. Lai, H. Li, An accurate and robust
12 HLLC-type Riemann solver for the compressible Euler
13 system at various Mach numbers, *Int. J. Numer. Methods*
14 *Fluids* 89 (2018) 430-463.
- 15 [24] E. Hairer, S.P. Nørsett, G. Wanner, Solving ordinary
16 differential equations II: Stiff and differential-algebraic
17 problems, second ed., Springer-Verlag, Berlin, 1996.
- 18 [25] D. Rettenmaier, D. Deising, Y. Ouedraogo, E. Gjonaj, H.
19 De Gersem, D. Bothe, C. Tropea, H. Marschall, Load
20 balanced 2D and 3D adaptive mesh refinement in
21 OpenFOAM, *SoftwareX* 10 (2019) 100317.
- 22 [26] B. Tekgül, P. Peltonen, H. Kahila, O. Kaario, V.
23 Vuorinen, DLBFoam: An open-source dynamic load
24 balancing model for fast reacting flow simulations in
25 OpenFOAM, *Comput. Phys. Commun.* 267 (2021)
26 108073
- 27 [27] Z. Jiang, G. Han, C. Wang, F. Zhang, Self-organized
28 generation of transverse waves in diverging cylindrical
29 detonations, *Combust. Flame* 156 (2009) 1653-1661.
- 30 [28] H. Shen, M. Parsani, The role of multidimensional
31 instabilities in direct initiation of gaseous detonations in
32 free space, *J. Fluid Mech.* 813 (2017) R4.
- 33 [29] X. Jia, Y. Xu, H. Zheng, H. Zhang, Direct detonation
34 initiation in hydrogen/air mixture: effects of
35 compositional gradient and hotspot condition, *J. Fluid*
36 *Mech.* 970 (2023) A22.