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Abstract:	<p>This work studies numerically the spontaneous initiation and sustenance of a detonation wave from a hot spot with a nonuniform initial temperature embedded within an H₂-O₂ mixture with and without O₃ addition. For the case with either no or just a small amount of O₃ addition, a weak reaction wave is auto-ignited at the hot spot, accelerates and then transitions to a pulsating detonation, which propagates along the temperature gradient and quenches as it runs into the cold fresh mixture. However, with increasing O₃ addition, the possibility of sustenance of a developing detonation within the gradient is significantly enhanced as it enters the cold mixture. Furthermore, the reduced induction time by O₃ addition leads to earlier appearance of the spontaneous reaction wave and detonation formation in the cold mixture, demonstrating that quenching of the detonation is largely related to the instability property of the mixture because the shortened induction time reduces substantially the instability. It is also noted that, for 5%O₃ addition, a low-temperature flame produced by the O₃ reactions is present in front of the spontaneous reaction wave, inducing a local pressure wave, which facilitates spontaneous initiation and sustains the detonation entering the cold mixture. Moreover, O₃ addition renders the critical temperature to induce the minimum spontaneous wave speed higher than the crossover temperature, while they are very close for the case without O₃.</p>

Title Page

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Spontaneous Initiation and Development of Hydrogen-Oxygen Detonation with Ozone Sensitization

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Spontaneous Initiation and Development of Hydrogen-Oxygen Detonation with Ozone Sensitization

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Abstract: This work studies numerically the spontaneous initiation and sustenance of a detonation wave from a hot spot with a nonuniform initial temperature embedded within an H₂-O₂ mixture with and without O₃ addition. For the case with either no or just a small amount of O₃ addition, a weak reaction wave is auto-ignited at the hot spot, accelerates and then transitions to a pulsating detonation, which propagates along the temperature gradient and quenches as it runs into the cold fresh mixture. However, with increasing O₃ addition, the possibility of sustenance of a developing detonation within the gradient is significantly enhanced as it enters the cold mixture. Furthermore, the reduced induction time by O₃ addition leads to earlier appearance of the spontaneous reaction wave and detonation formation in the cold mixture, demonstrating that quenching of the detonation is largely related to the instability property of the mixture because the shortened induction time reduces substantially the instability. It is also noted that, for 5% O₃ addition, a low-temperature flame produced by the O₃ reactions is present in front of the spontaneous reaction wave, inducing a local pressure wave, which facilitates spontaneous initiation and sustains the detonation entering the cold mixture. Moreover, O₃ addition renders the critical temperature to induce the minimum spontaneous wave speed higher than the crossover temperature, while they are very close for the case without O₃.

Keyword: temperature gradient, spontaneous reaction wave, spontaneous initiation, detonation

1. Introduction

In industrial explosions from the leakage of combustible gas and within internal combustion engines, hot spots may be produced by the turbulent mixing of hot products and cold mixture. The resulting medium of nonuniform temperature and concentration can then generate spontaneous reaction waves when the characteristic time of turbulent mixing is smaller than the induction time of the resulting mixture [1, 2, 3]. As such, the study of detonation initiation by a hot spot with initial nonuniform temperatures and concentrations in cold mixture is of practical importance.

The mechanism of spontaneous initiation has been extensively studied theoretically and numerically [1-3], including identifying the conditions for spontaneous initiation by Zeldovich [4] and a SWACER (shock wave amplification by coherent energy release) mechanism by Lee [5]. Bradley et al. [6] proposed the boundaries of reaction waves from subsonic to supersonic combustion with a diagram of detonation peninsula. He & Clavin [1] showed that a developing detonation quenches for an initial hot spot with a linear gradient of initial temperature embedded in a cold uniform mixture, and further found that the quenching may be attributed to the negative role of the gradient [2,3]. Liberman & Wang et al. [7, 8] found that the sustenance of detonation initiated by spontaneous reaction wave is closely related to the ambient temperature and pressure at the end and outside of the temperature gradient. Dai, Qi & Chen et al. [9] studied the development of a spontaneous reaction wave in a hot spot with high initial pressure and temperature for large hydrocarbon fuels with low-temperature chemistry which is prone to exhibit the negative temperature coefficient (NTC) phenomena. Pan & Wei et al. [10]

investigated numerically detonation development inside and outside a hotspot with a temperature gradient for different fuels, and observed that a developing detonation can be self-sustaining as it leaves the hot spot, suggesting the significant role of mixture reactivity in detonation development outside the hotspot. Radulescu, Sharpe & Bradley [11] identified a unique parameter, $\chi \sim \tau_{\text{ind}}/\tau_e$ that can characterize the detonability of reactive media, and highlighted its role in amplifying the pressure waves within it. These studies identified that quenching of a developing detonation exiting a hot spot is closely related to the reactivity of the mixture associated with the initial temperature, pressure and fuel type, which are associated with a critical parameter, namely the induction time τ_{ind} (ignition delay time) of the mixture.

We next note that ozone has been studied in various combustion applications, including its use as an additive in measuring laminar flame speeds [12,13] and in spark ignition engines [14,15]. Sepulveda & Ju et al. [16] found that ozone addition reduces drastically the deflagration-to-detonation (DDT) time and the onset distance for microchannel detonation transition in acetylene mixtures. Crane et al. [17] isolated the effects of induction time on the detonation structure for hydrogen-oxygen detonation promoted by ozone, and confirmed that the detonation structure is controlled largely by chemical length scales. Liang, Wang & Law [18] found that O_3 catalysis modifies significantly the ignition delay time (induction time) and the explosion limits.

In this work, we have isolated the effects of induction time on the spontaneous initiation and detonation development inside and outside of a hot spot embedded within a cold $\text{H}_2\text{-O}_2$ mixture, with ozone addition. The goal is to identify whether quenching of a

developing detonation along a temperature gradient is spontaneous or controlled, and the relation of the quenching and induction times associated with detonation stability.

2. Methodology

The governing equations for the numerical simulations can be found in the literature [19] and are also listed in the Supplementary Materials. The kinetic and transport properties are evaluated using the CHEMKIN [20] and TRANSPORT [21] packages. We adopt the H₂-O₂ mechanisms of Burke [22], comprising of 19 species and 32 reactions, together with an O₃ sub-mechanism [23] consisting of eight steps. The physical flux is split by the WENO-LF method [24] and the spatial discretization of the advection and diffusion terms by the 5th-order WENO and the 6th-order central difference schemes. To solve the stiffness problem, an explicit-implicit additive Runge-Kutta scheme [25] was used in the time discretization. Eventually, the method based on conservation variables was used to solve the equations, which guarantees conservation and also yields good solution with the shock speed evaluated accurately.

3. Results and discussions

3.1 Autoignition and ZND Structure with O₃ Addition

The mixture is stoichiometric H₂-O₂ mixture with 0.05%, 0.1%, 0.5%, 1% and 5% O₃ additions. The initial pressure is $p_0=1\text{atm}$ and the initial temperature is given by:

$T_i(t=0, x) = T^* - 72(T^* - T_0)x$ for $0 < x < 0.06\text{m}$; $T_0 = 300\text{K}$ for $x > 0.06\text{m}$, where $T^* = 1200\text{K}$.

The length of the computational domain is 0.12m and grid resolution is 20 points per induction zone, which is sufficient to capture the detonation structure.

Figure 1 shows the ignition delay time as a function of temperature for different O_3 additions. The ignition delay time shows the crossover behavior, namely at certain temperature, the ignition delay time suddenly drops, which is mainly due to the second limit for $\text{H}_2\text{-O}_2$ mixtures. When the temperature reaches this value, the kinetic time becomes much faster as it crosses the boundary from the slow reacting regime controlled by the HO_2 kinetics to the fast reacting regime controlled by the H+O_2 chain branching. It is seen that O_3 addition substantially shortens the ignition delay time, namely the induction time. In addition, O_3 makes the slope of the ignition delay time versus temperature substantially increase, which also facilitates spontaneous initiation as it strongly depends on the derivative $\partial\tau_{ind}/\partial T$. Increasing the initial temperature substantially influences the ignition delay time in the ambient of a hot spot, while the CJ detonation velocity is slightly affected, as shown in the insert of Fig. 1. Since the CJ velocity is only controlled by the initial state and the final equilibrium state, this indicates that O_3 addition mainly changes the kinetic behavior, while thermodynamically it has little influence on the detonation structure. Furthermore, steady ZND solution with different O_3 additions (Fig. 2) shows that, while slightly varying O_3 addition can substantially affect the induction time, the thermicity peak is minimally affected, which is consistent with results in Fig. 1.

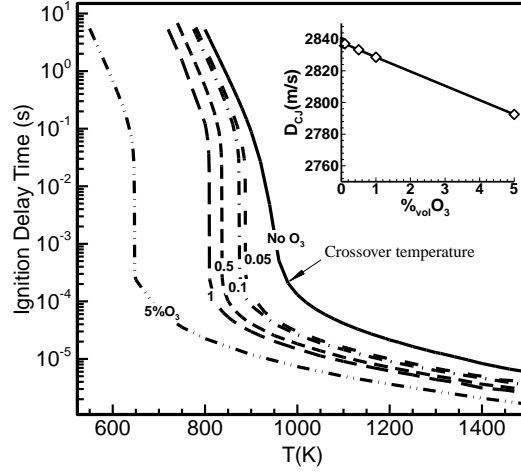


Fig. 1 Ignition delay time as a function of temperature for $\text{H}_2\text{-O}_2$ system with different O_3 additions at $p_0=1\text{atm}$: using Burke's mechanism [22].

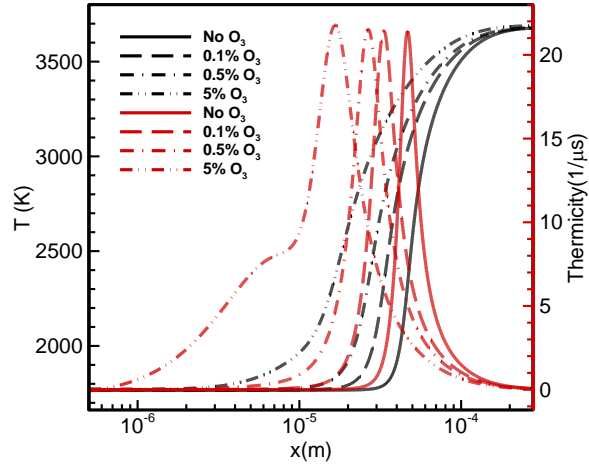


Fig. 2 Steady ZND of detonations for different O_3 additions.

In a region with temperature gradient, the reaction begins at the minimum ignition delay time, and then it progresses along the temperature gradient by spontaneous autoignition at neighboring locations where the induction time is longer, namely spontaneous reaction wave. The velocity of the spontaneous reaction wave in the direction of the temperature gradient is evaluated as [4, 26] $U_{sp} = |d\tau_{ind}/dx|^{-1} = |(\partial\tau_{ind}/\partial T)^{-1}(\partial T/\partial x)^{-1}|$, where $\tau_{ind}(x)$ is the induction time and $U_{sp}(x)$ depends only

on the steepness of the temperature gradient and $\partial\tau_{ind} / \partial T$. In general, the velocity of the spontaneous wave decreases along the temperature gradient and reaches minimum at a certain temperature, where the spontaneous wave can be coupled with the pressure wave generated behind the high-speed spontaneous wave front. After the intersection of the spontaneous wave front and the pressure wave, the spontaneous wave evolves into a combustion wave and the pressure wave steepens into the shock wave. The pressure peak becomes large enough and steepens into a detonation wave [7]. This process is defined as a spontaneous initiation. Successful detonation initiation requires that the spontaneous wave can be caught up and coupled with the pressure wave. Consequently, the necessary condition for triggering a detonation can be written in the form,

$$U_{sp}(T_c) = \left| (\partial\tau_{ind} / \partial T)^{-1} (\partial T / \partial x)^{-1} \right|_{T_c} = \left| (\partial\tau_{ind} / \partial T)^{-1} \right|_{T_c} \frac{L}{T^* - T_0} \geq a_s(T_c)$$

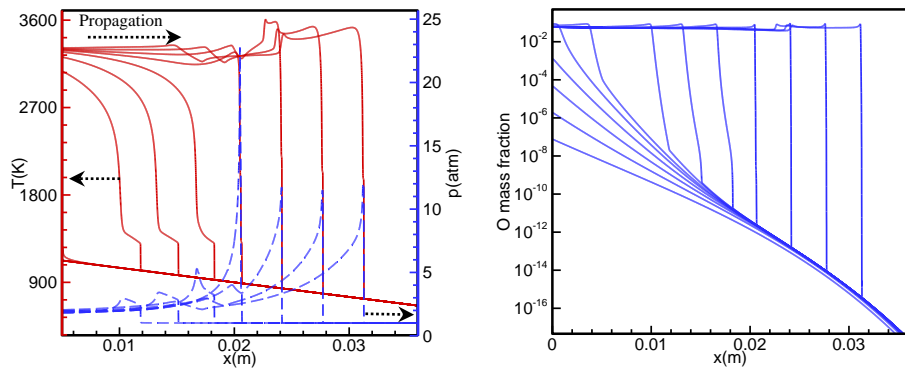
where $a_s(T_c)$ is the sound speed at the point corresponding to the minimum of the spontaneous wave speed and T^* is the highest temperature along the gradient and T_0 is the initial temperature in the uniform region. Using this condition we can estimate the maximum steepness of the temperature gradient, or the critical gradient length (the minimum size of the hot pocket, L_c) for successful detonation initiation. Consequently, as fixed $T^*=1200\text{K}$, the length of 0.06m is used for the present simulation.

3.2 Formation of spontaneous initiation for different O_3 additions

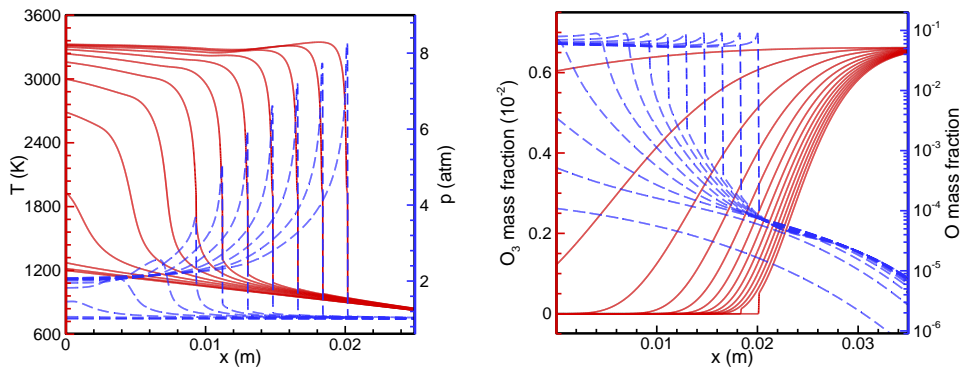
Figure 3 shows the pressure, temperature and mass fraction profiles in the process of spontaneous initiation for different O_3 additions. It is seen that spontaneous initiation

can occur within the temperature gradient for the different cases. The spontaneous reaction wave starts in the high-temperature region; and it is coupled with the pressure pulse produced by the energy released in the reaction. Consequently, a pressure peak is formed at the reaction front and grows with the energy released in the reaction. After the pressure peak becomes large enough, it steepens into a shock wave, forming a detonation wave. For the case without O₃, spontaneous initiation occurs at $x=0.02\text{m}$, and the overdriven detonation forms and then decays rapidly, propagating at the local CJ speed along the gradient, shown in Fig. 3(a). It is seen that the O concentration is still very low as there is no O₃ addition. In the gas ahead of the reaction wave, temperature is increased slightly, while reaction in the preheat zone does not occur, as substantiated by the O mass fraction ($\sim 10^{-8}$) shown in Fig. 3(b). However, with O₃ addition, the distance to attain spontaneous initiation is reduced significantly, with O₃ starting to be consumed and radical O mass fraction increases through the reaction $\text{O}_3 + \text{M} = \text{O}_2 + \text{O} + \text{M}$ ahead of reaction wave, while the concentration of the O radical (mass fraction $\sim 10^{-5}$ - 10^{-4}) still is low, as shown in Fig. 3(b). When the spontaneous reaction wave progresses into the region with reactive O, a detonation is easier to be initiated spontaneously at $x \sim 0.006\text{m}$. With increasing O₃ addition, spontaneous reaction wave becomes stronger and its initiation is promoted substantially due to the “catalytic” role of O₃ in the premixed gas. For larger O₃ addition, higher spontaneous wave speed leads to longer distance to initiate a detonation. For 5% O₃, it is seen that a low-temperature flame caused by O₃ catalysis (O mass fraction, $\sim 10^{-4}$ - 10^{-2}) appears ahead of the spontaneous wave and the temperature is increased to $\sim 1200\text{K}$ due to the partial release

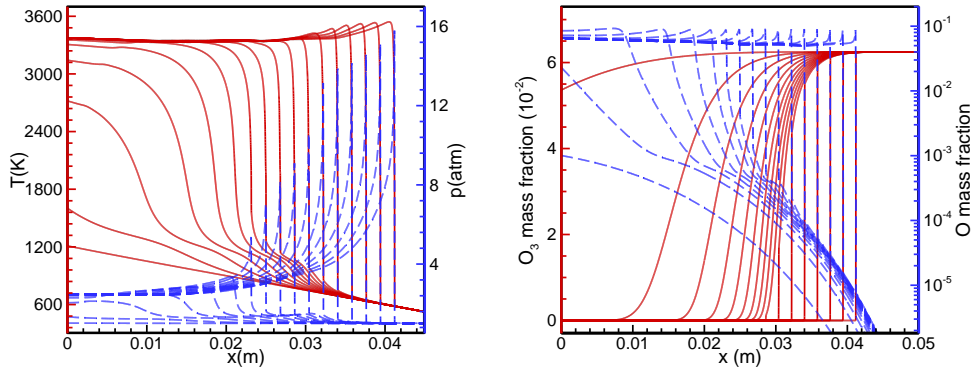
of the energy at $x \sim 0.015 - 0.03\text{m}$. The low-temperature flame elevates the local temperature and leads to a locally lower temperature gradient. By $U_{sp} = (\partial\tau_{ind} / \partial T)^{-1}(\partial T / \partial x)^{-1}$, the small gradient produces very large speed of the spontaneous wave, $\sim 2840\text{m/s}$ at $x \sim 0.015\text{m}$, which decreases to the minimum of $\sim 1980\text{m/s}$ at $x \sim 0.024\text{m}$. The low-temperature flame causes the pressure to increase by $\sim 0.5\text{atm}$, and is followed by a hot flame. The spontaneous initiation occurs at $x \sim 0.024\text{m}$. The detonation then catches up with the low-temperature heat release at $x \sim 0.032\text{m}$. Meanwhile, the shock pressure increases abruptly because the potential energy in the fresh mixture is still not released as there is no low-temperature reaction.



(a) No O_3



(b) 0.5% O_3



(c) 5% O₃

Fig. 3 Evolution of spontaneous reaction wave and the spontaneous initiation for different O₃ additions.

In summary, O₃ addition significantly influences the evolution of spontaneous reaction wave and the occurrence of initiation from a hot spot within the cold mixture. For lower O₃ concentrations, spontaneous initiation occurs within a shorter distance as compared to that without O₃ addition; O₃ catalytic reaction can enhance slightly the local temperature ahead of reaction wave, but a low-temperature flame is not observed ahead of the spontaneous reaction wave. From Fig. 4(a), in the initial phase the pressure rise is due to the heat release from chemical reaction while the increase of the specific volume is due to expansion after passage of the pressure wave, although the O₃ catalysis enhances slightly the temperature ahead of the spontaneous wave. However, for 5% O₃ the spontaneous reaction wave runs much faster and the spontaneous initiation occurs at the lower temperature region; a low-temperature flame produced by O₃ catalysis is present in front of the spontaneous wave, which is able to produce local compression waves, as shown in Fig. 4(b).

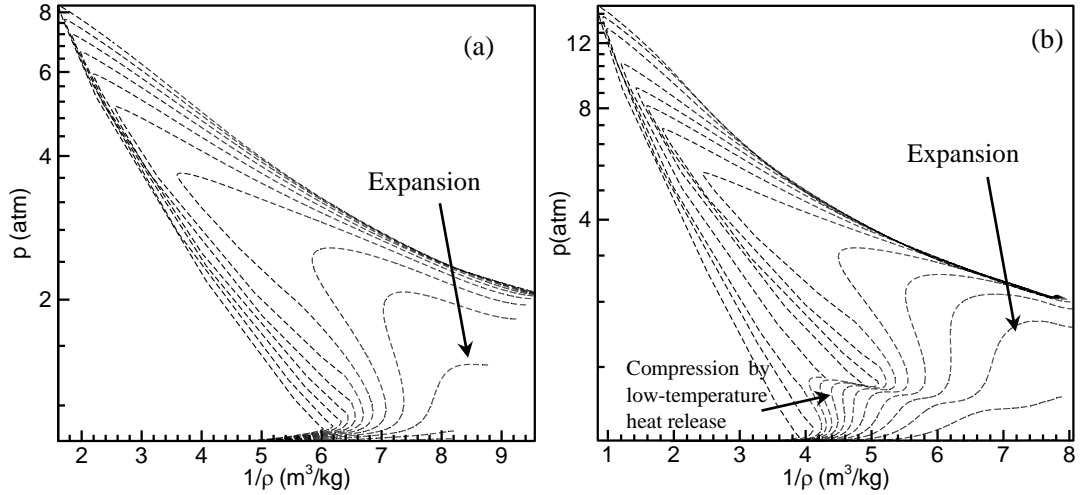


Fig. 4 Diagram of pressure vs. specific volume, p - v for the particles at the locations in Fig. 4: (a) 0.5% O_3 , (b) 5% O_3 .

3.3 Propagating dynamics of reaction wave for different O_3 additions

A spontaneous wave speed can be defined as $U_{sp}(x) = (d\tau_{ind}(x)/dx)^{-1}$, where the profile of the induction time $\tau_{ind}(x)$ is associated with the initial temperature profile $T_i(x)$. When U_{sp} is larger than the local acoustic speed $a_s(x)$, a nearly constant volume explosion takes place within this region. However, since $U_{sp}(x)$ is small compared to the local acoustic velocity $a_s(x)$, a deflagration is always formed within this region [1]. Figure 5 shows the velocity of the reaction wave inside and outside the gradient. It is seen that for all cases, the entire process of the propagation includes four stages: 1) ignition; 2) spontaneous wave; 3) developing detonation; 4) quenching or sustenance in the cold uniform region. Except for the case without O_3 , the velocity of the spontaneous reaction wave can increase rapidly to the local peak and then decreases to the minimum value at a certain temperature. As it reaches the minimum value, the pressure wave catches up with the spontaneous wave, triggering spontaneous initiation; and then the formed detonation propagates at the local CJ value and up to the CJ value

in the uniform flow. For the case without O_3 , initially the spontaneous wave speed, U_{sp} , is close to and even slightly less than the local sonic speed. As it accelerates along the gradient, an overdriven detonation is developed at $x \sim 0.02m$, with the speed of $\sim 4000m/s$, and then decays to the CJ state and propagates along the gradient at the local CJ velocity. As it reaches the cold mixture with $T_i = 450K$ at $x \sim 0.055m$, pulsating instability appears, with the peak of the velocity being $3400m/s$ and finally, the velocity decreases below the $0.5CJ$ value as it enters the cold uniform mixture, showing that the detonation quenches completely. For 0.05% and $0.1\%O_3$, the velocities of the spontaneous wave are much higher than the local sonic speed, while they are lower than the CJ velocity. At $x \sim 0.005m$ ($t=9.38\mu s$), they reach the minimum of $\sim 1850m/s$, demonstrating that spontaneous initiation occurs. As it reaches $x \sim 0.055mm$, quenching occurs after a strong pulsating instability for these two cases, similar to that in the case with O_3 . For $0.5\%O_3$, U_{sp} is obviously larger than that with $0.1\%O_3$, although it still is lower than the CJ value; the minimum U_{sp} is $1900m/s$ at $x \sim 0.075m$ ($t=9.38\mu s$), at which spontaneous initiation happens. The resulting detonation propagates at the local CJ velocity and still sustains after pulsation as it enters the cold uniform mixture. For $1\%O_3$, U_{sp} increases further and initially the maximum speed is slightly larger than the CJ value; then it decreases to the minimum of $\sim 1900m/s$ at $x \sim 0.01m$ ($t=9.29\mu s$), where transition to detonation occurs. Entering the cold region, the formed detonation tends to be stable after undergoing oscillation, with the CJ speed in the cold uniform mixture. For $5\%O_3$, the maximum U_{sp} ($\sim 6000m/s$) is much higher than the CJ value and slows down to the minimum at $x \sim 0.02m$ ($t=8.31\mu s$), at which spontaneous initiation occurs.

Meanwhile, the developing detonation propagating at the local CJ velocity does not undergo any oscillation as it exits the gradient and becomes sustained in the cold uniform medium.

For 0.05%, 0.1%, 0.5%, 1% and 5% O₃, the crossover temperature is respectively 900K, 880K, 850K, 810K and 650K (Fig. 1), while the numerical results show that the corresponding minimum U_{sp} is at $x \sim 0.0035, 0.005, 0.0075, 0.01$ and 0.02m , and the temperature is $\sim 1147.5\text{K}, 1125\text{K}, 1087.5\text{K}, 1050\text{K}$ and 900K respectively. Consequently, O₃ addition makes the critical temperature substantially higher than the crossover temperature, while for the case without O₃, spontaneous initiation occurs at $T \sim 900\text{K}$ ($x \sim 0.03\text{m}$), which is close to the corresponding crossover temperature.

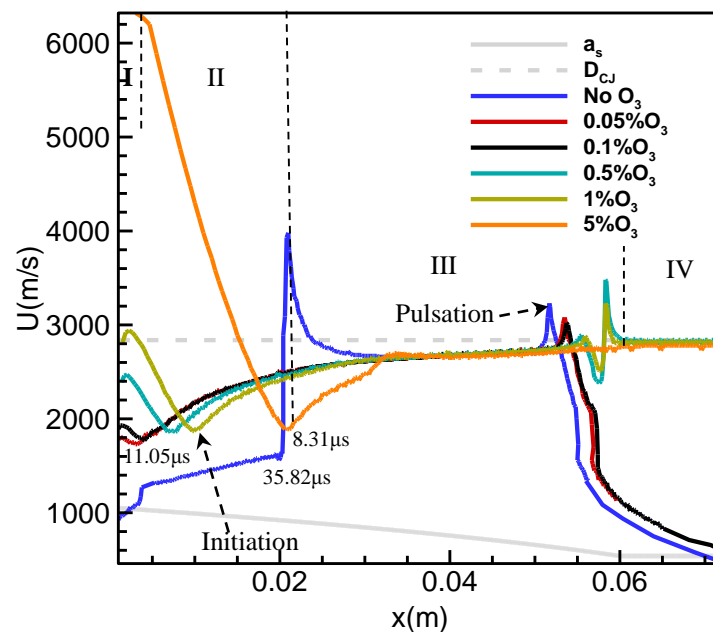


Fig. 5 Spontaneous wave and detonation velocities as a function of distance for different O₃ additions: I, ignition; II, spontaneous reaction wave; III, developing detonation; IV, quenching or sustaining.

The above discussion then demonstrates that for lower O₃ additions, a developing

detonation along the temperature gradient always quenches. He & Clavin [1, 2, 3] showed that cold fresh medium is easy to cause quenching, and the criterion for initiating a detonation in the cold uniform mixture at T_0 must require $T_c < T_0$, where T_c is the critical initial temperature. The present result shows that as the induction time is reduced through increase in the O_3 addition, a developing detonation along a temperature gradient is prone to survive as it enters the cold mixture. Consequently, it can be known that quenching of a developing detonation exiting a hot spot is not spontaneous while it is controlled by detonation instability, associated closely with the induction time. This is also substantiated by the fact that when a detonation enters the cold mixture the pulsating instability weakens as O_3 addition increases and the induction time shortens, as shown Fig. 5.

Figure 6 shows trace of the maximum pressure as a function of distance for different O_3 additions. It is seen that for all cases, the developing detonation along the gradient follows the local CJ value in the middle stage of propagation after the spontaneous initiation, except for departures from the CJ detonation in the early and later stages. Before spontaneous initiation, a constant volume explosion occurs for all cases, which was explained by the Zeldovich's criterion [4]. For the case without O_3 addition, the spontaneous initiation is abrupt at $\sim 0.02m$, accompanying a strong pressure pulse with the peak of $\sim 28atm$; subsequently a developing detonation propagates along the gradient at $x \sim 0.022-0.05m$. At $x \sim 0.055m$, the second pressure pulse appears, with $\sim 30atm$, and subsequently quenches as it moves into the cold mixture, with the reaction wave separated from the leading shock, shown in Fig. 7(a).

For 0.05%O₃, the spontaneous initiation is smooth after a short period of volume explosion, without the pressure pulse. In the initial stage of developing detonation at $x \sim 0.03$ -0.045m, the shock pressure is lower than the theoretical value; similar to that without O₃, the pulsating instability leads to quenching at $x \sim 0.055$ m as it moves into the cold mixture. For 1% and 5%O₃, the detonation produced by spontaneous initiation can sustain with stable mode in the uniform cold fresh mixture, with coupling of shock and the reaction wave, as shown in Fig. 7(b). In the uniform fresh medium, the shock pressure for 1% and 5%O₃ are slight lower than the CJ value.

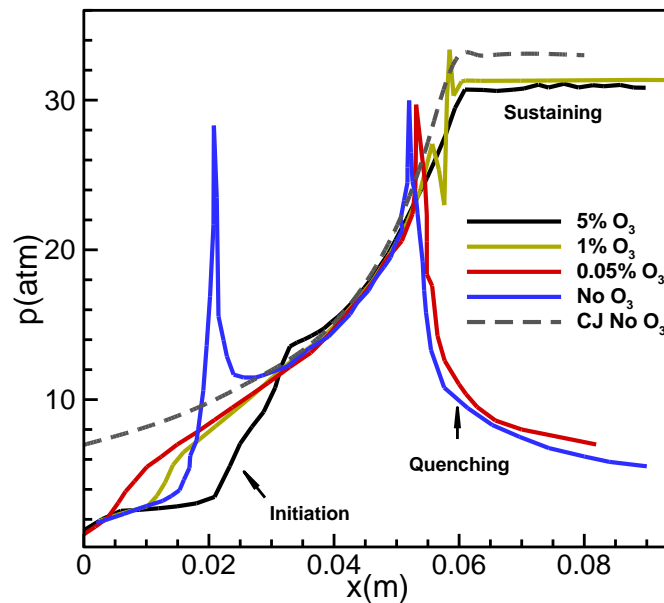


Fig. 6 Maximum pressure histories for detonation at different O₃ additions.

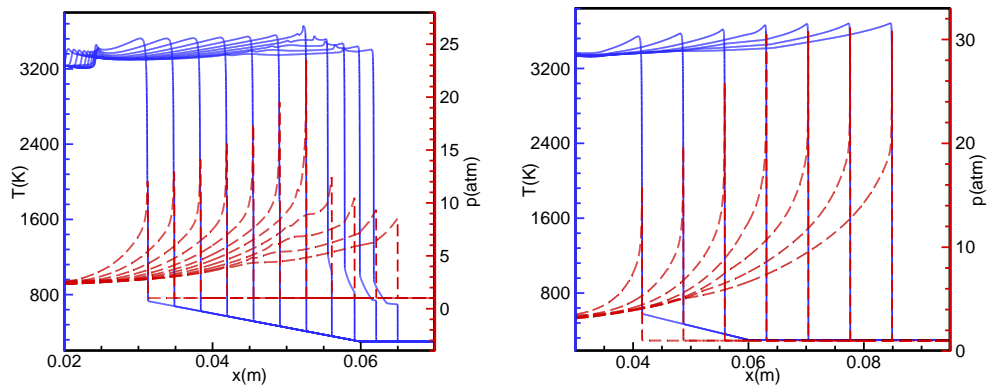


Fig. 7 Evolution of detonation propagating from a gradient to uniform regions: (a) without O_3 , (b) 5% O_3

4. Concluding Remarks

The effects of O_3 addition on spontaneous initiation and development of detonation from a hot spot with the cold mixture are numerically studied. In summary, O_3 addition modifies substantially the spontaneous initiation and the sustenance of the detonation entering the cold fresh mixture. As the amount of O_3 increases, the spontaneous wave speed is enhanced substantially. When a detonation enters the cold fresh mixture, its sustenance depends on the extent of the O_3 addition. For the higher $O_3\%$, it is easier to sustain a detonation in the cold mixture. He & Clavin [2] suggested that the temperature gradient may prevent the sustenance of a developing detonation and the transmission of detonation to the uniform fresh mixture. However, the present results show that quenching of the detonation is more related to the instability of the mixture, through the induction time. Consequently, the induction time may be the critical parameter for detonation quenching in the cold fresh mixture, which is associated closely with the stability factor, as discussed in Radulescu & Bradley et al. [11] and Ng et al. [27]. He

& Clavin [28] and Radulescu et al. [29] indicated that strongly pulsating instability can extinguish an established detonation wave in a 1-D simulation. For a one-step reaction model, the stability factor, $\chi = \tau_{ind}/\tau_e Ea/RT$ indicates the detonation instability. For the uniform cold mixture, the induction time τ_{ind} reduces significantly with O₃ addition and therefore the stability factor decreases, demonstrating that the mixture tends to be more stable. Consequently, the sustenance of a detonation entering the cold mixture becomes more possible. This is why for the higher O₃ addition a detonation is easier to sustain as it exits the gradient.

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Figure Captions

Fig. 1 Ignition delay time as a function of temperature for H₂-O₂ system with different O₃ additions at $p_0=1\text{atm}$: using Burke's mechanism [22]

Fig. 2 Steady ZND of detonations for different O₃ additions

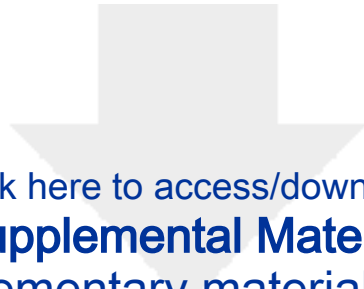
Fig. 3 Evolution of spontaneous reaction wave and the spontaneous initiation for different O₃ additions

Fig. 4 Diagram of pressure vs. specific volume, p - v for the particles at the locations in Fig. 4: (a) 0.5%O₃, (b) 5%O₃

Fig. 5 Spontaneous wave and detonation velocities as a function of distance for different O₃ additions: I, ignition; II, spontaneous reaction wave; III, developing detonation; IV, quenching or sustaining
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Fig. 6 Maximum pressure histories for detonation at different O₃ additions

Fig. 7 Evolution of detonation propagating from a gradient to uniform regions: (a) without O₃, (b) 5%O₃



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