Numerical Study on Hydrogen Detonation Initiation through an Inhomogeneous Thermal Explosion

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Abstract. Detonation initiation through an inhomogeneous energy source is studied using one-dimensional simulations. The energy source is divided into two segments, called segment A and segment B. The initial temperature and the length of two parts energy source are varied to provide different auto-ignition delay time and strength of the leading shock. Detailed chemical reaction mechanism is used for a stoichiometric hydrogen/oxygen mixture diluted by 70% Argon. According to the initial thermodynamic parameters, four different regimes of detonation initiation were found in the present study, namely high-critical, low-critical, low-subcritical and high-subcritical regimes. The critical temperature and internal energy in the inhomogeneous energy source to initiate the detonation are analyzed. It was found that, as we fix the length and temperature of segment B, by changing the temperature of segment A, there are two critical temperatures, called high critical temperature and low critical temperature. When the temperature of segment A higher than the high-critical temperature or lower than the low-critical temperature, there is no detonation occurs. As we change the length ratio of segment A and B, the same results was found. In addition, the relationship between the length ratio of segment A and B and the energy to initiate detonation are also studied.

1. Introduction

The initiation of gaseous detonations can be obtained by many ways. As we know, a detonation is essentially a strong shock wave supported by chemical reactions. Previous studies have suggested that initiation of detonation could be achieved by a strong incident or reflected shock wave in reactive mixtures [1, 2, 3]. Smirnov et al. [4] showed that both regimes of combustion to detonation transition and regimes including deflagration waves lagging behind the shock waves are possible. Grogan and Ihme [5] investigated weak and strong ignition regimes in a shock-tube system, they found that the transition from ignition kernel to detonation is well described by the SWACER mechanism. Kiverin and Yakovenko [6] elucidated the process of ignition kernel formation and subsequent detonation onset behind the shock wave propagating in the shock tube, and found that shock-induced compression of the test mixture provides conditions for the self-sustained acceleration of the combustion wave, and finally, the detonation onset takes place.

Ignition behind a shock is also sometimes seen in DDT cases in which two shocks produced by an accelerating flame merge, resulting in a transmitted shock and a contact discontinuity. The contact surface drives the shock and hence behaves like a piston. Thus the ignition process between the leading shock and contact surface has also been studied by many researchers [7, 8]. Parkins [9] used high-activation-energy to examine the reactive-acoustic induction domain
between a contact surface and shock. Sharpe and Short [10] carried out a systematical study of the dynamics of ignition between a contact surface and a shock wave using a one-step reaction model with Arrhenius kinetics. In addition, the complete spatial and temporal ignition evolution of hydrogen combustible mixtures of different concentrations was studied numerically by Melguizo-Gavilanes and Bauwens [11].

Blast wave is another way to initiation the detonation. Ng and Lee [12] studied a powerful ignition source driving a blast wave into a gaseous combustible mixture to generate a Chapman-Jouguet (CJ) detonation numerically by using a three-step chain-branching chemical kinetic model. Detonation in less reactive mixture can also be initiated by a transmitted detonation rather than by a shock, as studied by Mooradian and Gordon [13] and Gordon et al. [14]. Temperature gradient is another common way to initiation detonation, which has also been extensively studied [15, 16, 17, 18, 19]. In addition, the initiation can also be obtained by the addition of the heat at a prescribed rate of heat flux through the wall [20] or energy deposition in a finite space with a certain depositing rate [21, 22].

All these initiation processes have already been studied for many years by different researchers as classical problem. However, the complicated interaction between hydrodynamics and chemical reactions is still not fully understood. Based on the above considerations, one-dimensional simulations on hydrogen detonation initiation through an inhomogeneous thermal explosion are conducted and detailed chemistry is employed. By choosing arbitrary temperatures and length of driver section, different types of detonation initiation mentioned above are expected to be reproduced, the details of the inhomogeneous initiation is revealed. The main objective of this paper is to elucidate further the complicated shock/reaction interaction process, scale effect and critical energy associated with the inhomogeneous initiation of detonation.

2. Numerical methodology
The governing equations employed to describe the detonation dynamics are one-dimensional reactive Euler equations.

2.1. Governing equations
Which have the following form:

\[ \frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = \mathbf{S}(\mathbf{U}) \]  

(1)

Where the vector \( \mathbf{U} \), the flux \( \mathbf{F} \), and the source term \( \mathbf{S} \) are defined as:

\[ \mathbf{U} = \{ \rho, \rho u, E, \rho_1, \rho_2, \ldots, \rho_{N-1} \}^T \]  

(2)

\[ \mathbf{F}(\mathbf{U}) = \{ \rho u, \rho u^2 + p, (E + p)u, \rho_1 u, \rho_2 u, \ldots, \rho_{N-1} u \}^T \]  

(3)

\[ \mathbf{S}(\mathbf{U}) = \{ 0, 0, 0, \omega_1, \omega_2, \ldots, \omega_{N-1} \}^T \]  

(4)

Where \( \rho, u, p \) and \( E \) denote the density, velocity, pressure and total energy, respectively. \( N \) is the number of species, and \( \rho_i = \rho Y_i \) in which \( Y_i \) is the mass fraction of the \( i \)-th species (Note that \( Y_N = 1 - \sum_{i=1}^{N-1} Y_i \)). \( \omega_i \) is the mass production rate of the \( i \)-th species. The total energy and the equation of state are given by,

\[ E = \rho h - p + \frac{\rho u^2}{2}, \quad h = e + \frac{p}{\rho} \]

(5)

Where \( h, p \) and \( e \) represent the enthalpy per unit mass, pressure and specific total energy, respectively. In order to investigate the influence of viscosity, a case as also simulated by using reactive Navier-Stokes (NS) equations.
2.2. Chemical mechanism

A detailed chemical reaction model comprised of 9 species and 48 elementary reactions is employed to describe a hydrogen-oxygen-argon detonation. The chemical reactions can be expressed as:

\[ \sum_{i=1}^{9} v'_{ik} x_i \rightleftharpoons \sum_{i=1}^{9} v''_{ik} x_i, k = 1, 2, 3, \ldots, 48 \]  

(6)

Where \( v'_{ik} \) and \( v''_{ik} \) denote the reactant and product chemical stoichiometric coefficients of the \( i \)-th species in the \( k \)-th reaction, and \( x_i \) is the mole fraction of the \( i \)-th species. The finite production rate \( \omega_i \) is defined as

\[ \omega_i = W_i \sum_{k=1}^{48} \left( v''_{ik} - v'_{ik} \right) \left\{ \sum_{i=1}^{9} \alpha_{ik} C_{xi} \right\} \times \left\{ k_{f,k} \prod_{i=1}^{9} C_{x_i}^{v''_{ik}} - k_{b,k} \prod_{i=1}^{9} C_{x_i}^{v'_{ik}} \right\} \]  

(7)

Where \( W_i \) is the molecular mass, and \( C_{xi} = \rho_i / W_i \) represent the molar concentration of \( i \)-th species; \( \alpha_{ik} \) is the third body coefficients of the \( i \)-th species in the \( k \)-th reaction; \( k_{f,k}, k_{b,k} \) represent the forward and backward reaction rate constants of the \( k \)-th reaction, which follow Arrhenius law and can be expressed as:

\[ k_{f,k} = A_k T^{nk} \exp \left( -E_{ak} / RT \right) \]  

(8)

\[ k_{b,k} = \frac{k_{f,k}}{k_{c,k}} \]  

(9)

\[ k_{c,k} = k_{p,k} \left( \frac{p_{atm}}{RT} \right) \sum_{i=1}^{9} (v''_{ik} - v'_{ik}) \]  

(10)

\[ k_{p,k} = \exp \left( \sum_{i=1}^{9} \left\{ (v''_{ik} - v'_{ik}) \left( \frac{S_i^0}{R_i} - \frac{h_i}{R_i} T \right) \right\} \right) \]  

(11)

Where \( A_k \) is the pre-exponential constant; \( nk \) represents the temperature power; \( E_{ak} \) denotes the activation energy; \( p_{atm} \) is the atmospheric pressure, and \( S_i^0 \) is the entropy at the standard state. In addition, \( R_i = R_u / W_i \) in which \( R_u \) is the universal gas constant.

2.3. Numerical methods and Simulation setup

To resolve the detailed structures during the detonation initiation process, it is necessary to use a sufficient fine resolution in the numerical simulation. To fulfill this requirement, a parallel AMROC code with a block-structured adaptive mesh refinement (AMR) method after Berger and Colella was used in the present work to dramatically reduce the computation time and memory requirement. The AMROC code developed by Deiterding [23] has been widely used for hydrodynamics with chemical reactions. It is fully accepted that the AMROC code can resolve the detonation problem with high accuracy, efficiency and robustness [24, 25]. The entire computational domain was covered by a coarse grid, and a fine mesh was superimposed on the coarse grid in the vicinity of discontinuities.

The setup of the framework is shown in figure 1. The initial temperature \( T_0 \) and pressure \( p_0 \) to the right of the diaphragm are set as 298 K and 6670 Pa respectively for all cases. To the left
of the diaphragm, the inhomogeneous driver section is divided into two segments, called segment A and segment B. The total length of segment A and B is 10 cm, which is unchanged for all cases. The initial temperature $T_a$ and the length ratio of two segments $r_L = r_a / r_b$ are varied to provide different auto-ignition delay time and strength of the leading shock. The pressure of segment A $p_a$ and B $p_b$ are set as 122 kPa that is the critical pressure of homogeneous driver section at the same total length. The temperature of segment B $T_b$ is set as 1800 K for all cases. The pre-mixed combustible mixture placed in the whole domain is a stoichiometric hydrogen/oxygen mixture diluted by 70% Argon. The left boundary is set as a solid wall in the present study unless specified. The right boundary is always set as an outflow condition.

![Figure 1. Computation setup](image)

3. Results and discussions

A series of detonation initiation cases with a fixed length of the energy source ($r_a + r_b = 10$ cm) is systematically studied, and the length ratio of segment A and B $r_L = 1$.

3.1. Low-subcritical and low-critical regimes

We first consider lowering the temperature in section A and keeping other variables constant. Two different regimes, corresponding to the so-called low-critical (figure 2 (a)), low-subcritical (figure 2 (b)) regimes, are observed in the present study. In the current state, the lowest temperature to successfully initiate a detonation is 939 K.

![Figure 2. Different regimes of detonation initiation with $r_L = 1, T_b = 1800$ K, $p_a = p_b = 122$ kPa, (a) low-critical case ($T_a = 939$ K), (b) low-subcritical case ($T_a = 930$ K).](image)

For the critical regime case, after the initial thermal explosion and shock reflected from the left boundary, an overdriven detonation is immediately formed. However, the detonation wave
first decays and then re-accelerates to an overdriven detonation, which asymptotically decays to a self-sustained CJ detonation, as shown in figure 2 (b).

For a subcritical regime case, with Ta=930 K, as plotted in figure 2 (b), the pressure pulse in the energy source increases to about 250 kPa as a result of a thermal explosion and reflected shock, chasing the leading shock wave. However, the reflected shock wave is not sufficiently strong to form a CJ detonation subsequently. Finally, the leading shock wave relaxes to an acoustic wave due to the influence of the rarefaction wave.

Figure 3. Profiles of (a) pressure and (b) temperature in the low-critical case of Figure 2(a).

To demonstrate the detailed processes of the detonation initiation, the pressure and temperature are plotted in figure 3-figure 4, corresponding to the low-critical and low-subcritical cases as shown in figure 2 (a) and (b) respectively.

As show in figure 3 (a1) and figure 3 (b1), at the very early stage, because of low temperature in segment A($T_a$) and high temperature in segment B($T_b$), a shock wave is immediately generated at the interface of A and B towards left. We can also see clearly in figure 3 (b1) a chemical reaction occurred in segment B but no chemical reaction occurred in segment A because chemical reaction occurs with heat releasing after an auto-ignition delay time that is inversely correlated to principally the initial temperature. At the same time, a leading shock wave is generated near the interface between segment B and driven section, and racing into the quiet gas followed by a contact surface. A rarefaction wave is also formed, sweeping backward and expanding the hot gas. As show in figure 3 (a2), a pressure pulse(or more obviously as a temperature pulse), which is essentially a reaction wave, appears near the left boundary, generated by the reflected shock wave and fast chemical release. The reaction wave amplifies itself as it advances forward then decays. When the temperature pulse catches up the contact surface, another temperature pulse is generated near the contact surface, and then transforms into an overdriven detonation, as shown in figure 3 (a3) and figure 3 (b3). Finally, the overdriven detonation decays to a self-sustained CJ detonation wave after a long distance.

In a subcritical case with $T_a = 930$ K, as shown in figure 4 (a1) and figure 4 (b1), the initial stage is consistent with the above critical case. However, in the present low-subcritical case, the pressure appears near the left boundary is much lower than the low-critical pressure pulse,
and thus no re-acceleration to an overdriven detonation occurs, as shown in figure 4 (a2). The temperature pulse still propagates until has caught up with contact surface. In contrast, no temperature pulse generated near the contact surface. Finally the pressure wave relaxes to a sound wave, as shown in figure 4 (a3).

3.2. High-subcritical and high-critical regimes

Then we consider increasing the temperature in segment A and keeping other variables constant. Similar to before, two different regimes, corresponding to the so-called high-critical (figure 5 (a)), high-subcritical (figure 5 (b)) regimes, are observed in the present study. In the current state, the highest temperature to successfully initiate a detonation is 1828 K.

As for the high-critical regime case, after the initial thermal explosion, the leading shock front undergoes a quasi-steady state with constant velocity and pressure ($0.5p_{VN}$) prior (about
80 cm long) to re-accelerate to an overdriven detonation, which asymptotically decays to a self-sustained CJ detonation, as shown in figure 5 (a).

For a high-subcritical regime case with an initial temperature $T_a$ of 2500 K as plotted in figure 5 (b), the pressure in the energy source increases to about 200 kPa as a result of a thermal explosion, generating a leading shock wave simultaneously. However, the leading shock wave is not sufficiently strong to form a CJ detonation subsequently. Finally, the leading shock wave relaxes to an acoustic wave due to the influence of the rarefaction wave.

![Figure 6. Profiles of (a) pressure and (b) temperature in the high-critical case of Figure 5(a).](image)

The detailed processes of the detonation initiation, the pressure and temperature are plotted in figure 6-figure 7, corresponding to the high-critical and high-subcritical cases as shown in figure 5 (a) and (b) respectively.

High-critical regime and low-critical regime are very different at the early stage, there is no shock wave generated at the interface of A and B towards left, because the temperature $T_a$ is higher than $T_b$. In addition, chemical reaction occurred in segment A and B, as shown in figure 6 (a1) and (b1). However, same as low-critical regime, a leading shock wave is generated near the interface between segment B and driven section, and racing into the quiet gas followed by a contact surface, as plotted in figure 6 (b1). As shown in figure 6 (a2), there is a plateau at the front of the pressure curves, the flow states of the plateau almost remain unchanged, referring to the so-called quasi-steady period. This quasi-steady period terminates when fast chemical reaction occurs at the tail of the plateau after induction, resulting in a high-amplitude temperature pulse, corresponding to a typical shock wave initiation, as plotted in figure 6 (b2).

As shown in figure 6 (a3), the pressure pulse amplifies and broadens itself, and finally transforms into an overdriven detonation with steepen front. The overdriven detonation, subsequently, merges with the leading front, which forms a detonation asymptotically decaying to a self-sustained CJ detonation wave after a long distance.

In a subcritical case with $T_a = 2500$ K, as shown in figure 7. The major difference between high-subcritical and high-critical regime is the initial stage. At early stage of high-subcritical regime, due to the high temperature difference between segment A and B, the intensity of the rarefaction wave becomes larger than high-critical regime. As a result, there is no detonation occurs.
3.3. Critical temperature and energy
We also study the relationship between the length ratio $r_L$ and the critical temperature $T_a$, and the relationship between critical energy to initiate detonation and length ratio. Figure 8 shows the critical temperature $T_a$ as a function of the length ratio $r_L$ for the detonation initiation processes in the present study.

![Figure 8](image_url)

**Figure 8.** Critical temperature $T_a$ for detonation initiation with respect to the length ratio of $r_L$, (a) low-critical cases, (b) high-critical cases.

The change of low-critical temperature with respect to the length ratio $r_L$ is plotted in figure 8 (a). It is observed that, with the decrease of the length ratio $r_L$, the low-critical temperature first decreases and then keeps constant, resulting in a minimum low-critical temperature. However, less low critical energy in the energy source is required to successfully initiate a detonation with the increase of the length ratio $r_L$, which can be clearly observed in figure 9 (a). It suggests...
Figure 9. Critical energy for detonation initiation with respect to the length ratio of $r_L$, (a) low-critical cases, (b) high-critical cases.

that the reflected shock from left boundary does have a significant effect on the scaled critical energy.

As show in figure 8 (b), the high-critical temperature needed to successfully initiate a detonation increases with the decrease of the length ratio $r_L$. This is obviously caused by the length of segment A $r_a$, as the decrease of the length ratio $r_L$, $r_a$ becomes short, in order to provide sufficient initiation energy, $T_a$ needs to be larger than before. This can also be proven in figure 9 (b), the high-critical energy in the energy source is required to successfully initiate a detonation remains unchanged with increase of the length ratio $r_L$.

4. Conclusions
The initiation of detonations through an inhomogeneous thermal explosion in a stoichiometric hydrogen-oxygen mixture diluted by 70% Argon has been systematically studied in the present study. The inhomogeneous driver section is divided into two segments, called segment A and segment B. The initial temperature in the segment A $T_a$ is varied to provide different energy to initiation detonation, and four different regimes of detonation initiation were found in the present study, namely high-critical, low-critical, low-subcritical and high-subcritical regimes. As for the low-critical and low-subcritical regimes, the reflected shock from left boundary plays an important role. However, for the high-critical and high-subcritical, rarefaction wave which is generated from the surface of segment A and B is the most important factor. In addition, the critical temperature and energy used to successfully initiate a detonation respect to the length ratio $r_L$ is also analyzed. It is found that with the decrease of the length ratio $r_L$, the low-critical temperature first decreases and then keeps constant, resulting in a minimum low-critical temperature. However, less low critical energy in the energy source is required to successfully initiate a detonation with the increase of the length ratio $r_L$. The high-critical temperature needed to successfully initiate a detonation increases with the decrease of the length ratio $r_L$, but the length ratio have no effect for the high critical energy.

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