NUMERICAL AND THEORETICAL STUDIES ON DETONATION INITIATION BY A SUPERSONIC PROJECTILE

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Conditions of detonation initiation induced by a supersonic sphere in a stoichiometric hydrogen/oxygen mixture with 70% argon dilution are investigated numerically and theoretically. Transitions of the two extremes, shock-induced combustion and detonation initiation, are examined over pressures ranging between 0.2 and 10 bar. Numerical results show a very distinct detonation initiation boundary that separates the detonable and undetonable regions. A good agreement is shown through the comparison of the numerical results with the recent experimental data. Additionally, a theoretical investigation on the determination of detonation initiation boundary is carried out by introducing a concept of the kinetic limit. The kinetic limit is defined by the ignition Damkohler number. A joint theory for the determination of the detonation initiation boundary is presented by relating the present kinetic limit defined by the unity ignition Damkohler number with the energy limit given by Lee. Comparison between the theory and the experiment over a wide pressure range shows that the detonation initiation boundary can be well defined by the present joint theory.

Introduction

Detonation initiation by a supersonic projectile has a renewed interest due to its fundamental significance in the theory of detonation and its close relevance to the operation of Ram accelerators [1]. Recent development of the supersonic propulsive device and control of the desired and undesired detonation initiation requires a clear understanding of both the mechanism of detonation initiation and the relation between the dynamic parameters such as the projectile velocity, size, as well as the mixture pressure. In the past 20 years, detailed flow regimes of supersonic blunt projectiles in combustible gases were examined by experiment and numerical simulation [2–8]. Efforts of these studies have been paid to the steady and periodic regular regimes of combustion at projectile speeds higher or slightly lower than the Chapman–Jouguet detonation velocity (CJ detonation velocity), particularly to the unstable oscillating phenomenon. However, quantitative conditions for detonation initiation are poorly understood, particularly at high pressures and subdetonative velocities.

Recently, an energy criterion defining the detonation initiation boundary induced by a supersonic projectile in an unconfined space is theoretically developed by Lee [9]. Experimental studies on detonation initiation are systematically performed by Higgins and Bruckner [10] and Belanger et al. [11]. Unfortunately, the comparison between the experimental data and the theory showed that the theory fails at high mixture pressures. In order to examine the effect of chemistry on detonation initiation, a numerical simulation with the same pressure conditions as the experiment is conducted by the present authors [12] using a detailed chemistry. Although the numerical simulation has a better agreement with the experiment [10], the experiment still shows a much lower initiation Mach number than the simulation at pressure 7.5 bar. This large difference makes the present authors question the effect of the diaphragm in the experiment. Recently, Higgins [13] improved their experimental facility by adding a buffer of argon ahead of the diaphragm on the dump tank side and matched the pressures on both sides of the diaphragm.

The object of the present work is to seek both numerical and theoretical determinations of the detonation initiation boundary and to compare it with the new experimental data.

Physical Models

As shown in Fig. 1, detonation initiation by firing a supersonic sphere into a detonable gaseous mixture is modeled by considering the shock-induced
computation or detonation with a blunt sphere fixed in an infinite supersonic flow. The inflow gas is a stoichiometric hydrogen/oxygen mixture diluted by 70% argon. The sphere diameter (D) is 12.7 mm in diameter, which is the same as that in the experiments [10,13]. The upstream and downstream boundaries are respectively D/2 and 3D from the front nose and rear surface, respectively. The outer boundary is located at 3D from the symmetric line. Curvilinear coordinate grid points generated by solving the Poisson equation are employed. The inflow Mach number varies between 2 and 5. In supersonic flow, a bow shock is formed around the blunt sphere. The bow shock induces chemical reaction and leads to an ignition behind. If the combustion wave is strong enough, the combustion wave will propagate upstream and begins to couple with the bow shock and finally results in a propagating detonation wave. If the combustion wave is not strong enough, the interaction between the two waves will be decoupled and results in a detonation failure. The interest of the present study is to determine the detonation initiation boundary over a wide range of initial pressure (0.2–10 bar).

In the numerical simulation, the two-dimensional, axisymmetric, time-dependent, chemically reactive Euler equations are implicitly solved using the LU-SGS algorithm [14]. A full chemistry, which was originally given by Stahl and Warnatz [15] and revised and tested by the authors [16] in the supersonic mixing layer, is employed. In order to exactly calculate the ignition at low temperature, where H$_2$O$_2$ is an important species, reaction H$_2$O$_2$ + H = H$_2$O + OH is supplemented. The mechanism includes 35 elementary reactions (see Refs. [15] and [16]) and 9 species (AR, O$_2$, H$_2$, H$_2$O, H, HO$_2$, OH, O, H$_2$O$_2$). Here, AR is considered reactively inert.

The Crank–Nicholson method is employed to achieve a second-order time accuracy. A CFL number of 0.2 is used in the current studies. 141 × 101 grid points are used in flow direction and its vertical direction, respectively. The upstream boundary condition is determined by specifying inflow temperature, pressure, velocity, and mole fraction of each species. At the outflow boundary, variables are extrapolated from their upstream values. On the outer boundary, variables are extrapolated from their values at inner grids. At inner boundary, sphere surface, and axis of symmetry, slip and adiabatic conditions are adopted.

In all the calculations, the converged flow field is first calculated by freezing the chemical reaction. This converged solution is then used as a start for the computation of detonation initiation. This procedure is analogous to the process of the supersonic projectile that suddenly enters the reactive mixture from the inert mixture. The unsteady disturbance due to the breaking of the diaphragm is neglected. Calculation is terminated when the leading shock wave runs out of the upstream boundary or the calculation time is longer than 1 ms, which is the largest traveling time of sphere in the detonable mixture in the experiment of Higgins and Bruckner [13].

**Numerical Results and Discussions**

Pressure contours for an inflow pressure of 1.5 bar at 0.007 and 0.018 ms are plotted in Figs. 2 and 3, respectively. The inflow velocity is 1260 m/s, which is the same as that in the experimental study [10]. At t = 0.007 ms, it can be seen that there is a pressure increase just at the front nose of the sphere. This increase is attributed to the ignition induced by the shock wave. The reaction zone (the region of pressure increase) locates far behind the standing off shock wave. At t = 0.018 ms, Fig. 3 clearly shows that the shock wave that is overdriven by the combustion wave propagates far ahead of the original location of the standing off shock wave. A subsequent
calculation shows that the propagating shock wave is coupled with the combustion wave and runs out the left boundary. This phenomenon indicates that the supersonic sphere successfully initiated a detonation wave. Therefore, the detonation velocity can be determined from the shock wave trajectory.

Figure 4 shows the trajectories of shock wave front and combustion wave front for initial pressures of 0.5 and 1.5 bar, respectively. The shock front position is defined where the local pressure is two times higher than the inflow pressure and the combustion wave is defined where the mole fraction H$_2$O is larger than 0.05. Of course, different definitions of the shock wave front and combustion may result in slightly different trajectories. However, when the propagating wave becomes quasi-steady, the definitions have no influence on the determination of detonation velocity. For initial pressure of 0.5 bar, inflow velocity is 1500 m/s, and the resulting stagnation temperature is higher than 1700 K. Ignition occurs immediately after the start of the calculation. After ignition, flame front propagates upstream and catches up to the standing off bow shock at 0.001 ms.

The shock wave is then overdriven by the chemical heat release and propagates upstream together with the combustion wave. However, from 0.002 ms, the combustion front begins to separate from the shock wave, indicating a beginning of decoupling of these two waves. As a consequence, both the propagating velocity of shock wave and combustion wave decreases. Finally, at 0.01 ms, the propagation of these two waves stops and results in a steady shock wave and combustion zone, showing the characteristics of shock-induced combustion. However, the case of 1.5 bar is quite different. The inflow velocity is 1260 m/s and the resulting stagnation temperature is about 1350 K. Ignition is slower than that of 0.5 bar. The combustion wave propagates upstream and overdrives the shock wave at almost constant velocity. No separation and decoupling process that is shown at 0.5 bar occur here. The resulting velocity relative to the inflow gas is 1673 m/s, which is within 2% of the CJ detonation velocity of 1703 m/s. This is a clear indication of a successful detonation initiation by a blunt sphere in a supersonic stream.

A boundary that separates the detonable and un-detonable region can be obtained by calculating all the shock-wave trajectory at projectile velocities below the CJ detonation velocity over pressures between 0.2 and 10 bar. A comparison between the numerical results and the experimental data obtained with [13] and without [10] an argon buffer is shown in Fig. 5. The argon buffer region is added to remove the pressure difference on both sides of the diaphragm of the test chamber. It can be seen that
the initial pressure jump across the diaphragm between the dump tank and the test chamber dramatically affects the measured critical Mach number for detonation initiation. The improved experiment with an argon buffer gives a lower detonation initiation Mach number on the low-pressure side but a higher initiation Mach number on the high-pressure side than the experiment without buffer. This discrepancy increases with an increase of the mixture pressure. At the mixture pressure of 7.5 bar, the experiment without buffer indicates that detonation can be initiated even when the projectile is as slow as Mach 2, which is too slow to ignite the mixture based on the stagnation temperature. However, the experiment with an argon buffer shows that the projectile below Mach 3.2 is unable to initiate detonation. This large difference is produced by the occurrence of the unsteady shock wave traveling from the high-pressure test chamber side to the low-pressure dump tank side when the projectile breaks the diaphragm and enters the test chamber at the experiment without buffer.

Because both the present numerical simulation and the theory exclude the occurrence of this unsteady shock wave, the experimental data with an argon buffer should be used when a comparison between the experiment and numerical simulation is made. As shown in Fig. 5, the present numerical results agree reasonably well with the experimental data on the high-pressure side, particularly at pressures 1.5 and 7.5 bar. On the low-pressure side, numerical results show a detonation limit of 0.65 bar, which agrees well with the limit of 0.8 bar obtained by the experiment. Furthermore, numerical data show there is a minimum critical Mach number near the mixture pressure of 0.8 bar. For mixture pressure below it, the predicted critical Mach number increases rapidly. This minimum critical Mach number corresponds to the second explosion limit of the hydrogen/air mixture, and the rapid increase of it is determined by the energy limit that will be discussed in the next section.

Theory for Detonation Initiation

Energy Limit

A theoretical study to estimate the energy limit required for direct detonation initiation of detonation by a supersonic projectile is conducted by Lee [9] using the hypersonic blast wave analogy. The theory equates the critical energy per unit length required for a cylindrical detonation initiation to the work done by the drag per unit length. Using the ideal blast solution to give the blast trajectory and assuming that the blast radius must be at least equal to a critical radius \(3.2\lambda\), the critical energy per unit length for the initiation of a cylindrical detonation is given by Lee as

\[
E_0 = 14.5p_0M_{CJ}^2\lambda^2
\]

where \(p_0\) is the mixture pressure and \(M_{CJ}\) is the Mach number of CJ velocity normalized by the sound speed \(c_0\) of the undisturbed mixture. \(\lambda\) is the detonation cell size.

On the other hand, the work per unit length done by the projectile at the critical Mach number \(M_{cr}\) is

\[
E_d = \frac{1}{2} \rho_0 \pi \eta^2 M_{CJ}^2 \left( \frac{\eta d^2}{4} \right) C_D
\]

where \(C_D\) is the drag coefficient and takes on a numerical value of 0.92 for a hypersonic sphere. \(\rho_0\) is the mixture density, and \(d\) is the diameter of the sphere. By equating the work done by the drag force per unit length to the critical energy for direct initiation of cylindrical detonation, the critical Mach number is given as [9]

\[
M_{cr} = M_{CJ} \left( \frac{116}{\gamma C_D d} \right)^{\frac{1}{2}} \lambda
\]

where \(\gamma\) is the ratio of the specific heats. Therefore, for given projectile diameter and mixture pressure, detonation initiation Mach number can be calculated directly from equation 3.

A comparison between the theory and the experiment is shown in Fig. 6. It can be seen that the theory agrees well with the experiment on the low-pressure side. However, for mixture pressure higher than 1.0 bar, the theory gives a much lower value than the experimental data. The reason for this discrepancy has been discussed in detail in our previous study [12]. Our conclusion is that the energy limit given by equation 3 does not include the requirement for auto-ignition. Therefore, quantitative determination of the detonation initiation needs another limit, the kinetic limit, which states the
requirement of the shock compression for auto-ignition.

Kinetic Limit Defined by the Unity Ignition Damköhler Number

In experimental determination of the detonation boundary, the test chamber has a finite dimension and thus the traveling time of the supersonic sphere in the test chamber will be limited both by the projectile speed and by the dimension of the test chamber. Therefore, a success of detonation initiation observed in experiment must require that the mixture should be ignited by the projectile at least within the traveling time. This requirement provides a natural definition of the kinetic limit (ignition limit) using the unity ignition Damköhler number as

\[ D_{\text{sig}} = \frac{\tau_0}{\tau_r} = 1 \]  

(4)

where \( \tau_0 \) is the traveling time of the supersonic sphere in the test chamber, \( \tau_r \) is chosen to be the auto-ignition time at the stagnation temperature \( T^* \) and at the pressure \( p^* \) behind the standing bow shock (this pressure rather than the total pressure is chosen for the weaker dependence of ignition time on pressure than on temperature). Thus, the detonation initiation Mach number can be determined by the following relation

\[ \tau_{\text{ig}} (p^*, T^*) = \frac{L}{M_{cr} c_0} p^* p_0 \left[ 1 + \frac{2}{\gamma + 1} (M_{cr}^2 - 1) \right] \]

\[ T^* = T_0 \left( 1 + \frac{\gamma - 1}{2} M_{cr}^2 \right) \]  

(5)

where \( L \) is the dimension of the test chamber; \( p_0 \) and \( T_0 \) are, respectively, the initial pressure and temperature of the mixture; and \( c_0 \) is the sound speed. With the initial values of \( T_0 \) and \( p_0 \) and a presumed value of \( M_{cr} \), a new \( M_{cr} \) can be calculated from equation 5. After several times of iterations, the critical Mach number for a given mixture pressure can be easily obtained.

The ignition time \( \tau_{\text{ig}} \) can be obtained both asymptotically and numerically. Numerical simulation shows that equation 4 can only be satisfied in a temperature range of \( T^* \) between 850 and 1050 K. This temperature is the same order with the crossover temperature, \( T_c \), defined by the competition between reactions \( H + O_2 \rightarrow OH + O \) (a) and \( H + O_2 + M \rightarrow HO_2 + M \) (b) for the ignition of the hydrogen/oxygen mixture. In this regime, the ignition time can be asymptotically expressed as \([17]\)

\[ \tau_{\text{ig}} = \left( \tau_0 + \frac{1}{A} \ln \frac{1}{K_c(T^*) c_{O_2}} \right) \]  

(6)

where \( \tau_0, A, \) and \( B \), are, respectively, the nondimensional time and functions of temperature. \( K_c \) and \( c_{O_2} \), are, respectively, the rate coefficient of reaction (a) and the initial oxygen concentration. As shown in Fig. 7, the kinetic limits calculated by both the numerical method and the asymptotic method agree well with the experimental data on the high-pressure side, although the asymptotic method slightly under predicts the critical Mach number.

Theory for Detonation Initiation

We have shown that the energy limit defined by Lee [9] gives a reasonable detonation boundary at low pressure while it fails at high pressure (Fig. 6). On the other hand, we also have shown that the kinetic limit can well define the detonation initiation boundary at high pressure but fails at low pressure (Fig. 7). These two facts suggest that a joint theory for detonation initiation can be built by combining the energy limit requirement with the kinetic limit requirement:

\[ M_{\text{cr}} = \frac{L}{\tau_{\text{ig}} (p^*, T^*) c_0} \]  

(7)

\[ M_{\text{cr}} = M_{CJ} \sqrt{\frac{\gamma}{2 \gamma - 1}} \frac{\lambda}{\sqrt{C_p D}} \]  

(8)

This definition is physically reasonable because a successful detonation initiation not only requires a shorter ignition time than the traveling time but also needs a larger energy input, the work done by the drag, than the minimum energy for the direct initiation of a cylindrical detonation wave. Therefore, the critical Mach number should be the larger of the two given in equations 7 and 8.

The comparison between the present joint theory...
with the experiment is given in Fig. 8. The upper-right region of curve AOB corresponds to the detonable region, and the lower-left part of curve AOB is the undetonable region. It can be seen that the detonation boundary AOB defined by the present joint theory agrees well with that measured by the experiment.

Conclusions

The problem of detonation initiation by a supersonic sphere is investigated numerically and theoretically. Comparison between the numerical results and the experimental data obtained with and without buffer shows that the pressure jump across the diaphragm between the test chamber and the dump tank in experiment has a dramatic effect on the measured results, particularly at high pressure. The numerical results reasonably agrees with the experimental data using an argon buffer. The theory presented by Lee correctly predicts the detonation initiation condition at pressures below 1 bar but no longer gives appropriate values as the pressure increases. A condition for kinetic limit of auto-ignition is shown to be required to quantitatively determine the detonation initiation boundary. A kinetic limit defined by the unity ignition Damköhler number reproduces well the experimental data. A joint theory presented by combining the kinetic limit and the energy limit agrees very well with the experiment. This agreement shows that a successful detonation initiation requires not only that the work done by the drag force of the projectile is larger than the minimum energy for direct initiation of a cylindrical detonation wave to keep from the decoupling of the shock wave and the combustion wave but also that the auto-ignition time at the stagnation temperature is shorter than the traveling time of the projectile in the test chamber. Future research is needed to address how the confinement of the test chamber affects the critical Mach number at high pressure.

REFERENCES

Andrew Higgins, McGill University, Canada. The difference between results with and without the buffer is not due to a shock wave traveling from the high-pressure test chamber to the low-pressure dump tank nor is it due to the flow of gas induced by the venting of the high-pressure gas into the dump tank. The supersonic projectile would outrun any rarefaction generated by venting. Rather, the initiation of detonation at anomalously low Mach numbers in the case without the buffer section is due to an unsteady shock sent into the test pressure gas by direct impact of the sphere on the diaphragm [1].

Also, the projectile transit time across the chamber is not the correct time scale to use in defining a Damköhler number. In all the experiments, initiation occurred within the first half of the chamber and in the case of the kinetic limit was extremely prompt, happening within a few μs.

Finally, the Lee theory does not fail at pressures greater than 1 bar. Pressure is not a relevant parameter, but rather velocity. The Lee–Vasiljev theory was formulated for superdetonative projectiles, where shock strength is always well above the autoignition temperature.

REFERENCE

Author’s Reply. Ref. [1] suspected the effect of the unsteady shock wave. However, this shock wave does not increase the total enthalpy that improves ignition. In addition, we need to know that ignition does not necessarily start in the front nose of the sphere. Recent experiment and simulation [2] shows that the high-pressure gas expansion through the diaphragm strongly affects the shock strength. Further direct experimental observations are necessary to understand this issue.

The transit time should be the time scale to define the Damköhler number in considering the detonation initiation in a closed chamber. Furthermore, ignition should occur within the first half of the chamber for a successful observation of the initiation. It should be noted that the kinetic limit is the bottom line of the initiation boundary. Initiation cannot occur below this boundary.

It should be realized that Lee theory is correct for a cylindrical detonation wave where ignition is already started. However, in discussing the detonation initiation below the detonation velocity in a finite chamber (the interest of Ref. [1] and the present paper), we need to consider the kinetic limit and the curvature effect of the combustion wave.

REFERENCE

Longting He, Princeton University, USA. The initiation of cylindrical or spherical detonation is controlled by the nonlinear curvature effect [1,2]. For successful initiation, the ignition source must be able to drive a detonation beyond the critical curvature radius, Re. The initiation of detonations by a supersonic blunt body corresponds to cylindrical detonation initiation only when the size of blunt body is smaller than Re and when the velocity of blunt body is much longer than the Chapman–Jouguet detonation velocity. At high pressure, the critical curvature radius becomes of the same order as the size of the blunt body. The initiation by the blunt body at high initial pressure is therefore close to planar detonation initiation, which is controlled by kinetic limits.

REFERENCES

Author’s Reply. Your comment is right when the sphere is much smaller than Re, and thus, the work done by the drag force is negligible. However, the sphere radius is 6.35 mm, which is comparable with Re at low pressure (say 1 atm). Numerical results confirmed that an onset of successful initiation occurs immediately after the catch up of the combustion wave with the bow shock. Therefore, the external work done by the sphere plays an important role to the onset of the detonation. As a result, the critical radius will be less than the predicted value. On the high-pressure side, the chemical heat release is large enough to balance the curvature effect for R > 6.35 mm. Therefore, only the kinetic limit is necessary.