Numerical Studies on Cellular Detonation Wave Subjected to Sudden Expansion

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Abstract

One of the primary concerns in the design of PDEs is that a successful transmission of detonation wave from a narrow pre-detonation chamber to a large main chamber. This problem is investigated in the present paper by simulating the fate of a two-dimensional detonation wave when it is subjected to a sudden expansion. It is found that the reflection of transverse waves at the walls and their collision within the chamber are critical in sustaining a detonation wave in a wider channel. Results obtained for both successful and unsuccessful transitions are presented and the role of transverse waves is discussed.

Introduction

Pulse Detonation Engines (PDEs) operate at a higher thermal efficiency than the conventional constant pressure combustion engines. PDEs also provide a very high specific impulse thrust at operating frequencies of a few hundred Hz. They can be designed without the use of any rotating machinery or valves in the flow path. However, the design and operation of the PDEs is complicated by the unsteady, high-speed, pulsed combustion. In order to reduce the deflagration-to-detonation transition time, it is generally accepted that the combustible mixture in the main chamber needs to be ignited using detonation wave that was generated in a much-smaller, pre-detonation chamber. One of the primary concerns in the design of PDEs is that a successful transmission of detonation wave from pre-detonation chamber to main chamber. This problem is investigated in the present paper using numerical techniques.

The detailed cellular structure of gaseous detonations has been studied using experimental techniques in 1960’s. However, only in the late 70’s Taki and Fujwara [1] and latter Oran et al. [2] were able to simulate the cellular detonation structure for the two-dimensional case numerically. The cellular structure was established in their numerical computations by subjecting a one-dimensional ZND (Zeldovich, von Neumann, and Doring) wave to a large perturbation (by providing inhomogeneous region with different chemical properties). Once disturbed, the two-dimensional cellular structure develops naturally and it was found that the cell size is independent of the strength and the number of perturbations. In other words, cells can be newly generated when fewer than initial perturbations are provided, and if more than the stable number of cells are generated initially from the perturbations, some will get attenuated and eventually vanish to give the same stable number of cells. Thus, the number of cells in a cellular detonation wave is a consequence of the chemistry of the problem which is characterized by the reaction zone length scale for the ZND wave. The cell size is also found to be independent of the channel width, suggesting that doubling the channel width gives twice the number of cells across the width of the channel.

An important concern in using cellular detonation wave as a source for the burning of the reactants stems from the stability of the cellular detonation wave. Experimentally it was found that the stability of the detonation wave increases with tube diameter. In other words, the stability of a detonation propagating in a tube where the diameter is one cell size (λ) is not the same as a detonation with 13 cells propagating in a tube whose diameter is 13λ. The latter is found to be extremely stable even to large perturbations. For example, a sudden increase in the tube diameter will not quench the detonation, if \( d > 13\lambda \). On the other hand, propagation of a one-cell detonation in a tube with \( d \sim \lambda \) is found to be in the limiting conditions. As shown by St-Cloud et al. [3] and Moen et al. [4], a finite perturbation may lead to complete destruction of such detonations. Therefore, a small but sudden increase in tube diameter may result in a deflagration wave. In the present paper the stability of the detonation wave is investigated by numerically simulating the expansion of detonation having different number of cells.

The governing equations used are of the Euler type with exothermic chemical reactions. They can be expressed in the following form

\[
\frac{\partial q}{\partial \tau} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + H = 0. \tag{1}
\]
Above equation represents conservation equations for mass, momentum, energy and the two progress variables depends on the variable ($p, \rho, u, v, e, \rho u, \rho v$, and $\rho\alpha$) used as $q$.

The gas mixture considered here is a stoichiometric hydrogen-oxygen fuel diluted with Ar/He by 70%. This mixture is known to generate a well-behaving detonation. The hydrogen-oxygen reactions are represented by the Korobeinikov model consisting of two-step reaction mechanism; 1) a non-exothermic irreversible induction reaction where the progress variable ($\alpha$) changes from 1 to 0, and 2) an exothermic irreversible recombination reaction with its progress variable ($\beta$) changing from 1 to $\beta_{eq}$. This two-step reaction model has been successfully applied in the past to address two-dimensional unsteady detonation problems [1,5]. The Chapman-Jouguet (C-J) Mach number of the premixed gas mixture considered is 4.8. A grid system that moves at an uniform velocity of C-J value is used.

The present simulation used an explicit 2nd-order MacCormack predictor-corrector technique with 4th-order FCT (Flux Corrected Transport) scheme for capturing the shock waves accurately. All the calculations were started from a plain ZND detonation wave. A stable multi-dimensional detonation wave was generated by placing a few exothermic spots just upstream of the leading shock front. These exothermic spots perturbed the plane C-J wave and developed transverse waves. Once the propagation of detonation became stable it was then subjected to a sudden expansion having different area ratios. By using different size main chambers, studies on the survivability of detonation in the expansion environment were performed. The grids are constructed with $\Delta x = \Delta y = 2L/9$. Here, $L$' is the induction length—a characteristic distance related to the unburnt gas mixture.

Results and Discussion

Calculations were initially made for a channel width of $9L'$. A stably propagating detonation having two transverse waves was established after ~1000 time steps. The interaction between the transverse and detonation waves results in a triple-shock structure and thereby a cellular detonation front. As the detonation propagates, these transverse waves travel toward the walls and reflect back when they interact with the walls. The structure of the detonation front propagating in the $9L'$ channel is shown in Fig. 1 at three instants. The iso-pressure plots shown in Figs. 1(a), 1(b), and 1(c) visualize the motion of the two triple shock structures between the lower and upper walls. Note that the grid system is moving at Chapman-Jouguet velocity and the detonation front is always located in the same region with a small amount of fluctuations resulting from the deviation in local propagation velocity. The wave velocities obtained at upper and lower walls and at the mid section are plotted in Fig. 2. This shows that the reflection of a triple shock from the wall and the interaction between two triple shocks resulting in similarly enhanced combustion (increased propagation velocity) locally. However, the average non-dimensional propagation velocity is 4.96, which is close to the C-J velocity for the mixture considered.

Calculations were continued further on this detonation by suddenly increasing the channel width to $18L'$. Results in the form of iso-pressure plots are shown in Fig. 3 at six different instants during the expansion process. It is clear that the detonation has transmitted successfully into a $18L'$-wide channel from a $9L'$-wide one. The entire transmission took about 100 µs and another 75 µs to establish a regular cellular structure in the $18L'$-wide channel that is appropriate for that size. Note from Figs. 3(b) and 3(c) that while the detonation wave tends to dissipate in the larger tube, the propagation of higher-energy, triple-shock intersection points tends to strengthen the detonation. After a few passes of these intersection points on the detonation wave front, the latter establishes into a self-sustained wave with three triple-shock intersections.

The velocity modulation at the detonation wave front in the bottom, mid and top sections during the transition period are shown in Fig. 4 and those for the stable detonation in the larger tube are shown in Fig. 5. The higher-than-usual jumps in velocity in Fig. 4 indicate the formation of super-energy detonations. The smaller jumps in velocity at the tube mid section in Fig. 5 suggest that triple-shock points are not interacting at that location due to the odd number of cells. Similar calculations performed for main chambers > $18L'$ could not yield successful transmission for detonation wave. An example of such unsuccessful transmission is shown in Figs. 6 and 7. In this calculation the channel size was suddenly increased from $9L'$ to $20L'$. As evident from Fig. 6(e), the reflection of transverse waves near the walls could not produce detonation wave and as a result the combustion waves further weakened as they propagated back into the channel.

References

Fig. 1. Structure of detonation wave in a 9L*-wide channel at (a) t₀ μs, (b) t₀+1.6 μs, and (c) t₀+3.2 μs.

Fig. 2. Propagation velocity at different locations for 9L*-wide channel.

Fig. 3. Transmission of detonation wave from 9L*-wide to 18L*-wide channel. (a) 0, (b) 2.6, (c) 5.2, (d) 13, (e) 36, and (f) 175 μs.

Fig. 4. Detonation propagation velocity at different locations during sudden expansion.

Fig. 5. Detonation propagation velocity at different locations for a 18L*-wide channel.
Fig. 6. Transmission of detonation wave from 9L*-wide to 20L*-wide channel. (a) 0 µs, (b) 2.8 µs, (c) 6.2 µs, (d) 11 µs. After 8 µs, detonation failed in the larger channel.

Fig. 7. Propagation velocity at different locations in 20L*-wide channel during sudden expansion.