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High resolution WENO simulation of 3D detonation waves

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A B S T R A C T

In this paper, we develop a three-dimensional parallel solver using the fifth order high-resolution weighted essentially non-oscillatory (WENO) finite difference scheme to perform extensive simulation for three-dimensional gaseous detonations. A careful study is conducted for the propagation modes of three-dimensional gaseous detonation wave-front structures in a long square duct. The numerical results indicate that, the instability of detonation, overdrive factor, transverse dimension and initial perturbation are the main factors that influence the appearance of spinning detonation. For unstable detonation with an overdrive factor $f = 1.0$, with the duct width decreasing, the transverse modes tend to be the lower ones. When the duct width is sufficiently small, detonation propagation is coupled to the lowest transverse mode in order to sustain itself. There is a maximum duct width for the appearance of spinning detonation. When the duct width is smaller than this value, the unstable detonation propagates in a spinning mode. When the duct width is larger than this value, spinning detonation disappears. For highly unstable detonation with an overdrive factor $f = 1.2$, the formation of the spinning detonation does not depend on the initial perturbation and it only depends on the high instability of detonation and channel dimension in the transverse directions. Both initial rectangular modes and initial diagonal modes can eventually evolve into spinning modes. For mildly unstable detonation with an overdrive factor $f = 1.6$, it is easier for the initial diagonal mode to trigger the spinning mode than for the initial rectangular mode. The formation of spinning detonation thus not only depends on the high instability of detonation and channel dimension in the transverse directions, but also depends on the initial perturbation. For the stable detonation with an overdrive factor $f = 1.1$, when the initial perturbation is in the transverse cosine mode, the front of the stable detonation has a rectangular structure and slapping waves appear on the walls. When the initial perturbation is in the symmetrical mode along the diagonals of the detonation front, the diagonal detonation is formed and the slapping waves on the walls disappear.

1. Introduction

Detonation is a complex supersonic flow phenomenon. Its front consists of a precursor shock wave that propagates into the unreacted medium at supersonic speed with a thin reaction zone immediately behind the shock. The precursor shock compresses the unreacted medium and increases its temperature. Burning occurs behind the front, which can release a large amount of heat that in turn supports the precursor shock wave to keep propagating forward.

Numerous experimental and numerical studies have been performed to study detonation. However, detailed numerical studies on detonation mostly remain in two-dimensional simulations. As is well known, detonation is essentially a three-dimensional phenomenon, and some important structural features cannot be obtained from two-dimensional simulations, such as the slapping waves and spinning structures. Unfortunately, a highly refined grid resolution is required for such computation, especially for unstable detonation, which makes three-dimensional numerical simulation of detonation tremendously computing-resource intensive. In this paper, we attempt to address this difficulty by developing a high order accurate weighted essentially non-oscillatory (WENO) solver with parallel implementation so that the desired wave structures can be resolved within acceptable computational time. WENO schemes have the advantage of high order accuracy and robust, sharp, and essentially non-oscillatory shock resolution [1–4].

Previous research in the literature indicates that the heat of the reaction, the activation energy, the overdrive factor and the ratio of specific heat all have some effects on the stability of detonation and cellular patterns [5,6]. Bourlioux et al. [7], Papalexandris et al. [8], He and Karagozian [9], and Daimon and Matsuo [10] carried out numerical simulation of one-dimensional detonations. Guirguis et al. [11], Bourlioux and Majda [12], Papalexandris et al. [13], Gamezo et al. [14], Hwang et al. [15], and Shepherd

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et al. [16] carried out numerical simulation of two-dimensional detonations. These numerical simulations have investigated the instability of detonation in details and have drawn some very important conclusions. The instability of detonation waves leads to irregular cellular structure which is caused by the transverse development of triple points (triple point lines in three-dimensional detonation waves) along the front. For unstable detonations, a very small initial perturbation will quickly develop transversely with time. Therefore, with different reactive parameters, such as the heat of reaction, the activation energy and the overdrive factor, and with a given initial perturbation and geometrical configuration, the detonation front structure may have different evolution processes, and hence the detonation modes may be different.

Detailed experimental study on three-dimensional gas detonation structures has been conducted as early as in the 1960s [17,18]. Recent numerical simulations and experimental results have shown that there are three main types of cellular detonation structures, namely rectangular, diagonal, and spinning modes [19,20]. Hanana et al. [21], by experimental study, pointed out that in rectangular tubes at least two types of detonation structures exist, namely the rectangular and diagonal structures. Through the soot-foil tracks on the walls, they showed the diamond-shaped cellular patterns. They also showed that the rectangular structure is characterized by straight triple lines emanating from the leading front that are parallel or orthogonal to the walls of the flow domain. Another characteristic feature is the occurrence of slapping waves on the walls. When the movement direction of the triple-line is along the diagonal line, the detonation front has a diagonal structure, and the direction of the transverse wave propagation has a 45° angle with the wall, while on the wall the slapping waves would disappear. They believed the ignition method was the key factor for the formation of different detonation modes. However, they did not give the relationship between different detonation modes, the front features of different detonation modes and the mechanism of their generation. Williams et al. [22] adopted a one-step reaction model and performed numerical simulation of three-dimensional detonation in a rectangular duct, and observed the front rectangular structure. Tsuboi et al. [23] carried out three-dimensional numerical simulation of detonation propagation in the rectangular duct, and further confirmed the detonation is divided into in-phase rectangular and out-of-phase modes. Deledicque and Papalexandris [24] studied the rectangular and diagonal structures of detonations in a three-dimensional rectangular tube by using a one-step chemical reaction model. When the overdrive factor $f = 1.1$, the heat of reaction $Q = 2.0$, and the activation energy $Ea = 20$, the detonation is in a rectangular out-of-phase mode under the transverse sinusoidal perturbation, and out-of-phase "slapping waves" are formed on the walls which are mutually perpendicular in the square tube. When they used a constant perturbation along the diagonals of the front, a diagonal detonation was formed. They also studied the rectangular mode of the unstable detonation for the activation energy $Ea = 50$, the heat of reaction $Q = 50$, and the overdrive factors $f = 1.2$ and $f = 1.6$ under a sinusoidal perturbation, but they did not study the evolution of the two unstable detonation fronts in perturbation along the diagonals of the front.

Campbell and Woodhead [25] identified the phenomenon of spinning detonations in small-diameter tubes near the detonation limits. They found that the pitch of the spin is about three times the diameter of the pipe, see also [26]. Lee et al. [27] observed a single-headed spinning detonation in a square channel through the soot-foil record, and the single helical trajectory from the four side walls of the square channel is unfolded to show the same soot characteristics as in the round duct. Recently, studies have revealed more information on spinning detonation in rectangular channels and round tubes [23,28–36]. Zhang et al. [26,30] conducted experimental studies on the two-phase flow detonation in a round tube, and showed that in a stable propagation of detonation, the transverse wave has played a leading role. Huang et al. [31] conducted experiments on spinning detonations with a detailed analysis of the shock structure. Experimental results indicate that the actual structure of the spinning detonation tries to match closely to the condition, where the state parameters (pressure and temperature) reach their maximum values. Tsuboi and co-workers [23,36–38] also carried out extensive numerical simulations on the detonation in round tubes and rectangular ducts. They pointed out that the formation of an unburned gas pocket behind the detonation front was not observed in their results because the rotating transverse detonation completely consumed the unburned gas. Dou et al. [39,40] investigated spinning detonation in narrow channels and detonation structures under different initial perturbations by numerical simulation. Their numerical results showed that the spinning detonation only exists in narrow channels. When the channel width is large enough, the spinning detonation goes away. These studies on the spinning detonation do not consider modes of propagation of detonation waves in tubes of different widths or when different chemical reaction parameters are selected. Therefore, with different chemical reaction parameters, the dynamical behavior and spinning mechanism of the spinning detonation remain unclear, and whether a change in duct width and initial perturbation can trigger spinning detonation warrants further study.

The main objective of this paper is to simulate numerically the detonation modes in different square tubes, with different chemical reaction parameters and under different initial disturbances, to provide a detailed front structure description for each detonation mode, to find out critical channel width for the appearance of spinning detonation, to investigate the effect of the overdrive factor on spinning detonations and to reveal factors that influence the transition from diagonal to spinning modes.

Before ending this introduction section, we would like to remark that recent study by Taylor et al. [41] indicates that a one-step overall reaction mechanism may not be able to give quantitatively correct descriptions of unstable detonations under extreme pressures and temperatures. The conclusions obtained in this paper are nevertheless expected to give at least qualitatively correct descriptions of the detonation features.

2. Governing equations and the WENO algorithm

The governing equations are the three-dimensional Euler equations with a source term that represents chemical reactions. In conservation form, these equations may be written in the compact form

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} + \frac{\partial H(U)}{\partial z} = S \tag{1}$$

where the conserved variable vector U, the flux vectors F, G, and H as well as the source term S are given, respectively, by

$$U = (\rho, \rho u, \rho v, \rho w, \rho E, \rho Y)^T \tag{2}$$

$$F(U) = (\rho u, \rho u^2 + p, \rho u v, \rho u w, \rho u(E + p/\rho), \rho u Y)^T \tag{3}$$

$$G(U) = (\rho v, \rho v u, \rho v^2 + p, \rho v w, \rho v(E + p/\rho), \rho v Y)^T \tag{4}$$

$$H(U) = (\rho w, \rho w u, \rho w v, \rho w^2 + p, \rho w(E + p/\rho), \rho w Y)^T \tag{5}$$

$$S(U) = (0, 0, 0, 0, 0, \rho\omega)^T \tag{6}$$

$$E = \frac{RT}{\gamma - 1} + YQ + \frac{1}{2}(u^2 + v^2 + w^2) \tag{7}$$

$$\omega = -K\rho Y e^{-(Ea/RT)} \tag{8}$$

$$p = \rho RT \tag{9}$$