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High resolution numerical simulation of triple point collision and origin of unburned gas pockets in turbulent detonations

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ABSTRACT

A key issue in pulse detonation engine development is better understanding of the detonation structure and its propagation mechanism. Thus, in the present work the turbulent structure of an irregular detonation is studied through very high resolution numerical simulations of 600 points per half reaction length. The aim is to explore the nature of the transverse waves during the collision and reflection processes of the triple point with the channel walls. Consequently the formation and consumption mechanism of unreacted gas pockets is studied. Results show that the triple point and the transverse wave collide simultaneously with the wall. The strong transverse wave switches from a primary triple point before collision to a new one after reflection. Due to simultaneous interaction of the triple point and the transverse wave with the wall in the second half of the detonation cell, a larger high-pressurised region appears on the wall. During the reflection the reaction zone detaches from the shock front and produces a pocket of unburned gas. Three mechanisms found to be of significance in the re-initiation mechanism of detonation at the end of the detonation cell; i: energy resealed via consumption of unburned pockets by turbulent mixing ii: compression waves arise due to collision of the triple point on the wall which helps the shock to jump abruptly to an overdriven detonation iii: drastic growth of the Richtmyer–Meshkov instability causing a part of the front to accelerate with respect to the neighbouring portions.

1. Introduction

Detonation combustion is an efficient means of burning propellant mixtures to release the chemical energy content. The very rapid energy conversion associated with detonation combustion can lead to more compact and efficient propulsion system designs relative to conventional systems presently in service. Recent interest in pulse detonation engines (PDEs) has resulted in several experimental and theoretical studies related to realizing multicycle detonations in tubes that simulate engine operating conditions [1–7]. These studies make a clear case that pulse detonation engines provide the potential for higher specific impulse, reduced complexity, and lower operational costs as compared to current gas turbine technology.

The pulse detonation engine (PDE) is an unsteady propulsion system that uses repeated detonation to generate thrust. The basic element is a tube that can be closed at one end by some sort of valve and open at the other. The basic cycle of operation is: i) the tube is filled with reactants, ii) a detonation is initiated and propagates through the tube, iii) the combustion products flow out of the tube, and iv) the tube is purged and refilled with reactants (e.g. [1,3,7]). The flow in a PDE is a challenging research problem, because

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it involves compressible, chemically reactive flow in complex geometrical configurations with moving boundaries. The goal of the present study is to study the successful propagation of a detonation in a tube that is crucial to the successful operation of the engine. In order to do that, we have to carry out a fully unsteady treatment of the flow processes within the tube.

A detonation is a violent chemical reaction that proceeds through the reacted material toward the unreacted material at supersonic velocity. The supersonic combustion event propagates at high velocities and produces a rapid and violent combustion of the reactants due to the strong shock wave leading the detonation. In a detonation the combustion reaction and shock wave propagation proceed in a totally coupled and mutually supporting manner. The shock imposed on the unreacted material by the supersonic combustion wave causes a rapid heating and subsequent combustion of the reactants to sustain the reaction [8–10].

Experiments have demonstrated that most self-sustaining detonations are intrinsically unstable with three-dimensional time dependent cellular structure [11]. The lead shock consists of weak incident wave and stronger Mach stem intersect at triple point with the transverse waves, which sweep laterally across the leading shock and collide with each other. The shear layer separates gas streams that have passed through portions of the lead shock with different strengths. The leading wrinkled shock consists of alternate weak incident shocks, stronger Mach stems and transverse waves that are interact at so-called triple points. Two types of detonation structure, weak and strong, corresponding to two distinct types of transverse wave are observed in experiments [11]. In the weak structure, the transverse wave is relatively weak and unreactive emanating from the triple point and extends back into the downstream flow. In strong structure, a portion of the transverse wave close to the triple point can act as a detonation itself that has its own transverse wave. In the previous numerical and experimental investigations, (e.g. [12–21]) both weak and strong types of structure have been observed. Trotsyuk [9] studied numerically studied the structure of detonation wave in hydrogen–oxygen–argon mixture within a wide range of initial pressures. The detonation cell size, its shape, and the relative height of the detonation front roughness were in good quantitative agreement with experimental results. For the case where the channel height is 1.5 times of the detonation cell and mixture with 60% argon dilution he observed trajectory of secondary triple point in the numerical smoked foil with two primary transverse waves and two secondary waves, indicating the existence of strong type transverse wave in detonation front. In another study Vasil'ev et al. [22] studied numerically the two-dimensional structure of the detonation wave in a stoichiometric hydrogen–oxygen mixture with addition of with addition of H_2O_2. They observed that in addition to an ideally regular structure with two practically symmetric transverse waves, there are also smaller and less intense disturbances on the wave front, which generates a system of weaker transverse waves. These transverse waves violate the flow symmetry in the wave front and also lead to additional curving of the shape of the leading shock front.

Strehlow and Crooker [17] observed regular structure detonation in hydrogen–oxygen–argon mixture and found that upon collision of a triple point with a wall, the structure was of the weak type. After some time the structure tended to develop a strong type structure. Importantly, the collision and reflection processes of a triple point with a channel wall or another triple point occur in a small region and within very short time. It is therefore extremely hard to capture these experimentally. Hence, numerical simulations are used to properly study the structure configuration in such processes. Furthermore, simulations need very high spatial and temporal resolutions to capture the small structures formed in this problem. So far only few numerical simulations have been performed on the collision and reflection of the triple points. Lefebvre and Oran [13] found that after the collision of a triple point, the structure was a single-Mach configuration with an associated weak transverse wave. However, as the structure evolved it changed to a double-Mach with more complex configuration, where a few kinks appeared along the strong transverse wave. Oran et al. [14] performed two-dimensional computations in a low-pressure mixture of hydrogen and oxygen and suggested the presence of a strong structure of regular detonation. Yet due to low grid resolution the structure configuration around the triple point was not so well identified.

Sharpe [16] used high spatial resolution of 64 cells in half reaction length and examined a regular structure of detonation in hydrogen–oxygen–argon mixture. He found that the detonation structure was of double-Mach configuration strong-type with no change in the structure configuration before and after collision of the triple point with a wall. He further commented that a very high spatial resolution was required to clarify the structure correctly. Hu et al. [12] conducted a two-dimensional numerical simulation with resolution of 440 cells per reaction zone length to acquire the detonation structure in regular structure detonation. They concluded that the structure configuration did not change much before and after the collision process, such that the single-Mach configuration appeared after the collision. However, it changed quickly to a double-Mach configuration. They further commented that a sufficiently high-resolution and detailed chemical reaction model are both essential to resolve the structure configuration around the triple point.

In summary, the above numerical simulations determined the structure configuration of laminar detonations characterised by their regular structure. It was found that during the structure evolution process the structure configuration remained unchanged after collision which was double-Mach configuration of strong type. However, both experimental and numerical results indicate the presence of two different types of structure in the mixtures with different activation energies. Smoke-foil technique has displayed irregular transverse wave spacing for high activation energy mixtures and regular cellular structure for low activation energy mixtures [18]. The transverse wave spacing or (i.e. cell regularity) depends on, the mixture composition, initial and boundary conditions [23]. Experiments also revealed that in contrast to the regular structure detonations, there exists an intense chemical activity in the vicinity of the