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NUMERICAL SIMULATION TO INVESTIGATE THE EFFECT OF OBSTACLE ON DETONATION WAVE PROPAGATION IN A PULSE DETONATION ENGINE COMBUSTOR

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ABSTRACT

Pulse detonation technology can be a revolutionary approach for propulsion system since it offers significant fuel efficiency, higher thrust to weight ratio and low cost. Although the design concept of a pulse detonation engine is comparatively simple, but the development and stabilization of sustainable detonation wave front is difficult. Consequently pulse detonation engine technology is still in active research stage. To accelerate the development of pulse detonation engine, there is a need to carefully pursue the experimental analysis of pulse detonation engine. At the same time, numerical simulation is equally important to understand the detonation phenomena in the PDE combustor. This paper deals with the numerical modeling and simulation of PDE tube with Hydrogen-Air mixture by using a commercially available CFD code. Pulse detonation engine combustor with and without obstacle has been numerically simulated. Simulation results of PDE combustor with and without obstacles have been analyzed and compared. The simulation results revealed the formation of reflection waves when the detonation wave interacted with the obstacles. The simulation results provided valuable insight into the interaction between detonation wave and obstacles which will be ultimately useful for design and development of pulse detonation engine combustor.

Keywords: Computational Fluid Dynamics (CFD), Detonation, Obstacle, Pulse Detonation Engine (PDE).

1. INTRODUCTION

Pulse Detonation engine is an unsteady propulsion system that operates cyclically and is based on supersonic mode of combustion. Supersonic mode of combustion causes rapid burning of a fuel-air mixture, typically tens of thousands of times faster than in a flame. Hence, there is not enough time for pressure equilibrium and the overall process is thermodynamically closer to a constant volume combustion process than the constant pressure combustion process typical in conventional propulsion system (i.e. gas turbines, ramjets, etc). A constant volume combustion process produces a lower entropy rise of the working fluid versus a constant pressure combustion process (deflagration). This result ultimately corresponds to an improved thermodynamic efficiency [1].

Pulse Detonation Engine cycle typically consists of four stages, filling of fuel/air mixture, combustion, blow down and purging. Out of these four processes, combustion is the most crucial one since it produces reliable and repeatable detonation wave. Detonation is a supersonic combustion process which is essentially a shock front driven by the energy release from the reaction zone in the flow right behind it.

Hence the high pressure ratio associated with detonation combustion due to reaction driven shock front, may eliminate the need for expensive high pressure feed system, thereby reducing propulsion system weight, complexity, cost, and packaging volume [2]. Therefore, pulse detonation engine has the potential to drastically reduce the cost of orbit transfer vehicle system as well as space vehicle attitude control system and can be used for wide range of military, civil and commercial applications. A final characteristic which makes PDE technology so appealing is the capability to provide transition from subsonic to high supersonic operational velocities without additional propulsion system or support vehicle.

Theoretically, the pulse detonation engine has many advantages over conventional propulsion system. The concept of PDE can be converted from the theoretical realm into real world applications after analyzing and solving some critical issues. One of the biggest challenges to make PDEs practical is the requirement for repeated initiation of detonation wave and sustainability of detonation wave throughout the length of the combustion chamber. Pulse detonation engine primarily relies on Deflagration-to-Detonation Transition (DDT) to avoid the high energy required for direct detonation initiation.

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DDT is the process whereby a deflagration is initiated using a weak energy source (typically tens or hundreds of milliJoules). The subsonic flame is accelerated via a series of gas dynamic processes, eventually transitioning to a supersonic detonation before exiting the combustion tube. A drawback of this approach for practical devices is the necessary length and time for transition to detonation (referred to as the run-up distance and time, respectively), which can limit cycle frequency. The run-up distance in fuel air mixtures can be significantly reduced by placing suitable obstacles inside the detonation chamber with little additional weight and complexity. Optimization for an obstacle-based DDT section is a trade-off between minimizing run-up distance via enhanced turbulence, and minimizing performance loss (total pressure losses) via less obstacles or smaller blockage ratio.

A lot of work has been done to find out the effect of obstacles on the DDT (Deflagration-to-Detonation Transition) process in detonation tubes. However, intensive study needs to be done to examine the effect of obstacles on detonation wave propagation since the interactions between a detonation wave and an obstacle is a basic problem in detonation science. These interactions are known to affect the leading shock strength as well as temperature behind the shock wave and hence the chemical reaction rate. Therefore, there is a need to investigate the effect of obstacle on detonation wave propagation in a pulse detonation engine combustor. To accomplish this investigation, numerical modeling and simulation of Pulse Detonation Engine combustor with and without obstacle has been carried out by using a commercially available CFD code. A comparative study of simulation results has been performed by plotting pressure, hydrogen mass fraction and Mach number.

2. LITERATURE REVIEW

Detonation is an extremely promising technique for burning of a fuel-air mixture and releasing its chemical energy content effectively. However, detonations have been explored for propulsion applications only for the past fifty years or so because of the difficulties involved in initiating and sustaining a detonation in a controlled manner in fuel-air mixtures. The development of the concept of Pulse Detonation Engine (PDE) has been traced back to the pioneering work of Hoffmann described by Nicholls et al. [3]. Nicholls also explored the concept of intermittent (or pulse) detonation waves for propulsion applications. Both single cycle and multi-cycle operations with hydrogen or acetylene as fuel and oxygen or air as oxidizer were demonstrated. The basic set up was a simple detonation tube, open at one end with co-annular fuel and oxidizer injection at the closed end. Chan et al. mentioned about the existence of a critical Mach number of 1.5 that the flame must reach to achieve transition to detonation [4].

They further concluded that the "existence of a critical flame Mach number implies that the dominant mechanism for DDT in H_2-air mixtures is related to the strength of its precursor shock". This was related to the shock-focusing phenomenon, induced by obstacles or end walls, which created local hot spots of high enough temperature in the mixture to directly initiate detonation.

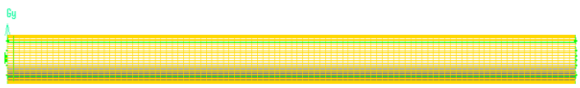
Use of Detonation in pulse detonation engine has been reviewed by kailashnath [5]. In order to understand the nature and structure of a detonation wave used for various propulsion applications further analysis is required. Numerical analysis can help to reduce the cost and time to understand these phenomena. The first numerical simulation of the detonation wave was performed by Taki and Fujiwara for 2D detonation in oxyhydrogen mixture [6]. Wilson et al. implemented the fully implicit, finite volume algorithm for 2D axisymmetric flow to a detailed H_2-air reaction for supersonic combustion phenomena [7]. Most of these computations have been conducted on structured meshes because the analysis of detonation phenomena requires higher order accuracy for capturing fine details. Bussing and Pappas provided a detailed description of the basic operation of an idealized PDE [8]. They also reported one-dimensional study of Pulse Detonation Engines burning hydrogen-oxygen and hydrogen-air mixtures. The detonation was initiated near the closed end of the engine using a high temperature and high pressure region.

3. CFD MODELING

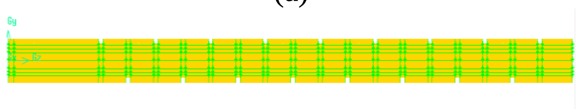
Computational simulation is now an integral step in research and development of any system. This process reduces the need to conduct numerous experiments as well as minimizes the cost. A three dimensional CFD modeling of reactive gas flow in the pulse detonation engine combustor (with and without obstacle) has been performed using a commercially available CFD code. CFD simulations presented in this paper are to mainly illustrate the effect of obstacles on detonation wave propagation.

3.1 Geometry and Mesh Generation

Geometry of Pulse detonation engine combustor is very simple as compared to the other conventional engines.



(a)



(b)

Fig.1. Discretized flow domain showing the mesh (a) Simple PDE combustor, (b) Obstacle laden PDE combustor

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It basically consists of a cylindrical tube, whose one end is closed while the other end is open to the atmosphere as shown in figure 1.

For the purpose of creation of geometry and mesh, a commercially available modeling and meshing software was employed. To create the cylindrical geometry with 100 cm length and 5cm diameter a bottom up approach has been followed by using the same software. Apart from this, the computational domain was split into two zones, namely cold zone and hot zone. The hot zone was a small disc portion of the cylinder of very small thickness as compared to the length of the PDE combustor. It starts from the left end of the tube which is closed. The rest of the portion of the cylinder is referred to as the cold zone with the right face open to the atmosphere. Obstacles basically characterized by Blockage ratio (BR), geometry of obstacle and spacing between them as shown in figure 2 were generated to create obstacle laden PDE combustor. The blockage ratio is defined as the ratio of obstacle area to the tube cross-sectional area ($1\text{-}D^2_{Orifice}/ D^2_{Tube}$).

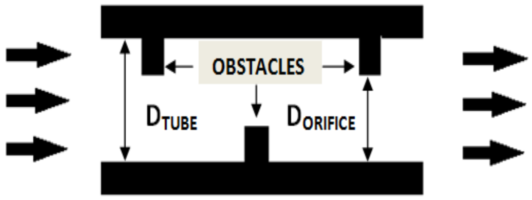

Fig.2. Schematic of obstacle laden tube

In experiments various kinds of obstacles such as circular, semi circular and shchelkin spiral are utilized. However, in the present work semi circular obstacles were used and the first obstacle was located 16 cm from the closed end. Blockage ratio and spacing of obstacles was kept 0.2 and 0.8 times of the diameter of the tube respectively. The computational domain for both configurations was discretized into hexahedra cells. Modeled and meshed PDE combustor without and with obstacles is shown in the figure 1(a) and 1(b) respectively.

3.2 Simulation Strategy

Initial and boundary conditions were set after mesh generation. The complete tube was filled with the premixed stoichiometric mixture of hydrogen and air. The cold zone initial pressure and temperature were kept at 1.0 atm and 300 K, respectively. To initiate detonation, hot zone was patched with high pressure and temperature conditions. Wall boundary conditions were created at left end and cylindrical surface of the PDE combustor. At the wall, no slip as well as adiabatic condition was imposed. In addition, outlet boundary condition was defined at open end for the combustor.

A detonation wave is sustained by the energy released by combustion. Therefore, simulation must include combustion kinetics. Hence, a single-step reduced chemical kinetics for hydrogen-air was used to model chemical reactions.

A 3D unsteady compressible RANS solver was used with K-ε turbulence model.

4. RESULT AND DISCUSSION

In this study, the gaseous mixture of hydrogen and air detonation was simulated and the results are compared with NASA CEA code. At the same time comparison between the results of simple and obstacle laden PDE combustor were performed to investigate the effect of obstacle on detonation wave propagation. These results can be very useful design guidelines and recommendations for the future development of pulse detonation engine (PDE).

The motive of present study was to analyze the effect of obstacle on detonation wave propagation. Therefore, there is a need to create detonation wave. Two methods are primarily utilized to ignite a mixture for detonation; one being direct initiation by depositing the required amount of energy in the system at a very high rate and in the other ignition starts with a deflagration and transits to detonation within a finite time and distance. This transition is known as deflagration to detonation transition (DDT). In literature, many researchers have used high temperature and pressure zone to initiate direct detonation [8, 9]. Therefore, in present simulation, detonation was initiated by patching a very small section (Hot zone) with high temperature and pressure.

In simulation, hydrogen mass fraction and pressure contours were studied and they gave an understanding of the flame development as well as the pressure wave formation. Hydrogen mass fraction disintegration and pressure plot are shown in figure 3 with a time interval of 20 µs between each step.

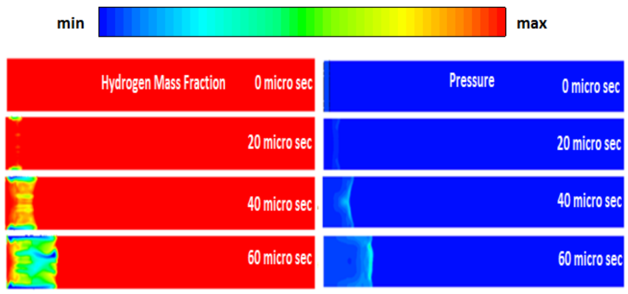

Fig.3. Hydrogen mass fraction and pressure contour plots for 50 cm long part of combustor.

It can be observed from the hydrogen mass fraction contour plots that disintegration of hydrogen starts near the wall and at the interface of hot zone and cold zone. It is well know that the ignition of stationary reacting mixture is easy as compared to the moving one. Therefore, the possible reason for this could be stationary reacting mixture at the wall due to no slip boundary condition. Later on flame develops due to heat release from the hot zone as well as chemical reactions. Looking at the pressure contours (figure 3), one could notice the development of the pressure wave as the hot and cold zones interacted and the start of the reactant disintegration at their interface.

It can also be clearly observed from the pressure contour that, pressure wave continuously strengthens due to the release of the energy from chemical reactions. Further it can be seen from the Mach no. plots that (Mach number) M = 1 is obtained in the flow after 5.5 cm from the closed end. This signifies the formation of shock wave. The plots of Mach no. for simple and obstacle laden PDE combustor are shown in figure 4. It can be clearly seen that the Mach no. plot is almost similar for both the cases since the initial condition and geometry were similar up to a distance of 16 cm.

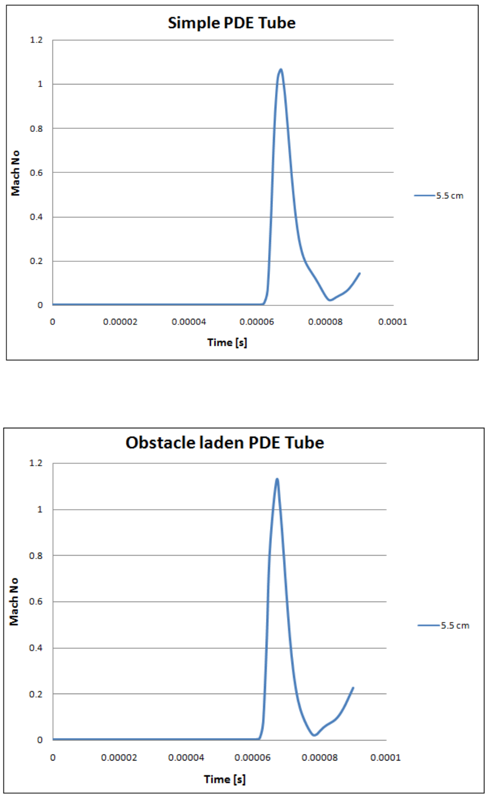

Fig.4. Mach number plot for simple and obstacle laden PDE combustor

The detonation velocity calculated from the simulation was compared with NASA CEA code results. The detonation wave velocity was determined by measuring the time of the pressure wave travelling across the two locations with a fixed distance apart. This is the most common approach used to determine detonation velocity in experiments and known as time of flight method. Hence, the pressure time history was plotted at two locations of PDE combustor for both configurations as shown in figure 5.

After a simple calculation, the velocity of the wave turned out to be around 2000 m/s for obstacle laden PDE tube while 1666.7 m/s for simple PDE tube at 19 cm the from the closed end. Additionally, calculation of Chapman-jouguet detonation velocity was done with NASA CEA (Chemical Equilibrium with applications) code for comparison [10].

The NASA CEA calculation predicted the C-J velocity of 1,966 m/s as per the initial conditions. The comparison between simulation results and NASA CEA code reveals the formation of detonation wave front in case of obstacle laden PDE tube while velocity deficit is observed in simple PDE tube. At the same time for both the cases pressure values were found to be relatively larger than C-J pressure value. Later on it was observed that in simple PDE tube the velocity reached 2000 m/s at 22 cm from the closed end, confirming the formation of detonation wave.

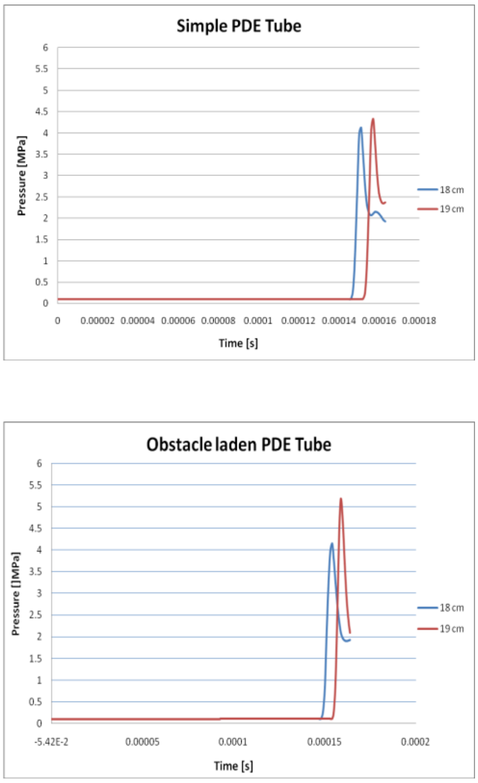

Fig.5. Pressure plot for simple and obstacle laden PDE combustor

The possible cause of early formation of detonation wave in obstacle laden PDE tube could be the interaction of flame front with obstacle. When the flame front passed over the obstacle, it gets stretched and wrinkled. This interaction ultimately created turbulence and increases the surface area of the flame front. The increase in flame surface area causes a surge in energy release rate into the un-burnt mixture. This resulted in the flame acceleration, strengthening of shock waves and ultimately reduced the deflagration to detonation transition distance.

Furthermore, the main objective of simulation study was to investigate the effect of obstacle on detonation wave. Thus to carry out the comparative study between simple and obstacle laden PDE combustor, pressure contours were plotted. For development of these contour plots over 50 cm length of the PDE combustor tube for both the configuration is shown in figure 6.

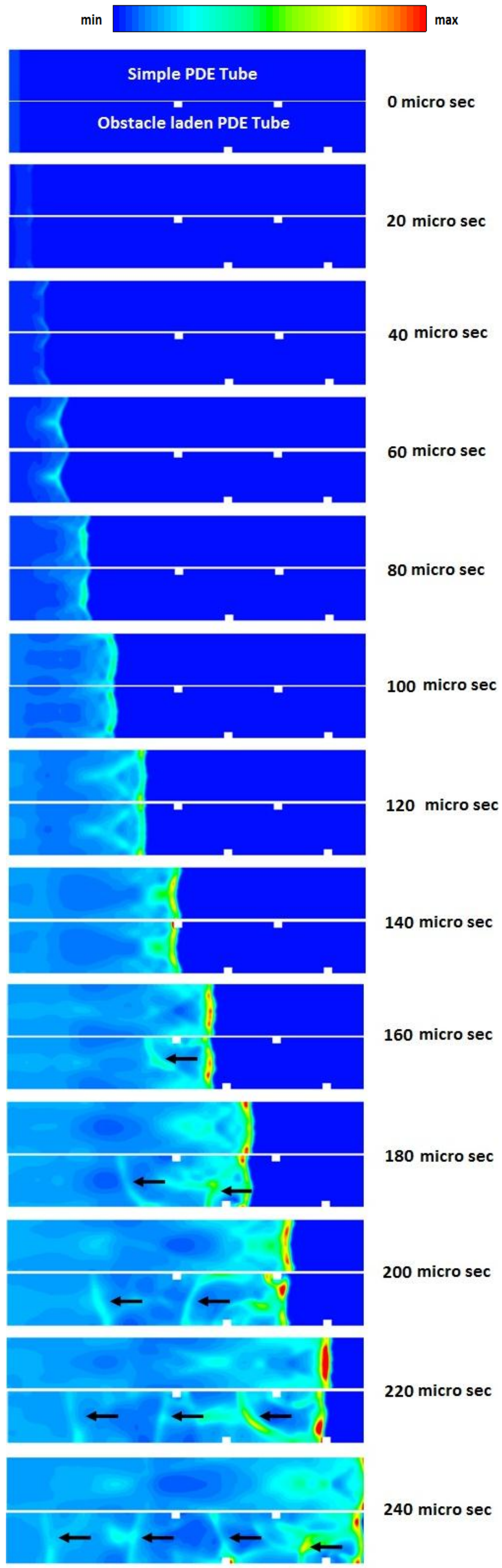

Fig.6. Pressure contour for simple and obstacle laden PDE combustor with 50 cm length

The high pressure and high temperature initial condition in the hot zone initiated combustion of the Hydrogen Air mixture. At the very beginning pressure wave can be seen to develop into a shock wave at 5.5 cm due to heat release from the chemical reaction as explained through Mach no. plot also. The shock wave transitions into a detonation wave after traveling certain distance, due to surge in energy release from the chemical reaction. Hence, shock wave is constantly supplemented and strengthened by heat from the exothermic chemical reaction zone. A closer look on figure 6 shows the formation of reflection wave (denoted by arrow) in case of obstacle laden PDE combustor. It can also be seen from the same figure, that when pressure wave interacts with the first obstacle a weak reflection is formed while when it interacts with second, third and fourth obstacle, a stronger reflection wave is created. The possible reason for this could be the transition to detonation as seen from the pressure time history shown in figure 5. The movement of these reflected pressure waves towards the closed end can also be observed from figure 6.

To see the complete development from pressure wave to propagating detonation wave, wide range of results from 0 to 500 µs are presented in figure 7. The time interval between each slice is 20 µs. In case of simple PDE tube, the formation of shock wave, detonation wave and subsequently accelerating detonation wave can be clearly seen. While in case of obstacle laden PDE tube, the formation of shock wave, detonation wave and almost stable detonation wave is observed.

A sustainable detonation wave needs continuous release of combustion energy from the reaction zone. The high temperature and pressure combustible products, just behind the shock wave expand instantaneously. This sudden expansion of combustible products ultimately pushes the shock wave like a piston, accelerating the detonation wave front. This could be the possible reason for the formation of accelerating detonation wave front in case of simple PDE combustor.

However, a stable detonation wave front was formed in the obstacle laden PDE combustor. In the simulation of obstacle laden PDE combustor, two prominent phenomenons were observed. One was turbulence in the flame front, while the other was strong reflection wave. Flame turbulence helps in formation and acceleration of detonation wave front due to surge in energy release rate. On the other hand strong reflection wave decreases the velocity and pressure of detonation wave. As seen from figure 6, interaction of a detonation wave with the obstacle created a strong reflection wave moving towards the closed end. The movement of these strong reflection waves also moved back the high temperature and pressure combustible product towards the closed end from the detonation wave. As a result, detonation velocity and pressure will be decreased. These two phenomenons might cancel out the effect of each other and result in the formation of a stable detonation wave front.

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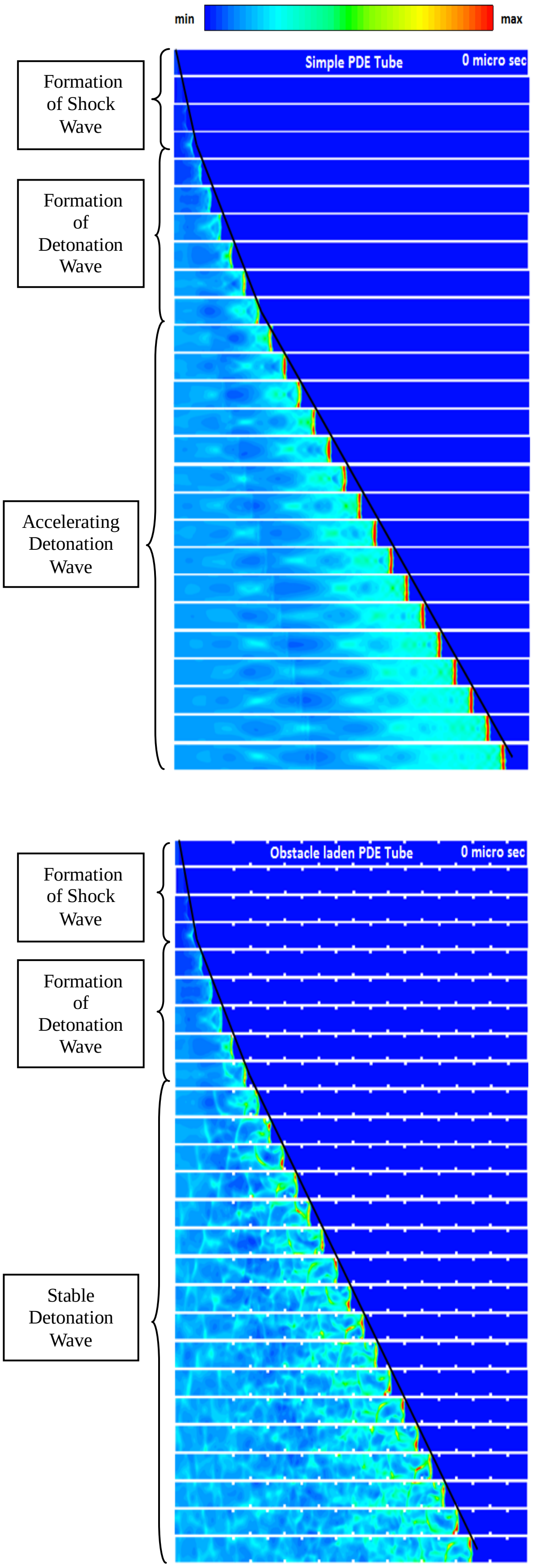

Fig.7. Pressure contour for simple and obstacle laden PDE combustor from 0 to 500 µs

It was also observed that value of pressure in obstacle laden PDE combustor was found to be less as compared to the simple PDE combustor as can be seen in figure 7. Therefore, one should be very careful while selecting the obstacle geometry, blockage ratio and spacing. The selection of inappropriate parameter of obstacles may lead to losses in the detonation velocity and pressure. Further, it might result in a decoupling of shock front and chemical reaction zone, ultimately leading to detonation quenching.

4. CONCLUSION

A simulation study on detonation wave propagation in a simple pulse detonation engine combustor and obstacle laden pulse detonation combustor has been performed. A high temperature and pressure zone was created to initiate combustion and detonation wave. The velocity obtained from the simulation has been compared with NASA CEA code results. The early formation of detonation wave has been observed in case of obstacle laden PDE combustor as compared to simple PDE combustor. This has been explained by sudden increase in energy release rate due to the turbulence caused by the obstacle. In order to investigate the effect of obstacles on detonation wave propagation a comparative study between simple and obstacle laden PDE combustor has been conducted. The formation of reflection wave was observed through pressure contours in the obstacle laden PDE combustor. One more interesting thing was observed from the pressure contours that when a shock wave interacts with obstacle it produces a relatively weak reflection wave. On the other hand, when a detonation wave interacts with obstacle it produces strong reflection wave. Furthermore, the pressure contours for wide range of results have been presented for both configurations. The results reveal the formation of shock wave, detonation wave and subsequently accelerating detonation wave in the case of simple PDE combustor. At same time, formation of shock wave, detonation wave and stable detonation wave was observed in the case of obstacle laden PDE combustor. These two have been explained by the mutually opposing effect of turbulence and reflection of pressure wave. Finally, it can be concluded that by CFD modeling of combustion of premixed hydrogen air mixture in a pulse detonation engine combustor, it is possible to predict and explain the complicated physical interaction between obstacle and detonation wave front. The results of analysis can be further expanded and used as an input for design and development of pulse detonation engine (PDE).

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