Computational fluid dynamics simulation of detonation wave propagation in modified pulse detonation combustor

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Abstract. In this paper effect of Schelkin spiral material on thermal load and detonation combustion wave propagation in pulse detonation combustor has been simulated. As detonation combustion is supersonic combustion process and energy release rate is very high. In this regards present researches are focusing on flame acceleration process to reduce the DDT run up length. Hence the Schelkin spiral is inserted in detonation tube, which creates a bluff body and enhanced the turbulence of flame propagation. During simulation three turbulence models are used to carry out the reliable and repeatable detonation wave in pulse detonation combustor near thin boundary layer of helical shape Shchelkin spiral. The computational fluid dynamics (CFD) simulation has been performed using Ansys fluent platform. The Large Eddy Simulation (LES), detached eddy simulation with realizable k-\(\varepsilon\) turbulence model and detached eddy simulation with SST k-\(\omega\) turbulence model are used for reacting flow simulation. From this simulation the LES turbulence model shows better turbulence initiation of detonation wave with velocity magnitude of 3040 m/s in detonation tube compared to other two turbulence models. This velocity is higher than C-J velocity of 1800 m/s. Further computational result shows that deflagration to detonation transition take place at several waves traveling region, in presence of Shchelkin spiral in detonation tube.

1. Introduction

The performance of pulse detonation engine can be obtained by generating detonation wave intermittently. The PDE system has potential advantages compared to conventional propulsion systems, due to reduced mechanical complexity, high specific impulse and thermodynamic efficiency \([1, 2]\). The several pulse detonation combustor geometry and operating conditions can accelerate the deflagration flame. The researchers and scientists have been studied on PDE with research gape and scope of future research work \([3, 4, 5]\).
The detonation front structure and characteristics of cell pattern depends on the duct or tube size and the properties of the fuels. To accelerate these deflagration to detonation Shchelkin spiral having 50 mm long with a blockage ratio of 0.42 at the closed end of the tube are placed in detonation tube. The detonation wave is typically used to evaluate the performance of PDE. The flow field inside the detonation tube is isentropic, considering these assumptions performance of detonation transition are simulated [6]. The deflagration is generated by an electric spark and produce detonation wave. Zeldovich, von Neumann and Doering (ZND) developed a model in the early 1940’s for detonation wave simulation. The detonation wave speed is depends on pressure, temperature and stoichiometric ratio of fuel and oxidizer [7].

The Shchelkin Spiral is one of the most accelerator devices for deflagration to detonation transition of reacting mixture in detonation tube [8]. Philip K. Panicker, et. al [9] studied on detonation enhance device by experimentally. They found that Shchelkin were able to withstand repeated tests and no deterioration when water cooled. Rocco Portaro, et. al [10] studied on gas phase detonation effect on surface treatment process. They found that pressure gain from detonation combustor can be utilized for green manufacturing process. Shengxi Jia, et. al [11] studied on wall thickness design and structural response of pulse detonation combustor. They found that weight of the combustor was reduced by detonation chamber thickness from 4 mm to 2.03 mm and found that success full detonation wave propagation in detonation tube with smaller thickness of combustor. Moreover, turbulence scales play a significant role in flame acceleration associated with burning rate [12]. Now a day numerical simulations are very powerful to obtain various combustion instability. Large eddy simulation (LES) is a technique that has been widely used to capture the unsteady swirling flows into the computational domain [13]. The turbulent is an irregular condition, small scale motion of combustion flame in both space and time, so statistically distinct average values can be discerned. The DNS have a very simple geometrical application, such as simple channel flows at low turbulent Reynolds numbers or jet flows [14]. The aim of LES type of turbulence model is directly simulated the larger turbulent eddies as this turbulence model have a complex interaction with the bulk flow, where the larger turbulent eddies is directly simulated [15]. LES models were previously used to simulated 3-D deflagrations for hydrogen-air mixture [16]. It is promising for deflagration simulation within less time and allows better prediction of highly non-isotropic turbulent flows and large scale flame flow interaction at the resolved level. The minimum numbers of computational grid points are required for numerical simulation using LES premixed combustion models [17]. The flame speed 200 m/s was found at subsonic flame speed for H2 ≲ 13% mixture. The flame speed reaches in supersonic flow at about 13% of H2. The quasi-detonation regime is formed at second transition and flame speed reaches 800 m/s at supersonic flow regime [18]. Edwards, D. H. et al. [19] experimentally observed the pressure and velocity deficits behind the detonation wave caused by effect of heat losses. Huang, Y., et al. [20] have studied experimentally kerosene as a combustion fuel to enhance DDT at 20, 42.5 and 50 Hz. The results indicate that the values of detonation wave pressures and velocities and detonation initiation times vary with frequencies. Lee, S. Y., et al. [21] have shown that obstacles in detonation tube play important role in establishing small or large scale turbulence that enhances flame acceleration from deflagration to detonation. Khokhlov A. et al. [22] studied the effects of viscosity, thermal conduction, molecular diffusion and chemical reactions to simulate the interaction of shock wave and DDT transition using two-dimensional reactive Navier-Stokes equation for an acetylene-air mixture. The simulation shows that pressure fluctuations generate the turbulence flame and hot spot in combustor. These hot spots may transit to detonation wave through the gradient mechanism. Vaagsaether, K., et al. [23] have simulated flame acceleration and DDT in hydrogen air mixture with a code based on flux
limiter centered method for hyperbolic partial differential equations. They calculated the energy source using Euler equations for the turbulent combustion and two step reaction model for hydrogen air reaction. However, it was unclear whether the physics of DDT was addressed. The 2D numerical simulation of DDT in hydrogen air mixture in an obstructed tube has been studied by Kratzel, T., et al. [24]. Their simulations were predicted to be in reasonably good agreement with their experimental data for the actual deflagration and detonation process but failed to capture the DDT process. The effect of blockage ratio on detonation flame acceleration was studied computationally. The obtained computational results showed that small blockage ratio is suitable for detonation flame acceleration and transition Debnath, P. et al. [25]. Debnath P. et al. [26, 27] studied the ejector effect on detonation combustion wave in pulse detonation combustor. In this study it was observed that ejector can enhances the detonation wave velocity up to 2226 m/s in detonation tube, which is near about C-J velocity. Later on they found that shrouded ejector plays the vital role for vortex formation of reacting mixture in PDE combustor. The experiment was done using Liquid-gasoline/air mixture by Wei W. et al. [28] for detonation flame acceleration. The experimental results indicate that there was no detonation wave formed in the straight tube, but in all the selected spiral tubes fully-developed detonation waves have been obtained. An ejector was used in a small pulse detonation rocket engine (PDRE) as a pre detonator to initiate detonation Yan, Y., et al. [29]. K. Asato, et al., [30] have studied experimentally; a rotating flow field of gaseous mixture was established within the detonation tube due to strong wave velocity. The effectiveness of Shchelkin spiral parameters on DDT phenomenon was studied using propane-oxygen mixture at low energy ignition source. The various configurations like spiral blockage ratio and spiral length to diameter ratio was also studied. In shorter length configurations and highest blockage ratio successful and sustained DDT were achieved by New, T. K. et al. [31]. P. Debnath et al. [32] studied on deflagration to detonation transition in pulse detonation combustor with effect of Schelkin spiral. They found that Schelkin spiral accelerate the flame propagation. P. Debnath et al. [33] studied on exergy analysis of deflagration and detonation combustion process, they have found that deflagration to detonation transition takes place in presence of Schelkin spiral and control volume is defined by C-J velocity. Gamezo, V. N., et al. [34] studied flame acceleration from deflagration to detonation in obstructed channels using 2D reactive Navier-Stokes numerical simulations. In these studies computational performance for channel depends on obstacle per unit length. The DDT occurs more easily when obstacles spacing is large enough for Mach stem generation. P. Debnath et al. [35] studied on flame acceleration with effect of different type of nozzle at exit section of detonation tube. They found that divergent nozzle has more efficient for flame acceleration.

According to the author knowledge there are very few research work on numerical simulation on effect of Schelkin spiral on detonation wave propagation in pulse detonation combustor was found in open literature review. Although there are numerous flames acceleration methods like Jet turbulator, jet in cross flow, acoustic atomizer, obstacle in detonation tube and ejector at exit section of detonation tube. But selection of turbulence model for numerical simulation in detonation tube is still in debate. So, Schelkin spiral effect on detonation wave acceleration and comparison can be performed with clean configuration of detonation tube.

2. Numerical simulation materials

2.1 Physical model description

The Fig. 1 shows the pulse detonation combustor with Shchelkin spiral in detonation tube. The helical Shchelkin spiral was made from high-strength stainless steel. The computational domain of present study is a circular tube with 6 cm diameter and 60 cm length, which is defined as detonation tube. The Shchelkin spiral has been placed inside the detonation tube.
having length of 45 cm. The spiral having a pitch length 5.5 cm, coil diameter 4 cm and coil wire diameter is 0.4 cm.

**Figure 1.** Physical model of pulse detonation combustor with Shchelkin Spiral.

### 2.2 Computational domain discretization

The mesh generation of computational domain is shown in Fig. 2 including the detonation tube and Shchelkin spiral inside the detonation tube. The computational domain has discretized in to tetrahedral mesh. The computational mesh was created outer surface of spiral and mesh was interfaced with metallic spiral surface and combustible gas mixture inside detonation tube.

**Figure 2.** Mesh generation in computational domain with Schelkin spiral

### 2.3 Grid convergence study

The correctness of the results greatly depends upon resolution of computational domain. The various level of grid refinement are used to grid resolution study of computational domain are shown in Table 1. The refinement level consists of 220824 nodes and 1194577 elements for final simulation of computational domain with Shchelkin spiral configuration. The variations of detonation wave velocities are shown in Fig. 3. The velocity of detonation wave was taken as parameter for grid independence study of computational domain. After the refinement level five wave propagation velocity fluctuations is very less.
Table 1. Mesh refinement level of computational domain with Shchelkin spiral

<table>
<thead>
<tr>
<th>Grid Refinement Level</th>
<th>Number of Nodes</th>
<th>Number of Elements</th>
</tr>
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<tr>
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<td>44078</td>
<td>224385</td>
</tr>
<tr>
<td>2</td>
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<td>1194577</td>
</tr>
<tr>
<td>6</td>
<td>303616</td>
<td>1655486</td>
</tr>
</tbody>
</table>

Figure 3. Grid independence test for computational domain with Shchelkin spiral.

2.4 Boundary conditions

The boundary conditions for computational simulations are specified by Dirichlet boundary conditions. The incoming flow of fuel and air is fixed at Mach number of 1.8. The detonation tube wall is assumed to be an adiabatic wall. The Shchelkin spiral inside the detonation tube was considered to be an obstacle wall. The rigid wall conditions were setup inner surface of detonation tube and no slip boundary conditions are adopted. The C-J pressure characteristic exit boundary conditions are used to be most appropriate conditions for detonation wave properties simulation.

3. CFD solver and methodology

The CFD Fluent solvers are employed as a platform for the realization of the several turbulence model effects. The double precision parallel versions of solver are used with explicit linearization of the governing equations. The second order upwind scheme was used for convection terms and central difference scheme for diffusion terms. Pressure-velocity coupling with SIMPLEC (Semi Implicit Method for Pressure-Linked Equations) method is used for good convergence stability.

3.1 Euler system of equations

The time dependent Euler Equations are used to describe on in viscid, non heat conducting, reacting gas flow with temperature model for thermal non-equilibrium. The governing equations can be expressed in generalized coordinates as:

\[
\mathbf{H} = \frac{\partial U}{\partial t} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} + \frac{\partial E}{\partial \zeta}
\]  

(1)
In these system equations the density $\rho(M, t)$ is the total density of the whole gas in position $M$ and at time $t$.

$\rho(M, t)$ is calculated as sum of mass fraction ($Y_i$) and density ($\rho_i$) of each species,

$$\rho = \sum_{i=1}^{\text{nt}} Y_i \rho_i$$  \hspace{1cm} (4)

Where, $i = 1$ to $nth$ species,

The following equations of state can also defined:

$$Y_n = 1 - \sum_{i=1}^{n} Y_i$$  \hspace{1cm} (5)

$$P = \frac{\rho R T}{M_m} \sum_{i=1}^{\text{nt}} Y_i M_i$$  \hspace{1cm} (6)

$$e = \frac{\rho}{\gamma - 1} + \beta \rho \Omega + \frac{1}{2} \rho u^2 + \frac{1}{2} \rho v^2 + \frac{1}{2} \rho w^2$$  \hspace{1cm} (7)

Where, $\rho$ is the density, $\gamma$ specific heat ratio and $q$ heat release per unit mass. The mass production rate of reactants

$$\omega = \frac{d\beta}{dt} = -A \beta \exp \left( \frac{-E_a}{RT} \right)$$  \hspace{1cm} (8)

In the above equations $\beta$ is the mass proportion of reaction gas mixture, $R$ is gas constant; $T$ is temperature and $E_a$ is active energy per unit mass.

### 3.2 Validation of present simulation

The flame is accelerated by rapid flame propagation and turbulence near Shchelkin spiral wall, which promoted by propagation velocity. The present computational wave propagation regimes are validated by experimental shadowgraphs cited from literature. The Fig. 4(a) shows the experimental shadowgraphs of flame propagation [36] at different times and Fig. 4(b) shows the contour plots of detonation wave at different run up distance. The flame propagates very first in combustion chamber toward radial and axial directions. In present computational study deflagration to detonation transition was found at $\delta=0.59$ m and $\delta=0.74$ m longitudinal distance in detonation tube with Shchelkin spiral effect.
4. Results and discussions

4.1 Effect of turbulence model

The detonation wave flow field in detonation tube near Shchelkin spiral inside the detonation tube is turbulent in nature and hence the selection of turbulence model is desired for computational simulations. The strong turbulence flow generally promotes the flame acceleration and propagation. The turbulence was promoted by helical Shchelkin spiral. The local strong turbulence may occur due to high circulating velocity. Three types of turbulence models such as Large Eddy Simulation (LES), Detached Eddy Simulation with Realizable k-ε model and Detached Eddy Simulation with SST k-ω turbulence models are used for simulations. The intensity of turbulence has taken as 1%. The turbulence intensity increases with increasing the propagation velocity. The turbulence combusting flows were characterized by continuous fluctuations of wave speed and pressure dynamics. The turbulence intensity leads to increase combustion wave propagation. Moreover, the effect of turbulence on the combustion physics is an important for combustor modeling. In this regards, various turbulence models have been proposed to cope with the problem of turbulence intensity near Shchelkin spiral wall. The Large Eddy Simulation of detonation wave velocity vector field at two axial locations is shown in Fig. 5(a). The LES turbulence model shows that hydrogen-air detonation in pulse detonation combustor with and without Shchelkin spiral zone in detonation tube and deflagration to detonation transition process was occur easily. The flame instabilities and recirculation region was initiated near Schchelkin spiral area. There is no initiation of detonation wave in δ=0.29 m and δ=0.89 m for without spiral zone, but in δ=0.49 m and δ=0.69 m distance the detonation wave created just near Shchelkin spiral wall. The turbulent intensity in terms of velocity vector magnitude is higher near Shchelkin spiral wall. The strong detonation velocity vector was obtained with a magnitude of 2070 m/s and 2300 m/s at δ=0.49 m and δ=0.69 m in wave travelling distance. The Shchelkin spiral wall surface generates flame turbulence which enhances molecular exchange processes and thereby increasing the turbulent burning velocity. Shchelkin spiral acts as an obstacle, due to this obstacle the flame velocity remains unchanged and the flame velocity deteriorate again after across the obstacles. The Fig. 5(b) shows the Detached Eddy Simulation-Realizable k-ε model for detonation wave velocity vector field at two axial locations in different planes. At δ=0.49 m and δ=0.69 m longitudinal distance the strong velocity vector colored by velocity variation of 1830 m/s and 1980 m/s. The flame propagation is purely governed by turbulent exchange process. The Fig. 5(c) shows velocity vector of detonation wave for DES-SST k-ω turbulence model. The detonation wave speed magnitude of 1590 m/s and 1772 m/s was found at δ=0.49 m and δ=0.69 m distance.
Figure 5. (a) Large Eddy Simulation, (b) Detached Eddy Simulation with Realizable k-ε turbulence model and (c) Detached Eddy Simulation with SST k-ω turbulence model of Detonation wave in pulse detonation combustor.
4.2 Shchelkin spiral effect on thermal load

The Fig. 6 shows the comparison of temperature contour plot of detonation wave propagation in PDE combustor with and without Schelkin spiral. The reflecting shock wave from boundary layer of Schelkin spiral are found in centre of the detonation tube. As the Schelkin spiral material is stainless steel thermal load can be sustain up to maximum limit. Contour plots also shows that the flame front propagation temperature contour is quite different from clean detonation tube. So far, strong combustion wave species temperature magnitude of 4321 K are found in detonation tube with Schelkin spiral.

Figure 6. Temperature Contour of detonation wave in PDE combustor (a) without schelkin spiral (b) with Schelkinspiral effect inside the detonation tube

4.3 Effect on detonation wave velocity

The velocity profile evaluation of Shchelkin spiral effected zone and clean configuration are shown in Fig. 7. As the flame travel through the Shchelkin spiral, it accelerates and eventually reaches in supersonic speeds. The propagating flame initiated near the Shchelkin spiral and combustion wave speed near Shchelkin spiral regime is often close to the Chapman-Jouguet speed. At 1.8 Mach number the average speed of detonation waves are equal to approximately 2060 m/s in Shchelkin spiral configuration and at the same incoming Mach number without Shchelkin spiral the detonation wave propagates at constant speed of 1190 m/s. The velocity rapidly reaches the level of the Chapman-Jouguet (C-J) detonation velocity in detonation tube. The overdriven detonation attains at highspeed and later on gradually sustain at stable detonation wave speed. The contour plots of detonation wave velocity clearly show that Mach stem is generated near Shchelkin spiral wall in long detonation tube. The successive stages of deflagration to detonation transition wave were achieved at δ=0.49 m and δ=0.69 m wave travelling distance, which is effected by bluff body structure like Shchelkin spiral. The hot spot zone was also generates in these detonation transition area. The galloping detonation mode was found at δ=0.49 m distance in detonation tube. The detonation wave velocity decelerates and gradually vanishes at δ=0.84 m wave traveling distance. The feature of detonation wave speed is affected by Shchelkin spiral area and influences of physical mechanism on transition to detonation wave. The Shchelkin spiral occupied high turbulence zone and the detonation wave consistently reaches the C-J velocity (near about 2500 m/s). The pickup detonation wave velocity was found at δ=0.69 m. The tendency of wave propagation is almost hemispherical form in detonation tube. The flame speed remains constant with uniform velocity in clean configuration.
4.4 Effect on detonation wave dynamic pressure

The Fig. 8 shows the comparison of three dimensional simulation of detonation wave pressure variation in detonation tube with and without Schelkin spiral. Detonation wave creates high pressure during combustion and shock wave pressure rapidly reached to the C-J pressure. The strong evident detonation wave pressure was found at $\delta=0.49$ m to $\delta=0.69$ m distance has been shown in Fig. 8(a). The reacting mixture pressure shows that shock produces by the spiral section. The Fig. 8(b) shows the pressure traces in clean configuration with poor performance at same operating boundary conditions. The stronger pressure wave travels faster than weaker one, which causes due to pressure gradient in the flow of steepen. The combustion wave appears to accelerate and transition to detonation at $\delta=0.69$ m but gradually fails for weak turbulence. The contour plot analysis shows the maximum level of detonation wave dynamic pressure behind the Schelkin spiral area is 26.1 bar. The pressure level 9.03 bar was found behind the clean configuration.

Figure 8. Shock wave pressure (Pascal) contour in detonation tube at iso-surface ($\delta=0.39$ m to 0.84 m) distance (a) with Shchelkin spiral and (b) without Shchelkin spiral effect.
4.5 Shock wave pressure oscillation in combustor

The Fig. 9 shows the comparison of dynamic pressure wave profile in detonation tube with and without Shchelkin spiral effect. This zone has strong promise to enhance detonation wave propagation. The pressure spike is gradually increased up to $\delta=0.69$ m distance, than it decreases at the end of tube. This dynamics pressure oscillation has great role for enhancement of propulsive power.

![Figure 9](https://example.com/figure9.png)

**Figure 9.** Comparison of shock wave Dynamic Pressure (a) with Shchelkin spiral effect and (b) clean configuration in detonation tube.

5. Conclusions

The computational simulation has been shown that combustion wave is highly unsteady in nature near Shchelkin spiral obstacle in detonation tube. Combustion wave turbulence are analysed using LES, detached eddy simulation with realizable k-ε turbulence model and detached eddy simulation with SST k-ω turbulence models with velocity vector flow field. The following conclusions are drawn:

- From this numerical investigation the LES turbulence model shows the more efficient for simulations. This detonation wave velocity magnitude is 3040 m/s, which is higher than Chapman-Jouguet velocity and it is stronger than other two types of turbulence model.

- It seems that strong turbulence flow promotes flame propagation and acceleration. From temperature contour plot it has been found that Shchelkin spiral prepared by stainless steel can withstand the wave propagation temperature magnitude of 4321 K.

- The effect of Shchelkin spiral on detonation wave at different transverse plane shows the wave propagation regime. The contour plot clearly shows that strong detonation wave initiated at $\delta=0.49$ m distance in detonation tube with Shchelkin spiral, which acts as a turbulator.

- The peak chamber pressure oscillation magnitude of 26.1 bar was observed in detonation tube with Shchelkin spiral and the dynamic pressure magnitude of 9.03 bar was found in clean configuration. The rapid flame propagation regimes are promoted by helical Shchelkin spiral. The detonation wave initiation is stronger in detonation tube with Shchelkin spiral and magnitude is quite different from clean configuration at Mach number of 1.8.
References


