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Numerical Investigation on detonation combustion waves of hydrogen-air mixture in pulse detonation combustor with blockage

Pinku Debnath*[1] and K.M. Pandey[2a]

[1]*Mechanical Engineering Department, National Institute of Technology Agartala, Tripura, 799046, India*
[2]*Mechanical Engineering Department, National Institute of Technology Silchar, Assam, 788010, India*

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Abstract. The detonation combustion is a supersonic combustion process follows on shock wave oscillations in detonation tube. In this paper numerical studies are carried out combined effect of blockage ratio and spacing of obstacle on detonation wave propagation of hydrogen-air mixture in pulse detonation combustor. The deflagration to detonation transition of stoichiometric (ϕ=1) fuel-air mixture in channel has been analyzed for effect of blockage ratio (BR)=0.39, 0.51, 0.59, 0.71 with spacing of 2D and 3D. The reactive Navier-Stokes equation is used to solve the detonation wave propagation mechanism in Ansys Fluent platform. The result shows that fully developed detonation wave initiation regime is observed near smaller vortex generator ratio of BR=0.39 inside the combustor. The turbulent rate of reaction has also a great significance role for shock wave structure. However, vortices of rapid detonation wave are appears near thin boundary layer of each obstacle. Finally, detonation combustor demonstrates the superiority of pressure gain combustor with turbulent rate of reaction of 0.6 kg mol/m^3-s inside the detonation tube with obstacle spacing of 12 cm, this blockage enhanced the turbulence intensity and propulsive thrust. The successful detonation wave propagation speed is achieved in shortest possible time of 0.031s with a significance magnitude of 2349 m/s, which is higher than Chapman-Jouguet (C-J) velocity of 1848 m/s. Furthermore, stronger propulsive thrust force of 36.82 N is generated in pulse time of 0.031s.

Keywords: computational fluid dynamics; deflagration; detonation wave; pulse detonation combustor; shock wave

1. Introduction

The pulse detonation combustor is potential pressure gain combustor and increases the propulsive power for next propulsion system. The detonation tube design for faster deflagration to detonation transition, which has vital role for several applications in the field of green manufacturing, process engineering, chemical plants, explosion safety, flame arresters and propulsion system. This technology is new exciting propulsive system for next generation of supersonic engines (*Ma*>1). Detonation combustion takes place inside the pulse detonation combustor due to the combustor design and operating conditions. The vortex generation

*Corresponding author, Assistant Professor, E-mail: er.pinkunits@yahoo.com
[a]Professor, E-mail: kmpandey2001@yahoo.com

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techniques are applied to generate vortices, recirculation, flow separation and reattachment in detonation tube channel flow, which enhance the mixing of fuel air mixture. The detonation waves are obtained by either direct or indirect ignition methods. Direct detonation initiation requires activation energy. Some researchers observed that the energy release and conversion is key issue of detonation combustion process Kailasanath (2000), Debnath and Pandey (2022), Glassman *et al.* (2008). Liu *et al.* (2020) studied on enhancement of thermal efficiency of a power plant by using a pressure gain combustor and they solved these reacting flows by RANS equations. Pandey and Debnath *et al.* (2016, 2021) studies various computational analyses, which address the performance of pulse detonation engine (PDE) and also indicate the further research scope. Eder *et al.* (2001) experimentally and analytically studies deflagration to detonation transition process and obtained results show that combustion efficiency of pulse detonation engine can be improved by their experimentation. Moen *et al.* (2003) studied on influence of obstacles on propagation of flame in the pulse detonation combustor. Hu *et al.* (2018) studied deflagration to detonation transition (DDT) in obstacle-filled detonation tube using an iso-octane vapor-air mixture by solving Navier-Stokes equation. The geometry of detonation tube condition for obstacles should be within DDT run-up distance. Teodorczyk *et al.* (2007) studied an experimentally flame propagation, acceleration and transition to detonation wave of hydrogen-air mixture an obstructed channel. They found that hot spot can create by shock reflection surface of obstacle. Gamezo *et al.* (2007) experimentally computed the flame acceleration and DDT in hydrogen-air mixtures in obstructed channels and observed flow regimes of supersonic turbulent flame, quasi-detonation and flame propagation in order to prevent the loss and consequently support the DDT process inside the tube with obstacle, which increases fuel-air mixture burning rate and facilitate flame acceleration. Detonation wave acceleration and deflagration to detonation transition in obstructed channel are studied by Gamezo *et al.* (2008). They observed that obstacles are involved in thermal expansion and flame-vortex interaction of combustion product. Johansen *et al.* (2009) investigated the effect of blockage ratio on flame acceleration in an obstructed square cross-section channel. They developed the flow field structure of unburnt gas ahead of obstacles. Valiev *et al.* (2009) studied that obstacle mechanism is much stronger for deflagration flame to detonation wave transition. Several researchers have found that numerical simulation of deflagration flame acceleration in an obstacle channel is quite different from Shchelkin spiral effect. Latter on mechanism of viscous heating can also be identified with proper modification of obstacle geometry. Johansen *et al.* (2009) studied on flame acceleration process in square shape obstructed channel. They found that size of vortex increases adjacent to obstacle wall. The effect of blockage ratio on energy release rate, flame acceleration and deflagration to detonation transition was simulated numerically. The flame propagation developed into a particular propagation regime depends on the channel geometry and flow condition (2009). Ciccarelli *et al.* (2010) studied experimentally the effect of obstacle blockage on the rate of flame acceleration and flame-tip velocity. The detonation transition occurs easily in an obstacle landed detonation tube, in this tube flame eventually accelerates with a velocity magnitude of 1000 m/s. Fence-type obstacles were placed inside square cross section channel with equal spacing and studied the flame acceleration by Johansen *et al.* (2010). The effect of obstacle blockage ratio on the development of unburnt gas flow field ahead of flame front in an obstacle channel is investigated using large eddy simulation (LES). The computational simulation indicates that turbulence increase with the increases of blockage ratio. Rudy *et al.* (2011) have been studied experimentally and computationally on flame propagation, acceleration and deflagration to detonation transition of hydrogen-air mixture with an obstacle tube. Ogawa *et al.* (2013) studied flame acceleration and DDT in square obstacle array and their computational results indicate that obstacle leads DDT process, stronger flame acceleration, burning flame speed and strong leading shock wave. Later on it is found that the effect of obstacle blockage ratio (BR) on detonation wave propagation and un-burnt gas flow field, which is investigated using varying obstacle height. Large eddy simulation of initial flame acceleration in an obstructed channel has been studied by Johansen *et al.* (2013). Debnath and Pandey *et al.* (2014) studied flame speed, which depends on obstacle geometry and contour of flame structure distribution inside the detonation tube. A small blockage ratio is desirable for flame acceleration and transition to detonation wave. Again, Johansen (2009) investigated flame acceleration in a channel having obstruction by experimentation. Their observation shows that flame interaction within turbulent flow and three-dimensional wave structure augmented the flame shape. Ashley *et al.* (2019) studied deflagration to detonation transition of stoichiometric hydrogen-air mixture in an obstructed channel. As a result vortex shedding is generating for flame acceleration. A computational study of mixing process of hydrogen-air turbulent non-premixed flame characteristics has been studied by Tabet (2012). The velocity and density of mixture have been studied by eddy dissipation model. Xuxu *et al.* (2020) studied obstacle thickness effect on detonation wave propagation. The critical conditions of detonation wave propagation can be quantified by hydraulic diameter and cell size of detonation wave. Xiao *et al.* (2020) studied on effect of shape of an obstacle for flame acceleration and DDT in circular, forward triangular and backward triangular shapes channel. Their obtained simulated result shows that square obstacle produces the strongest growth rate of flame surface area for flame-acceleration with shortest detonation onset time. The comparison shows that circular obstacle produces the weakest flame surface growth and thus they have least effect on promoting DDT. Debnath *et al.* (2017) studied exergetic efficiency analysis of hydrogen-air detonation in PDE combustor. Their CFD post processing result shows that detonation is thermodynamically more efficient than deflagration mode of combustion. Jeffrey (2018) studied supersonic heat addition in PDC. They observed that performance of specific thrust is characterized by free stream Mach number. Teodorczyk *et al.* (2009) studied DDT of hydrogen-air detonation in obstructed channel of BR=0.25, 0.5 and 0.75. Their result shows that higher blockage ratio leads separation of boundary layer of thin flame and also found that less important of lean mixtures (ϕ=0.6) on flame acceleration. Nguyen *et al.* (2018) studied on pulse detonation engine (PDE) from lean to rich ethylene-air mixture. The obtained result shows that maximum values of detonation wave velocity occur at equivalence ratio of 1.1. Debnath and Pandey *et al.* (2021, 2023) studied on detonation combustion propagation of liquid and gaseous fuel-air mixture in PDC with shrouded ejector. They found that shrouded ejector with a taper angle of α=+4° performed starting vortex generation with shortest possible time of 0.032 s. Heidari *et al.* (2014) studied chemical reaction mechanism of hydrogen-air mixture for different stages of flame propagation and acceleration. Min *et al.* (2021) studied on effect of obstacle ratio on hydrogen-air detonation in a channel with array of obstacles. They found that DDT transition takes place well in staggered obstacles with blockage ratio of 0.5.

The above literature review indicates that there are few researches are found in open literature on effect of obstacle on detonation combustion wave propagation and acceleration in fully develop mode in PDE combustor. So the objective of the present investigations are focus on combined effect of vortex generator ratio (BR) 0.39, 0.51, 0.59 and 0.71 with obstacle spacing of S=2D=8 cm and S=3D=12 cm on detonation wave pressure, temperature, combustion species and detonation wave velocity. Further propulsive thrust has been investigated for several pulse times for stoichiometric hydrogen-air mixture. Not only the thrust but also shortest possible time for deflagration to detonation transition has been studied.

2. Numerical methodology

The mathematical model of detonation combustion wave is solved numerically using CFD code in ANSYS Fluent platform. The governing equations are discretized by second order upward scheme with SIMPLE algorithm for one step chemical kinetics model. The density based solver is used to simulate the compressible flow. The simulation convergence criteria are set up to 10^{-6}. Initially pulse time varies between 0.021s to 0.033s (2017). So far, fully developed detonation wave pulse times of 0.031s have been taken for overall simulation.

2.1 Large eddy simulation modelling

The large eddy simulation (LES) is used for detonation wave simulation and energy release from fuel-air mixture during combustion. The turbulence is generated due to presence of obstacle in a channel. This turbulence is enhanced the mixing, so far energy transfer rate increase. The governing equations are given below to carry out on wide range of simulations of combustion wave. The continuity equation implies conservatives balance between the mass entering and leaving from a control volume and the density of reacting mixture is changed within this pulse time. The independent variables are solved by the following equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial X_i}(\rho U_i) = \dot{S} \tag{1}$$

The momentum equation of reactive flow is given below

$$\frac{\partial}{\partial t}(\rho U_i) + \frac{\partial}{\partial X_j}(\rho U_i U_j) = -\frac{\partial P'}{\partial X_i} + \frac{\partial}{\partial X_j}\left\{\mu_{\text{eff}}\left(\frac{\partial U_i}{\partial X_i} + \frac{\partial U_j}{\partial X_j}\right)\right\} + \dot{S}_{M_i} + \dot{S}U_i \tag{2}$$

$$\mu_{\text{eff}} = \mu + c_\mu \rho \frac{k^2}{\varepsilon} \tag{3}$$

$$P' = P + \frac{2}{3}\rho k + \frac{2}{3}\mu_{\text{eff}}\frac{\partial U_j}{\partial X_j} \tag{4}$$

The energy equation is derived from first law of thermodynamics and this equation is as following

$$\frac{\partial}{\partial t}(\rho c_p^g T^g) + \frac{\partial}{\partial X_i}(\rho c_p^g U_i T^g) = \frac{\partial}{\partial X_i}\left(\rho c_p^g \alpha_{\text{eff}} \frac{\partial T^g}{\partial X_i}\right) - \frac{\partial q_i^r}{\partial X_i} + \dot{S}_E + c_p^g T^g \dot{S} \tag{5}$$

Where, $\dot{S}_E$ is the energy source term. This energy absorbed from atomization of fuel-air mixture during heating-up period. The inter-phase transport and other energy are generated due to chemical reaction.

2.2 Species transport model

The stoichiometric fuel-air mixture and chemical species are modelled by species transport equation. The transport equation is given as Eq. (6) along with diffusion and source term of each chemical reaction species. The species conservation equation is solved for vaporization of fuel, oxygen and water vapor mass fraction, while nitrogen concentrations are ignored. The species mass fraction equations are as follows

$$\frac{\partial}{\partial t}(\rho C_j) + \frac{\partial}{\partial X_i}(\rho U_i C_j) = \frac{\partial}{\partial X_i}\left(\rho D_{\text{eff}} \frac{\partial C_j}{\partial X_i}\right) + \dot{S}_{C_j} \tag{6}$$

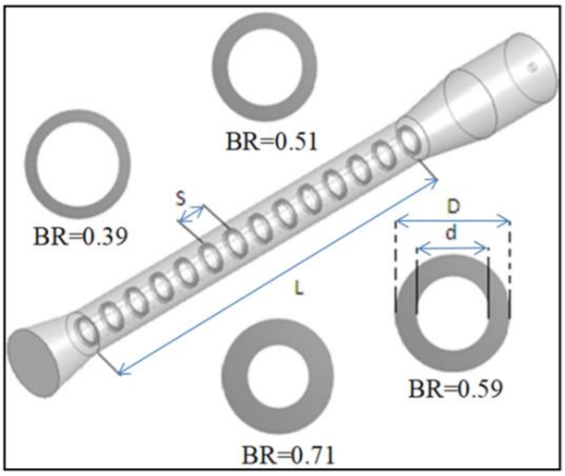


Fig. 1 The physical model of PDE combustor with array of obstacle

Where, U_i is the flame velocity, C_j is reaction progress variable and D_{eff} is diffusion coefficient term. The conservation equation for each species of fuel-air mixture contains a source term S_{C_j} is given by

$$S_{C_j} = -\omega M_f \qquad \text{for fuel vapor}$$

$$S_{Cj} = -\omega M_f \gamma \qquad \text{for oxidizer}$$

$$S_{C_j} = -\omega M_f (1+\gamma) \qquad \text{for the product (water vapor)}$$

Where, the rate of reaction ω is equal to min (ω_k, ω_d). The additional source term S_{C_j} is zero for all species except the fuel vapor.

2.3 Combustion modelling

The deflagration to detonation transition in PDE combustor with stoichiometric (ϕ=1) hydrogen-air mixtures, including thermodynamics parameters and one-step reaction kinetics parameters are adopted. The hydrogen (H_2)-air mixture is taken for detonation wave simulation with array of obstacle effect. The combustion reaction takes place inside the combustor with supersonic (*Ma*>1) flow regimes. The balanced reaction equations are as follows

$$\mathrm{C_m H_n} + (\mathrm{m}+\tfrac{\mathrm{n}}{4})\,(\mathrm{O_2} + 3.76\mathrm{N_2}) \rightarrow \mathrm{mCO_2} + \tfrac{\mathrm{n}}{2}\mathrm{H_2O} + (\mathrm{m}+\tfrac{\mathrm{n}}{4}) \times 3.76\mathrm{N_2} \tag{7}$$

$$\phi = \frac{F/A}{(F/A)_{st.}} \tag{8}$$

$$(F/A)_{st.} = \frac{1}{4.76(\mathrm{m}+\frac{\mathrm{n}}{4})} \times \frac{W_f}{W_a} \tag{9}$$

Where, ϕ indicates stoichiometric ratio, W_f and W_a are molecular weight of hydrogen fuel and oxidizer (air). As the hydrogen (H_2) is the pilot fuel for detonation wave propagation in pulse detonation combustor. For hydrogen-air combustion in reaction equation the subscript m=0 and *n*=2 are considered.

Table 1 Adopted mesh elements and nodes from four blockage (BR) with obstacle spacing

Blockage Ratio (BR)		0.39		0.51		0.59		0.71	
		Nodes	Elements	Nodes	Elements	Nodes	Elements	Nodes	Elements
Spacing (S)	8	223487	1214834	224389	1217672	224400	1216677	223817	1212636
	12	222625	1212571	222425	1210306	222637	1211103	222544	1209900

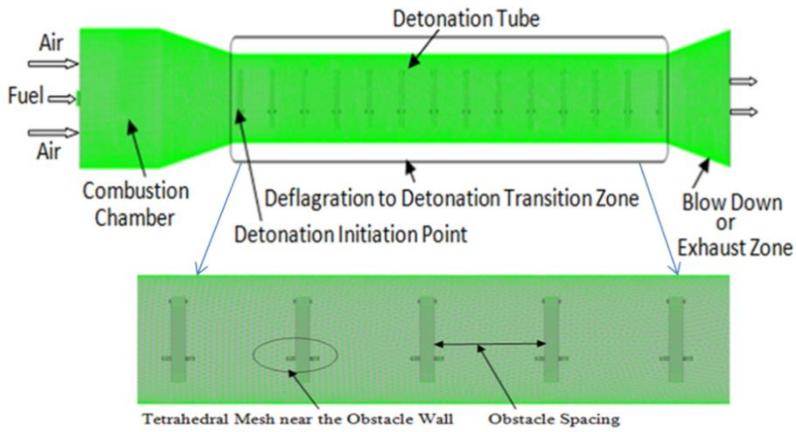


Fig. 2 Tetrahedral mesh of combustion domain with obstacles

2.4 Physical and computational model

The physical model of pulse detonation combustor is designed by inserting regular obstacle in channel with obstacle spacing is shown in Fig. 1. The total length of the combustor is divided into two sections, the first part having 10.5 cm and second part having length of 60 cm is known as detonation tube. The divergent type nozzle is attached in exit section of detonation tube, as the D-type nozzle can enhance the propulsive performance (2020). The three dimensional computational model is created in Ansys design modeller platform (2011). The obstacle blockage ratios (BR) are calculated using the mathematical equation (10). As the computational domain obstacle size is the same as blockage ratio (BR), so the vortex generator ratio is the same as BR. The starting vortex generator ratios of 0.39, 0.51, 0.59 and 0.71 are designed for simulations. The inner diameter (D) of detonation tube is 4 cm. These obstacles are placed inside the detonation tube having a spacing of S=2D=8 cm and S=3D=12 cm. There is fourteen number of obstacles are allocated and maintain the obstacle clearance from side tube wall the rod having diameter of 0.2 cm is kept for correct spacing inside the channel.

$$BR=1-(d/D)^2 \tag{10}$$

Where, d and D denote orifice and tube inner diameter respectively.

2.5 Mesh generation description

The grid generation and schematic view of grid arrangement in computational domain with detonation tube are shown in Fig. 2. The unstructured grids are generated to discretize the computational domain with obstacles. The inflation layer is added near obstacle surface to have $Y+$

Table 2 Mesh refinement test of PDE combustor

Grid Refinement Level	Number of Nodes	Flame Velocity (m s^{-1})	Error (%)
1	83567	2110	-
2	114914	2260	6.64
3	163102	2320	2.59
4	**223487**	**2349**	**1.23**
5	289816	2260	3.94

value close to one, so reacting flow physics near boundary wall is observed. The grid size of Δx=0.021 cm are taken for grid generation. The successive number of nodes and elements are listed in Table 1. So far, the accurate and smallest grid size consists of 223487 number of nodes and 1214834 number of elements for BR=0.39. These grid points are adopted based on detonation wave propagation velocity. The adopted grids reduce the convergence time and increase the grid resolution of detonation wave contour. After refinement of grid, final nodes and elements are taken for further simulation.

2.6 Grid independence test

In order to minimize the computational error and improve mesh quality the grid independence test is required. The accurate result greatly depends on successive smaller grid cell size and resolution. These grid refinement are done up to a certain limit, beyond this limit refinement does not have any significance effect on post processing result. This limit is called the Grid Independent Limit (GIL). The detonation wave velocity from higher resolution of contour plots are achieved using finer grid size. In order to resolve the combustion wave propagation physics, the several grid domains are used for simulation. The relative error of detonation wave propagation velocities are given in Table 2. The minimum error of 1.23% is found at optimum number of 223487 nodes. Beyond this 1.23% error the result does not change no more. As the flame propagation velocity difference is more between refinement level 4 and level 5. So the error is greater at the grid refinement level 5. The Fig. 3 shows the various level of refined mesh corresponding to flame velocity for the case model having spacing of S=2D and BR=0.39. Moreover, propagation speed of 2349 m/s is obtained at refinement level 4. Hence chocked flow condition takes place at this propagation velocity.

2.7 Initial boundary conditions

The simulation of detonation wave structure in obstacle landed tube has been done in Ansys Fluent platform. The boundary conditions of computational domain are defined as inflow, fixed wall and outflow. For present simulation the details of initial boundary conditions are present in Table 3. The hydrogen fuel is injected in to combustor with species mass fraction of 1.5% for simulation of detonation combustion wave. The inlet condition are taken as free stream velocity of stoichiometric fuel-air mixture and specified by Dirichlet boundary condition. As compressibility effect are acting on reacting fluid (Ma>0.3). So the inlet velocity (u_{in}) is formulated from Mach number (Ma). The outflow conditions are pressure outlet and Neumann boundary conditions are also applied. The obstacles are considered no-slip walls and outer surface of detonation tube has been provided symmetry. The species transport model with finite rate turbulence chemistry

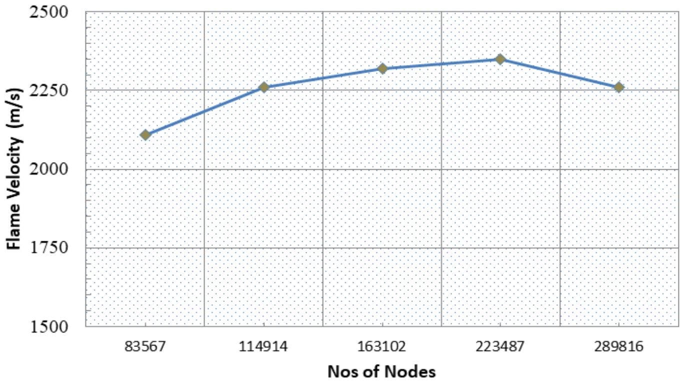


Fig. 3 Grid independence test of computational domain

Table 3 Initial boundary condition of hydrogen-air mixture are employed for PDE combustion simulations

Inlet Parameters	Air	Hydrogen
Mach number	1.889	2
Pressure [kPa]	4.0115	1.01325
Temperature [K]	780	298
H_2 mass fraction	---	0.015
O_2 mole fraction	0.2035	0
H_2O mole fraction	0.0303	0

Table 4 The comparison of detonation wave velocity from CFD analysis with different author's results

Authors	Detonation velocity (ms^{-1})	Blockage Ratio (BR)
Tangirala *et al.* (2005)	1867	BR=0.43
Alam *et al.* (2019)	1795	BR=0.50
Heidari *et al*. (2014)	1997	BR=0.50
Xiao. *et al.* (2020)	1993	BR=0.41
Present Study	2349	BR=0.39

interaction is used for exothermic chemical reaction process.

2.8 Validation of present model

The numerical simulation of detonation wave propagation in detonation tube required less time, but numerical model validation is required for accuracy. Hence, the present model of PDE combustor with obstructed channels in detonation tube is validated with experimental results of Tangirala *et al.* (2005) and other peer researcher. The Table 4 represents the comparison of present numerical simulation of hydrogen-air detonation wave propagation speed with different author's results from literature. The present propagation wave velocity is 2349 m/s and this value is higher than the C-J velocity of 1848 m/s (1996) and other author's cited results. This rapid flame acceleration is used for thrust generation in several pulse times. As the model is validated so the detonation wave pressure and temperature contour magnitudes are also justified.

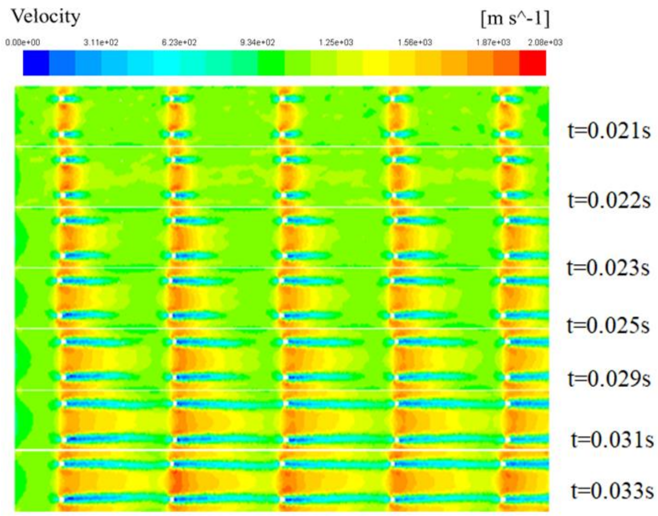


Fig. 4 Detonation wave propagation velocity in detonation tube for several pulse times

Assumptions and Idealization

- The flow is considered to be in unsteady and also in chemical and thermal equilibrium.
- The compressibility effect ($\frac{\rho_d}{\rho_u} \neq 1$) are considered and obeying the ideal gas law.
- The reactive Navier-Stoke equation is solved with second order accuracy.
- The combustion zone is considered as an adiabatic wall.

3. Results and discussions

The energy transfer from reacting mixture and detonation wave propagation in channel has been studied with effect of obstacle. The heat energy generates momentum of detonation wave. The combustion wave propagation is strongly promoted by an array of obstacles. However, the numerical analysis depends on initial boundary conditions but geometry of combustor has a significant role in flame acceleration process. The pilot fuel hydrogen is injected into the combustor through injector and finally air-fuel mixture is ignited by a spark.

3.1 DDT analysis

The unsteady flame propagation and transition to detonation wave in obstructed detonation tube are shown in Fig. 4. The vortex generator leads to increase flame surface area. These obstacles also performed the flame acceleration, which is strongly influenced by reacting flow and stretching interactions between crule of velocity circulation. In this regard, perturbation is initiated inside the combustor and increases momentum flux and vortices of reacting mixture and also reduces ignition delay. Furthermore, chocked flow developed before DDT process. The detonation wave varies from 0.021s to 0.033s. The flame is repeatedly accelerated and separation takes placed by vortices between upper and lower obstacles. The magnitude of flame front velocity is 2080 m/s is obtained from DDT period of 0.029s. The Prandtl-Meyer expansion wave takes place behind each

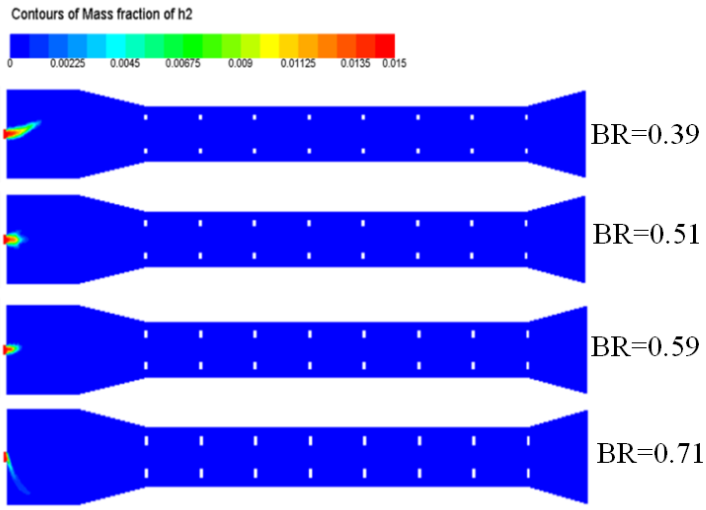


Fig. 5 Hydrogen species mass fraction contour of combustion product in detonation tube with obstacles effect

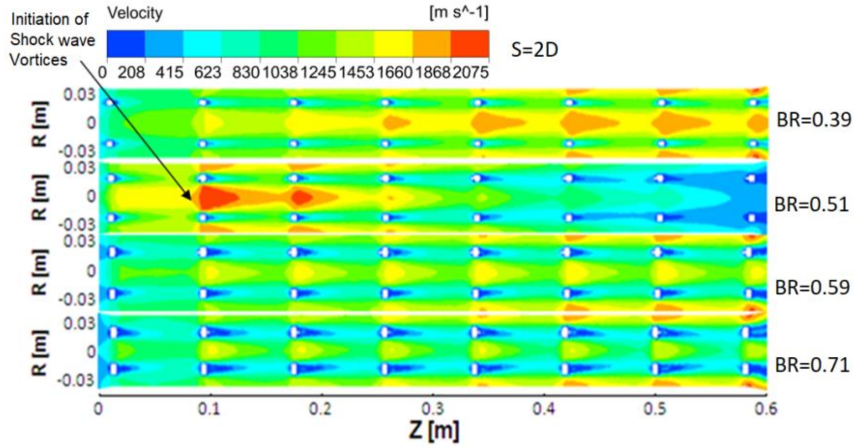
vortex generator, but more perturbation are found near *BR*=0.39. Thus propagation velocity of reacting mixture increases simultaneously. The deflagration to detonation transition occurs strongly appear at centre of detonation tube with maximum propagation speed magnitude of 2080 m/s. When operating pulse time increases, flame shape also reaches to fully developed regime. After certain time period of 0.031s flame surface growth is more and reaches to fully developed detonation wave. Moreover, the maximum thrusts are obtained in pulse time of 0.031s. Although in 0.032s the fully develop flame propagation regimes are present in flame propagation contour analysis, but magnitude of thrust retardation are there at this pulse time. So the minimum pulse times of 0.031s are required for fully develop detonation wave.

3.2 Hydrogen species mass concentration analyses

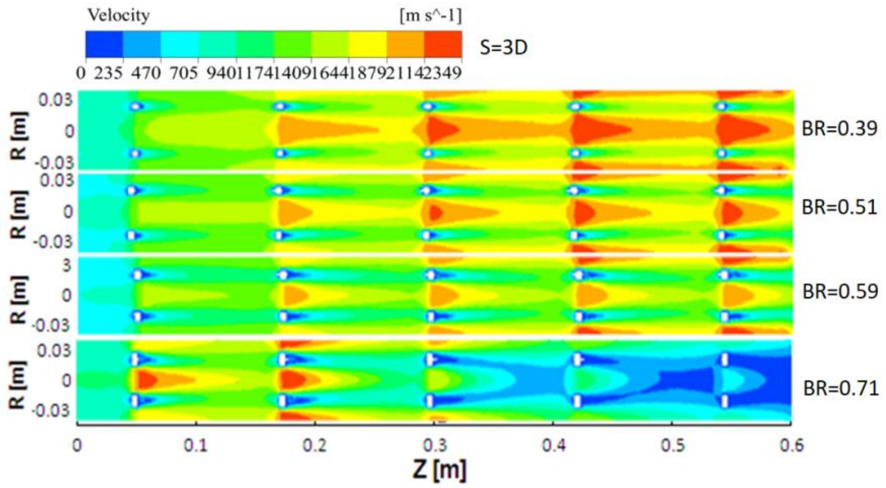
The different H_2 mass fraction contour analysis of detonation combustion wave in PDE combustor for blockage ratio of 0.39 and spacing *S*=2D in detonation tube as shown in Fig. 5. Although heat capacity increases with increasing more hydrogen fuel utilization and exothermic reaction take place. The thermo physical properties i.e., pressure, temperature and density are evaluated by using lesser hydrogen fuel mass concentration in combustor. The mass fraction contour plot analysis shows that maximum hydrogen mass concentration with magnitude of 0.015 is found in combustion chamber. The burned hydrogen mass fraction and faster flame acceleration contour is found in PDE combustor with a smaller vortex generator ratio of *BR*=0.39.

3.3 Effect on flame speed propagation

The comparison between shock wave formation in detonation tube for blockage ratio of *BR*=0.39, 0.51, 0.59, 0.71 and vortex generator spacing of *S*=2D and *S*=3D are shown in Fig. 6. Due to thermal explosion of combustion product, quasi-detonation flame fronts are formed at pulse time of 0.029s in central region of detonation tube. The vortex generator generates turbulence near



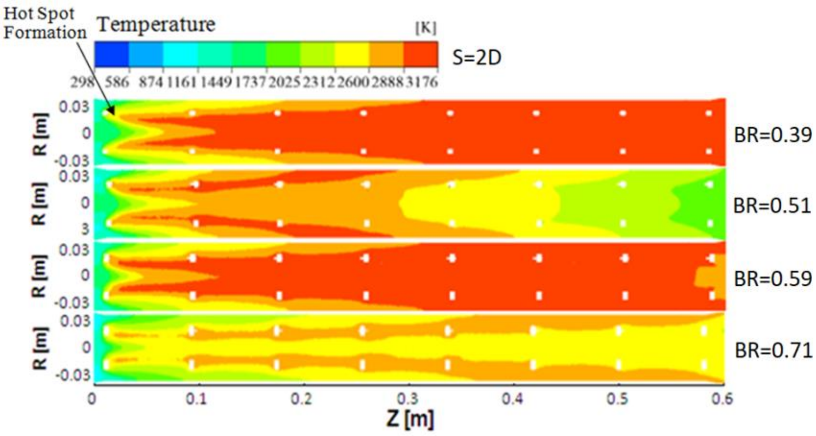
(a)



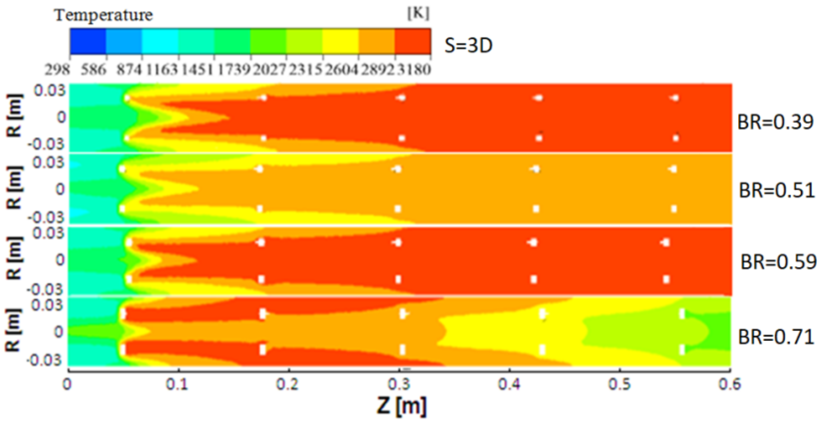
(b)

Fig. 6 Contours of detonation wave propagation velocity in detonation tube with obstacles for spacing (a) *S*=2D and (b) *S*=3D

thin boundary layer of obstacle surfaces and strong recirculation zone is created above speed of sound (*Ma*>1). The velocity fluctuation of detonation wave depends on Mach stem, which is generated by combustion wave. The vortex and recirculation zones also created when flame travels in small orifice channel. The flame oscillates in multiple pulse times and passes over each obstacle and smaller blockage ratio of *BR*=0.39 leads to greater amplitude of detonation wave. After crossing wave traveling distance of 0.3 m in longitudinal direction, the propagation velocity magnitude of 2075 m/s and 2349 m/s are found in detonation tube for vortex generator spacing of *S*=8 cm and *S*=12 cm. The flames are wrinkled due to high Reynold's number flowing ahead of flame front. Further stronger flame propagation is found in smaller blockage ratio of 0.39 for both obstacle spacing. The obtained detonation wave velocities from *S*=12 cm are very much higher than Chapman-Jouguet (C-J) detonation wave speed of 1848 m/s.



(a)

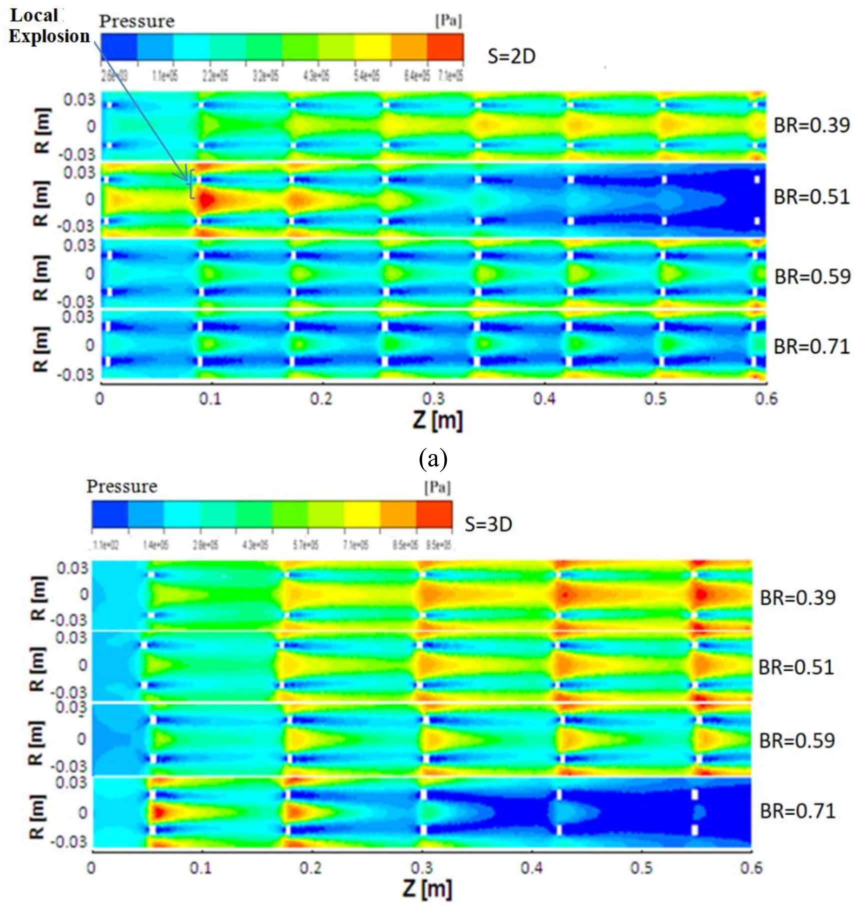


(b)

Fig. 7 Contours of detonation wave propagation temperature in detonation tube with obstacle for spacing of (a) S=2D and (b) S=3D

3.4 Propagation temperature contour analysis

The temperature variation at different positions in detonation tube is shown in Fig. 7. The effect of blockage ratio of BR=0.39, 0.51, 0.59 and 0.71 including obstacle spacing of S=8 cm and S=12 cm are analysed for propagation temperature contour. The detonation wave is eventually triggered in channel by hot-spot. These hot spots create due to formation of thermal explosion of hydrogen-air mixture and instantaneous heat releases takes place. So far, high temperature plays the role for successful detonation wave initiation. Subsequently, deflagration to detonation transition occurs due to appearance of hotspot behind each vortex generator wall and micro explosion. From contour plots analysis it is observed that gradient of temperature gradually rises up at rare end of detonation tube. The first stage of ignition occurred after crossing first obstacle and turbulent flame kernels developed inside the channel, which lead to the detonation wave front. In the smaller blockage flame recirculates and propagates very fast and quickly reaches adiabatic flame temperature. The temperature sharply increases due to heat release from ignition region in



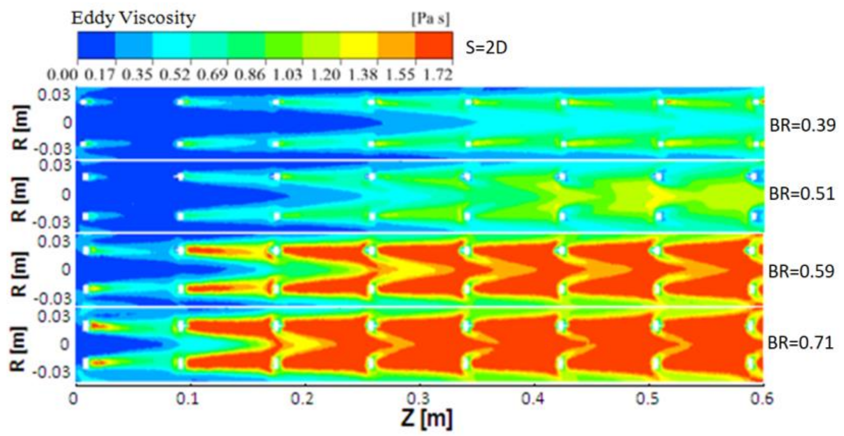
(b)

Fig. 8 Contours of detonation wave pressure in detonation tube with obstacles for spacing (a) *S*=2D and (b) *S*=3D

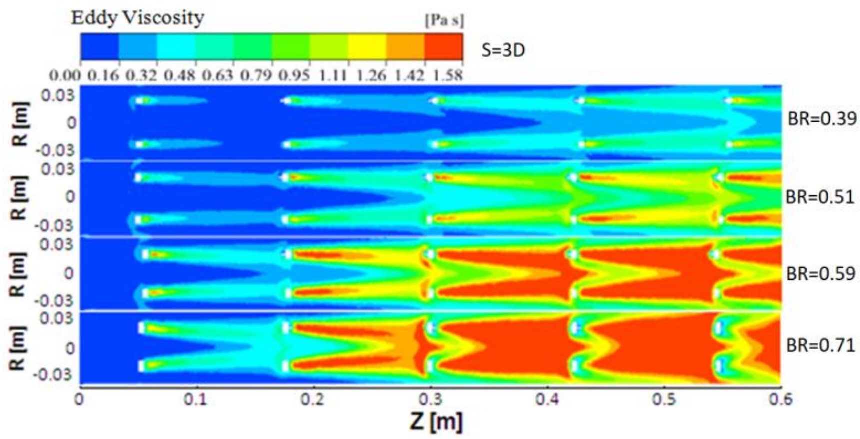
detonation tube. Therefore, leading flame edge is tried to burn fuel particles and produced hot spot regime in which flame accelerates with high propagation speed. The maximum detonation wave propagation temperature of 3176 K is obtained from spacing of *S*=8 cm and temperature of 3180 K is obtained from *S*=12 cm spacing geometry. The detonation wave temperature oscillation intensify near *BR*=0.39 for each spacing, but maximum flammable temperature is obtained from channel with *S*=12 cm spacing. This flame propagation temperature is desirable for chemical energy release from detonation combustion and ignores the ignition delay. The reflected shock wave is used to ignite a fresh fuel-air mixture in multiple pulse time.

3.5 Effect on combustor pressure

The pressure contour traces of shock waves along entire blockage laden channel are shown in Fig. 8. When the flame travels near obstacle wall, strong local explosions have occurred. Subsequently, micro explosion occurred near obstacle layer of detonation tube. So vortex flow



(a)



(b)

Fig. 9 Contours of eddy viscosity of reacting mixture in obstacle landed detonation tube with blockage for spacing (a) *S*=2D and (b) *S*=3D

circulations are found near each obstacle. The recirculation zone is generated between two obstacles. The strong pressure wave tip owing to detonation tube with blockage ratio of *BR*=0.51 and pressure gradient decelerated after crossing the second obstacle from left side of detonation tube. The overpressure magnitude of 7.5×10^5 Pa is obtained from detonation tube with vortex generator spacing of *S*=2D. The noticeable pressure rises ahead of corrugated flame during the flame propagation in detonation tube for *BR*=0.39 to *BR*=0.59 and reflecting shock are found from deflecting wall of detonation tube. For the same blockage ratio with spacing of *S*=3D, shock wave overpressure magnitude is 9.5×10^5 Pa. These shock wave pressures are directly related to propulsive thrust calculation.

3.6 Eddy viscosity contour analysis

The contour plots of eddy viscosity of detonation wave in channel from three dimensional computational simulations have been shown in Fig. 9 for obstacle blockage ratio of *BR*=0.39, 0.51,

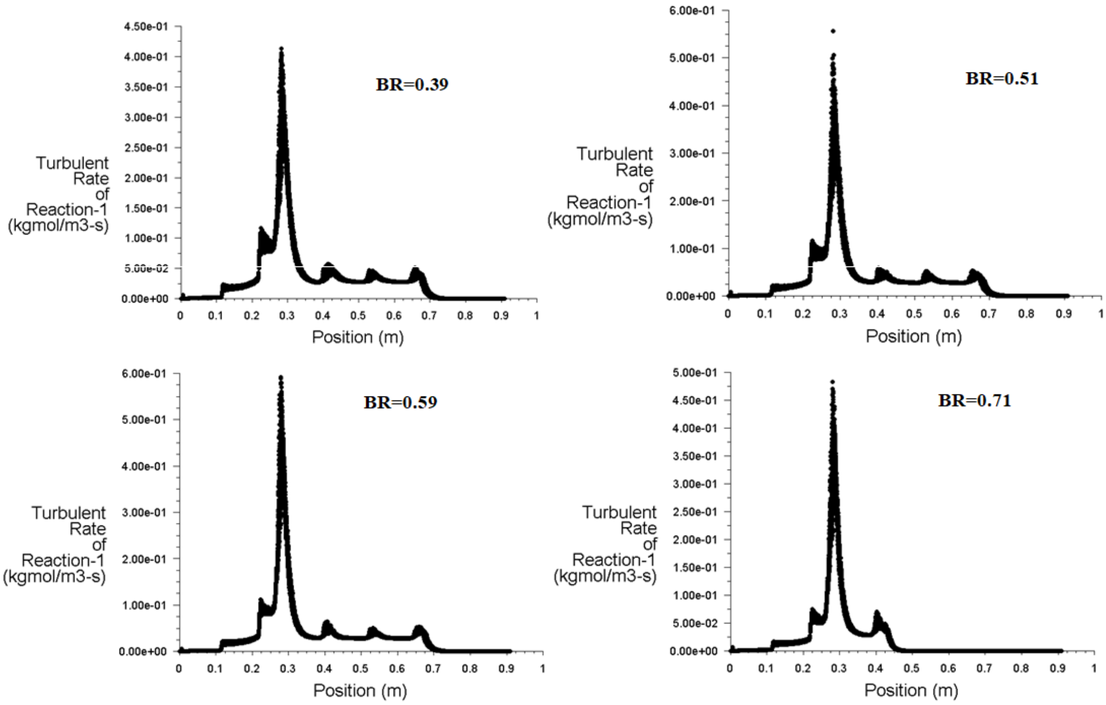


Fig. 10 Variation of turbulence rate of reaction in channel with different obstacles for *S*=12 cm

0.59 and 0.71 at spacing *S*=2D and *S*=3D. Furthermore, eddy viscosity gradually increases from 0.1 to 0.6 m wave traveling distance in detonation tube near *BR*=0.71 and contour plots also show that eddy viscosity is strong for both the aforesaid vortex generator spacing. The magnitude of eddy viscosity is found to be 1.72 Pa-s in spacing *S*=8 cm and 1.58 Pa-s from spacing *S*=12 cm in detonation tube. Moreover, weak eddy viscosity is found at *BR*=0.39 and *BR*=0.51 in aforesaid spacing, due to rapid obstacles. From the contour plots analyses the strong eddy viscosity and mushroom shape flame are appear near *BR*=0.59 and *BR*=0.71 in detonation tube. The weaker eddy viscosity of combustible mixture enhances the deflagration to detonation transition and energy release rate is also increases. From the contour plots of eddy viscosity comparison, it is observed that the undesirable eddy viscosity is found near *BR*=0.71 for both spacing of *S*=8 cm and *S*=12 cm.

3.7 Effect on turbulence rate of reaction

The turbulence rate of reaction of detonation wave propagations inside the detonation tube in longitudinal distance is shown in Fig. 10. The mechanism of DDT is initiated by turbulence rate of reaction in intermediate regime of blockage ratio (0.39<*BR*<0.71) in the channel. So far, Mach reflection occurred behind each obstacle. The combustion instability and flame turbulence near boundary layer of vortex generator contribute to generating the large flame surface area. The excess flame surface area presents the faster depletion of wave and additional energy release is caused by rate of reaction. The turbulence is non equilibrium and propagation energy is transferred into large scale range simultaneously. In small obstacle spacing region very little expansion of

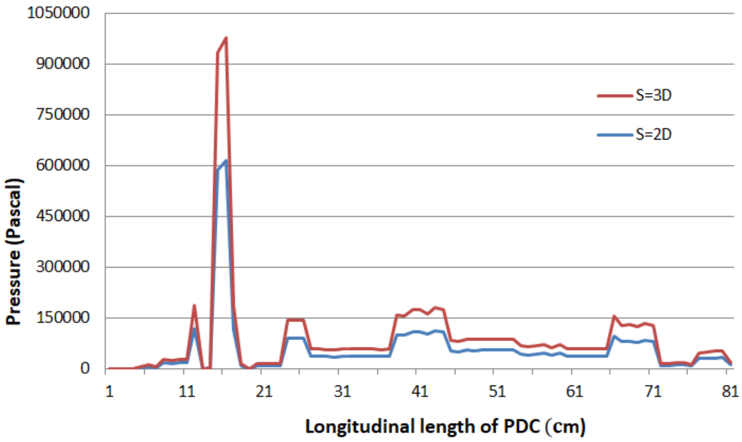


Fig. 11 Detonation wave pressure fluctuation at different wave traveling distance in detonation tube at pulse time of 0.031s

reacting flow occurred and suppressed large scale of turbulence reaction between two obstacles. The detonation wave reaches easily to strong turbulence wave near obstacle affected area. Here the obstacles are examined to simulate the turbulent rate of reaction in detonation tube. The obstacle generates turbulence wave and it increases rapidly by changing the pulse time. The strong turbulence rate of reaction of 0.6 kg-mol/m^3-s is found for spacing S=12 cm with BR of 0.51 and 0.59. It is also found that turbulent rate of reaction varies from Gaussian to bimodal form and later on decreases toward the end of detonation tube. The large activation energy is needed to break the chemical bond of hydrogen molecule, so temperature significantly rises. So far, reaction rate has changed exponentially. The blockage ratio of 0.51 leads to larger growth rate of reaction-flame front surface thus enhancing the heat released from combustion.

3.8 Combustor pressure oscillations analysis

The detonation flame pressure oscillation at several waves traveling distance along the obstructed detonation tube is shown in Fig. 11. The combustor pressure oscillation takes place from PDE combustor to converging section then detonation tube and exit diverging section. Due to change of cross sectional area of physical model, the pressure fluctuation takes place along with longitudinal direction. The obstacles are act as a vortex generator and sustainability of these vortices depends on obstacle spacing (S). So the pressure variations are occurs at different wave traveling distance for aforesaid spacing. Initial flame acceleration pressure magnitude is strong at 0.15 m wave traveling distance and immediately reduces after crossing 0.21 m distance in channel for BR=0.39. The pressure variation comparison has been done for detonation tube having S=2D and S=3D. The pressure magnitude of 11×10^5 Pa at 0.15 m run up distance in channel with spacing S=3D are observed and gradually decreased exit of detonation tube. So the stronger detonation wave pressure gain are found in detonation tube having S=3D at pulse time of 0.031s.

3.9 Effect on propulsive thrust

The propulsive performance of pulse detonation combustor is computed by thrust generation.

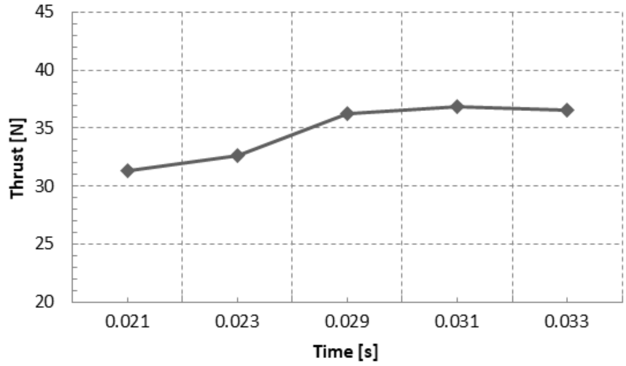


Fig. 12 Propulsive thrust variation in PDC with different pulse time

Therefore, the propulsive thrust is directly depends on detonation wave speed and overpressure generated inside the obstructed channel. The ideal cycle thrust of PDE combustor is analysed by the following identical numerical formula.

$$F_{PDE} = \dot{m}_{exit} \sqrt{2c_p T_{t-wee}[1 - (\frac{P_a}{P_{t-wee}})^{\frac{\gamma-1}{\gamma}}]} \quad (11)$$

Where, "a" stands for ambient state conditions and "t" indicates stagnation condition and "*wee*" represents the wave ejector exit state supplying the nozzle at very short duration time, $\dot{m}_{exit}$ indicating the mass flow rate of isentropic expansion of combustion product.

The dynamic thrust through periodic pulse time from exhaust combustion products is shown in Fig. 12. This thrust generation has been analysed for obstacle spacing *S*=3D having blockage ratio of *BR*=0.39 on operating cycle time of 0.021s, 0.023s, 0.029s, 0.031s and 0.033s. The thrust generation varies from 31.32 N to 36.82 N inside the channel with obstacle effect on aforesaid pulse time. These pick propulsive thrust magnitudes of 36.82 N are obtained at pulse time of 0.031s.

4. Conclusions

The present research work is to investigate the numerical study on acceleration of detonation combustion wave in pulse detonation combustor. The detonation tube has been designed to increase the flame acceleration in combustor. The shock wave initiation and detonation wave propagation in vortex generated detonation tube with combined effect of blockage and obstacle spacing. Further detonation wave propagation is performed for turbulent reaction by species transport model. The following conclusions are drawn from the simulations:

- Flame propagation and fully developed detonation wave transition takes placed within pulse time of 0.031s in operating cycle with significant magnitude of 2349 m/s. Furthermore, lesser fuel mass fraction utilization of 0.15 in channel with smaller blockage ratio of *BR*=0.39 is more effective for flame acceleration and lesser eddy viscosity of compressed air-fuel mixture.
- The diffracting shock from reflecting wall was found in smaller blockage ratio of *BR*=0.39 in each obstacle spacing. Furthermore, the larger vortex generator spacing of *S*=12 cm plays significant role for stable detonation wave with magnitude of 2349 m/s and this value is higher

than that of propagation velocity of 2075 m/s, which is obtained from channel with spacing of *S*=8 cm. Both these velocities are much higher than the C-J velocity of 1848 m/s.

• From temperature contour plot analysis it is observed that nucleation of hot spot area ahead of corrugated flames have appeared in the vicinity of thin boundary layer near obstacle. The propagation temperature of 3180 K is obtained from channel with spacing of *S*=12 cm, this magnitude is higher compared to vortex generator spacing of *S*=8 cm inside the detonation tube. The strong turbulent rate of reaction of 0.6 kg-mol/m^3-s is found in a blockage ratio of 0.51 in the channel with obstacle spacing of *S*=12 cm.

• In propulsion application maximum thrust are required to be obtained in minimum pulse time. The propulsive thrusts are gradually increased up to a fully developed detonation wave. So from the simulation the strong thrust forces of 36.82 N are found at pulse time of 0.031s.

The obtained results from this numerical analysis prevent the energy losses and enhance the fast DDT process to overcome the delay of flame front propagation. Further research work can be carried out for detonation wave speed propagation of different liquid and gaseous fuel-air detonation in channel with triangle, rectangle and semi-circular shape vortex generator.

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CC

Abbreviations

BR	Blockage ratio
C-J	Chapman Jouguet
CFD	Computational Fluid Dynamics
DDT	Deflagration to detonation transition
GIL	Grid Independent Limit
LES	Large Eddy Simulation
Ma	Mach number
PDE	Pulse Detonation Engine
S	Spacing
ϕ	Equivalence ratio