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Numerical Investigation of Predetonator of Pulse Detonation Engine Tube

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Abstract: Pulse detonation engine (PDE) is future propulsion technology that involves detonation of fuel to produce thrust more efficiently than the available current engines. The PDE can provide static thrust for a ramjet or scramjet engine, or operate in combination with turbofan systems. The objective of present study was to observe the effect of predetonator (having disturbances in the form of Shchelkin spiral) on the detonation velocity, pressure and length of PDE tube. In this project a new design has been developed for Predetonator. Initiation and propagation of detonation waves inside predetonation tube has been done by two-step detonation initiation method, low energy ignition system (total energy of 50mJ), and effective Shchelkin spiral of blockage area ratio of 0.43. Liquid kerosene, gaseous oxygen and nitrogen were used as fuel, oxidizer and purge gas respectively with 420mm predetonator, a convergent-divergent nozzle and a 415mm long tube for main detonation has been used. In the present study the filling processes is modeled numerically using CFD code FLUENT. Calculations for the gas flow are carried out by solving the Navier-Stokes equations coupled with the k ε "turbulence model. Numerical analysis of the geometry made has been done by using GAMBIT and FLUENT for two dimensional predetonator model and results have been observed in the form of pressure, velocity and temperature contours at different time step. Numerical analysis obtained results have been compared with the calculated results from NASA CEA code for respective conditions.

Keywords: Detonation, Deflagration, Predetonator and Pulse Detonation Engines (PDE).

I. INTRODUCTION

Aircraft engines are the propulsion system or component of propulsion system which are used to generate mechanical power. At the starting of twentieth century aircraft engines were very simple and low powered machines. These types of engines were designed for one specific type of aircraft. Earliest engines used in aircraft were stationary and then these types of engines were succeeded by rotary engines. The Antoinette series and Gnome and Le Rhone were commonly used at that time. The Antoinette engines were strong, safe and fairly powerful and generating 50 horsepower while the Gnome was rotary engine generating same amount of power.[?]

During the world war high speed aircrafts were greater in demand therefore to achieve higher speed different types of aircraft were designed and manufacture, these modern engines generates much more power and having greater efficiency than the previous types of engines which were available at that time. As per requirements different engines were designed and manufactured for different kind of aircraft.

1.1. Detonation Engines

Energy release rate in detonation is much higher than in deflagration, also engines utilizing detonation have higher thermodynamic efficiency, and they are easier to scaling as compared to conventional engines which use declarative combustion. If detonation combustion is applied to jet engine, efficiency of the engine cycle can be theoretically increased even more than 15 percent. This is due to the fact that during detonation specific volume of reacting mixture is decreased, so the theoretical efficiency of the cycle is even higher than for constant volume combustion and specific impulse for such propulsion systems is much higher than for conventional engines.[21; 20; 6]

1.2. Detonation versus Deflagration

In detonation the reaction front in fuel-air mixture propagates with the velocity of order of km/s, and produces a significant pressure increase. Detonation velocity for fuel-air mixtures is usually over 1.8 km/s, and creates pressure increase of more than ten times.

In the mixtures with oxygen, detonation velocity can be as high as 3 km/s and the pressure rise can be higher than 20 times. For marginal conditions, quasidetonation (or degraded detonation) can propagate with the velocity of the order of one km/s. In past the detonation most often occurred in accidental explosions, and since, in detonation the pressure increases significantly, damages are usually much more severe than those in non-detonative explosions. Up to now, practical applications detonative combustion has been very limited. Only recently the detonation process is being applied to Detonation Engines.[22; 21] In contrast to detonation, deflagration flame velocity is of the order of dozens m/s, so combustion also has to be organized at the stoichiometric ratio (higher burning velocity) what results in a high combustion temperature and in production of high concentration of NOx. Since in jet engine temperature of burned products is very high, it is necessary to mix extra air before turbine, which makes the design more complicated. Also in the combustion chamber the pressure drops due to the combustion.

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In contrast to deflagration the combustion zone in detonation is very small. If the detonation propagates in a lean mixture, the combustion temperature is relatively low, so a low emission of NOx is expected (also due to a small residence time). Thus there is no necessity to add extra air before the turbine (in turbojet engines). In addition due to the detonative combustion the pressure in chamber is increased. So application of the detonation to jet engines offers significant improvement to its performance.[6; 19; 18; 3].

1.3. Pulse Detonation Engine

A pulse detonation engine (PDE) is a new type of propulsion system that utilizes detonation waves to combust the fuel and oxidizer mixture. The engine is pulsed because the mixture must be renewed in the combustion chamber between each detonation wave and the next. Theoretically, a PDE can operate from subsonic up to a hypersonic flight speed of roughly Mach 5. An ideal PDE design can have a thermodynamic efficiency higher than other designs like turbojets and turbofans because a detonation wave rapidly compresses the mixture and adds heat at constant volume. Consequently, moving parts like compressor spools are not necessarily required in the engine, which could significantly reduce overall weight and cost. PDEs have been considered for propulsion for over 70 years. Key issues for further development include fast and efficient mixing of the fuel and oxidizer, the prevention of auto ignition, and integration with an inlet and nozzle. PDE differs from conventional system in two major ways: detonation combustion and unsteady operation.[9; 16] Extensive researches have been done over past few decades in the field of detonation engines and among all detonation engines pulse detonation engine has attracted considerable attention due to its potential advantages in thermodynamic cycle efficiency, reliability, simplicity in hardware, and operational stability. Despite extensive research in PDE over the past several decades, it is not yet to be used in practical volume-limited propulsion application where the preferable fuel is liquid hydrocarbon. A number of fundamental challenges and engineering issues needs to be solved in developing PDE with high performance. One of the key barriers to the realization of an operation PDE lies in the difficulty to rapidly and reliably initiate the detonation with low energy source in a short distance. Detonation can be initiated either directly or indirectly by a deflagration-to detonation transition (DDT) process, which describes the acceleration of a subsonic deflagration created by low initiation energies to a supersonic detonation. Direct detonation initiation requires a prohibitive amount of energy being deposited, and the minimum ignition energies are approximately 26000 J for several hydrocarbon/ air mixtures therefore indirect detonation initiation by a DDT process.[6; 15; 17; 11]

1.3.1. Deflagration to Detonation Transition (DDT)

This begins with the deflagration initiated by some relatively weak energy source which accelerate through interaction with its surroundings into a coupled shock wave reaction zone structure characteristic of a detonation. DDT is the general process through which a subsonic combustion wave (flame or deflagration) becomes a supersonic combustion wave (detonation). After a deflagration is created, it may decelerate or accelerate to steady state velocity or accelerate and then abruptly transition to detonation. This process can be divided into four phases. [21; 1]

- Deflagration initiation: A relatively weak energy source such as an electric spark is used to create a flame. The energy release from the initiator device along with radical production and energy release from the mixture compete with loss processes including expansion of the reacting flow field and thermal conduction and species transport away from the flame front. Flammability limits which result from this competition have been extensively researched.[3; 5; 14]
- Flame acceleration: Increasing energy release rate and the formation of strong shock waves are caused by flame acceleration. The observed mechanisms for flame acceleration are outlined above.
- Formation and amplification of explosion centers: One or more localized explosion centers form as pockets of reactants reach critical ignition conditions (the so-called explosion within the explosion). Critical temperatures are typically around 1500 K and 2000 K for fuel-oxygen and fuel-air mixtures, respectively. The explosion centers create small blast waves which rapidly amplify in the surrounding mixture.[8; 12]
- Formation of a detonation wave: The amplified blast waves and existing shock reaction zone complex merge into a supersonic detonation front which is self-sustaining. [15; 21]

1.3.2. Factors Affecting DDT

- Blockage Ratio
- Obstacle Geometry and Spacing
- Length
- Position of obstacle section in tube
- Fuel/Air Equivalence Ratio
- Fuel/Air Mixing
- Fuel valve open / close time
- Inlet air velocity
- Inlet Pressure and Temperature

II. NUMERICAL MODELLING AND MESHING

Two dimensional geometry of predetonator has been made using GAMBIT Tool and an axis symmetric model has been preferred because this type of model was simple to design, easy to mesh and analyzed and results with less error and reduced computational time has been observed. GAMBIT version 2.2.30 has been used in this case.[4; 2] A cylindrical tube or predetonator of length 420 mm and outer Diameter 30 mm has been modeled. Predetonator consists of Reactants injector, Ignition section, DDT chamber and Test section. The blockage area ratio of the Shchelkin spiral welded inside the DDT chamber was 0.43 and length of DDT chamber was 360 mm. Due to the consideration of axis symmetric model, diameter has been reduced to 15 mm but length of predetonator remain unchanged. Four type of commands i.e Point, Edge, Face and Volume commands has been used for modeling of our geometry.

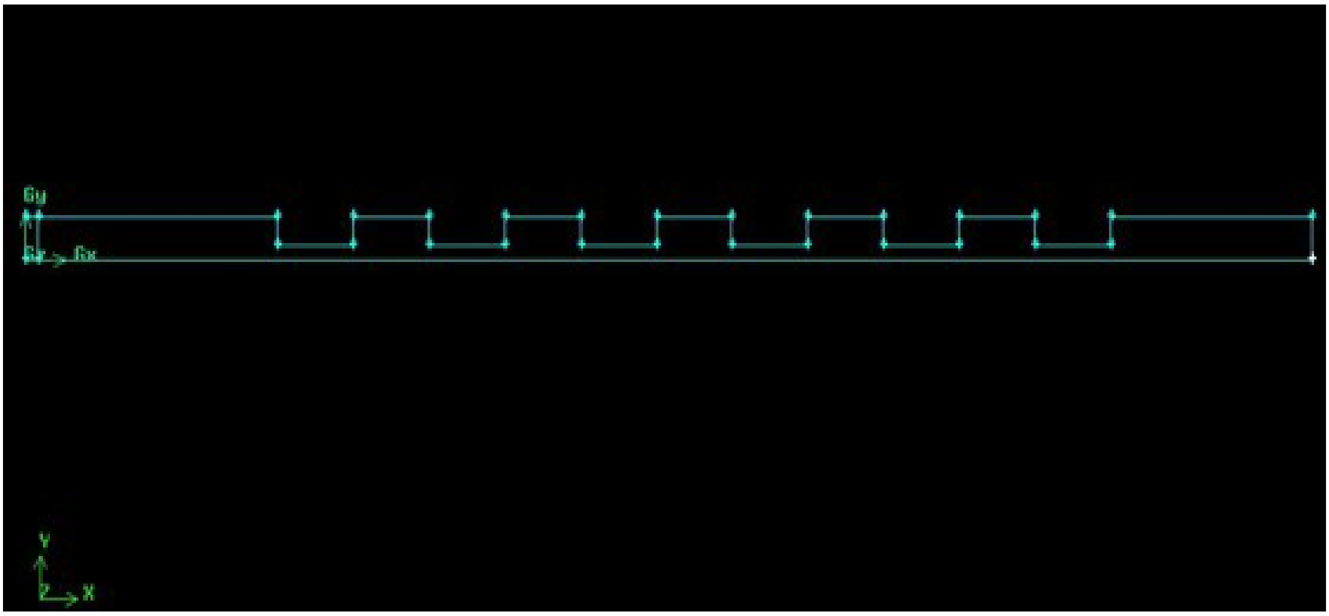

Figure 1: 2D model of Predetonator.

Principle of structured mesh in the design software GAMBIT has been utilized for meshing. Edge mesh has been performed by providing interval counts and this was followed by generating face mesh with the help of tetrahedral mesh principle. If number of interval counts has been given on the edges of the geometry that has been modeled inside the GAMBIT this would lead to start the process of mesh like this modeling software that was nothing but the GAMBIT would start creating the meshing nodes and hence mesh on the entire edges have been created. The next step was to create mesh nodes by the specific values that were given for the problem this could be triangular shaped, tetrahedral shaped or both types too. Mesh was uniform throughout the section and this has been shown in the Fig 6.

Table 1: Mesh details of Predetonator tube

Cells	Faces	Mesh Quality
93600	Face1, Face2	100%

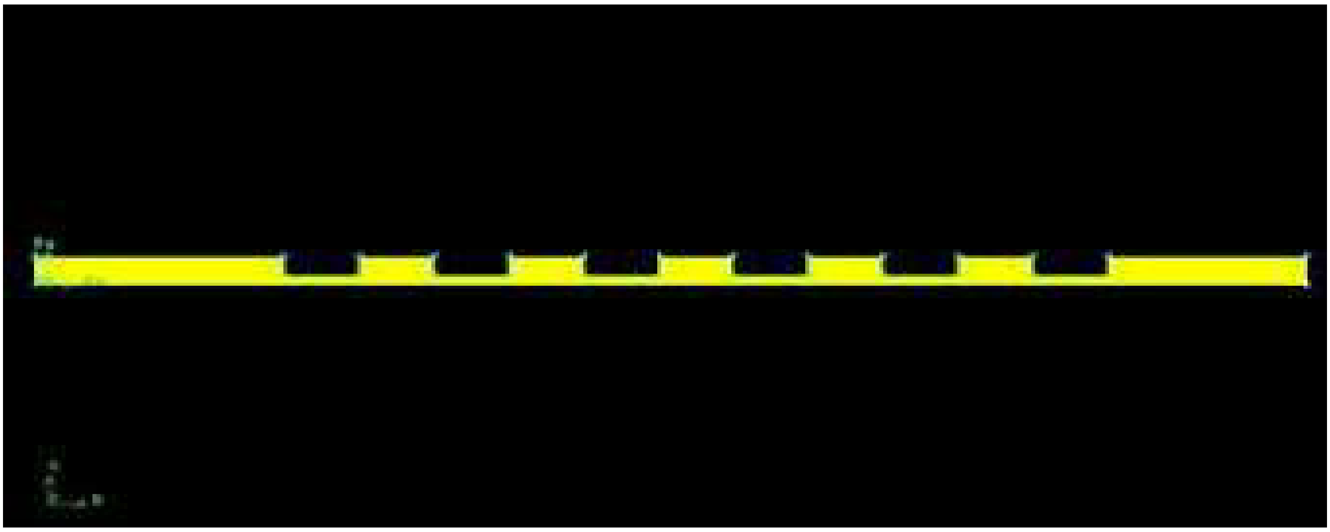

Figure 2: Meshed view of 2D Predetonator Tube.

2.1. Zone specification and Boundary Conditions

Two different zones i.e Hot and Cold zone have been specified which has been shown in the next Fig. and physical properties of the fluid has been defined separately for these two zones. Patching the zones in the solver part has provided the propagation of shock wave inside the combustion chamber. An axis symmetric model has been used and the boundary surrounded by the pre detonation chamber has been defined as the wall. Cold zone temperature has been maintained at 300K and pressure at 1 atm while hot zone temperature was nearly about 2600K and pressure was about 5.5 atm. In both zones kerosene mixture has been used. Due to the occurrence of no slip condition at the walls and the temperature of 1000K has been maintained to calculate temperature difference which leads to detonation in- side the combustion chamber.

The wall's material was Aluminium having 202.4 W/MK amount of thermal conductivity and backflow temperature was maintained at 1000K.

Table 2: Values of Different Properties

Properties	Kerosene-air mixture
Viscosity	1.72 e-05 kg/m-s
Mass Diffusivity	2.88 e-05
Specific Heat	1005 J/kg-K
Thermal Conductivity	0.0454 W/m-K

2.2. Simulation and Solver Model

Following steps were required to solve this problem

1. Define the boundary and cell zone conditions
2. Monitor the solutions
3. Inspect and save the results obtained
4. Until we reached to the converged the solution we have to check again and again for the different numerical value that we are given for solving the problem

FLUENT Tool has been used as a solver in this study and finite volume system has been used to solve the continuity, momentum and energy equation with the accompanying boundary conditions. Partial differential equations has been solved by using SIMPLEC finite volume method.[13] The propagation of the reactants entering PDE during filling stage was important therefore an unsteady solver has been selected. Boundary conditions and application of material properties of the fluid play major role in computational analysis of the flow. Adequate model properties and boundary conditions has been required for result converging. To consider the turbulence effect in the present research the simplest k- model with default setting has been preferred.

The direction of the flow was normal to the inlet boundary and outlet was specified as pressure out therefore outlet boundary pressure was 1 atm. Each time step has been determined and monitored by the solver and time step (Dt) has been calculated by using the following formula:-

Pressure implicit formulation has been used to obtain the better solution and to reduce the time steps. The flux type which has been used in the solution method was the Roe-FDS. Green–Gauss cell based spatial discretization technique has been used to get a faster solution rate where second order upwind has been used in the flow. In this problem our flow was highly turbulent with changes in density of mixture that was kerosene and air, therefore the type of solver which has been used here was Density based to solve this problem. As the detonation in the combustion chamber was changing instantaneously with the time so transient type of solver has been preferred.

The simulation has been initialized by taking the physical properties of kerosene air. The solution has been initialized so that the flow parameter values can be calculated by using the initialized boundary conditions. The operating pressure was maintained at 1 atm and temperature of the outside of the combustion chamber was 300 K. The discretization scheme was chosen to be second order upwind scheme for all flow and the convergence criteria has been fixed to 1e-03 for momentum, energy and continuity equations.

III. RESULTS AND DISCUSSION

Combustion process has been initiated via weak spark of 50 mJ timed to closely coincide with the end of fill cycle. The spark plug is located near head end of predetonator tube. Blockage ratio of 0.43 has been used to reduce the run up distance to detonation.

Detonation waves create a rise in pressure during combustion. Consequently, the pulsed detonation engine (PDE) must use a system of valves that close off the combustor while the wave is formed and then open for refueling. Mechanical valves could be used for cycle frequency of about 100 Hz but in our study cycle frequency was about 5 Hz therefore valveless system has been preferred for multishot pulse detonations. Convergence has been determined by inspecting the scaled residuals and confirming that they were less than 10-3.

3.1. Pressure and Velocity Contour

The value of pressure would leads to the further propagation as the detonation moves in forward direction and the pressure contours has been calculated at the time step 0.009 second and showed up to the 0.18 second. The model has been considered as converged when the continuity, momentum and energy equations approach constant values. Pressure contours has been plotted at different time steps. In the Fig.9 pressure contours showed that there was ignition of spark inside the combustion chamber because of pressure and this value would lead to the further propagation as the detonation would move in forward direction, Ignited combustion was propagating which has been shown by the second and third pressure contours of the Fig.9 and this propagation was due to the change in static pressure with respect to change in position of the tube.

Magnitude of detonation wave velocity at three different time step has been shown in the form of velocity contours. After the initiation process, detonation waves have formed and these detonation waves accelerated at certain speeds and due to the

Shchelkin spiral in the path, speeds of these detonation waves has been disturbed and.

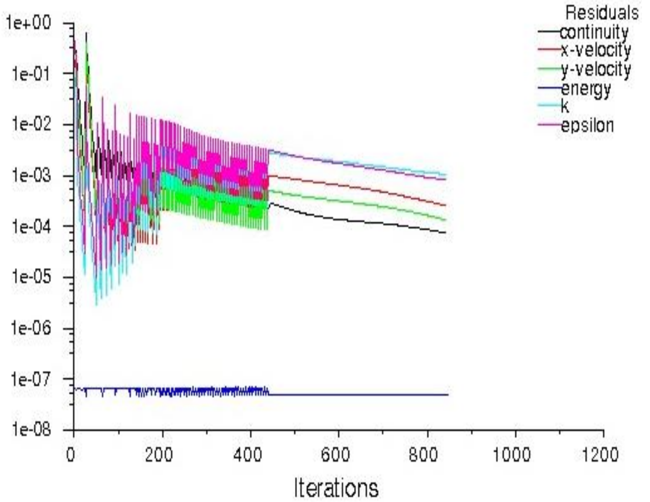

Figure 4: Residual Plots of Model with Closed End Inlet.

This may cause sharp rise in the speed. The first contours of the velocity show that there is initiation in value of velocity inside the combustion chamber because of this the whole combustion mixture will propagates at higher speed and like this we can observe the detonation inside the given domain and the velocity contours is calculated at the time step 0.009 sec which has been shown in Fig.11. At time step 0.035 sec, this has been shown (Fig.12) that there was increment in thevalues of velocity as compare to last time step value hence what we assumed in the last was true. The explanation of above statement was clearly shown in the Fig.12. At the last time step that is 0.18 sec we observed that finally up to a certain level the value of velocity is propagating and this will surely provide us at the final value of velocity.

Velocity magnitude rises from 0 because it also include initiation process after the initiation process and formation and propagation of detonation wave these value has increased sharply. Due to the disturbances in their way some detonation waves have been decelerated which could be seen in the above velocity contour plots. These plots include accelerated and decelerated both type of detonation waves. At the time step 0.18 second 2D and 3D (isometric) view of pressure and velocity contours have been plotted and these plots gave the clear vision of propagation of detonation wave and the magnitude of detonation velocity and detonation pressure.

3.2. Temperature Contour

The red colour regions in the temperature contours was representing the high temperature zones and showing the temperature contours of the two-dimensional model. As noticed from the temperature contours, the flow in the detonation tube has become relatively uniform when the time reaches 0.18 second. Just after the initiation when detonation wave has been formed static temperature has been rising very sharply but after certain time of starting of propagation of these waves static temperature nearly becomes constant which has been shown in the Fig.14 and Fig.15.

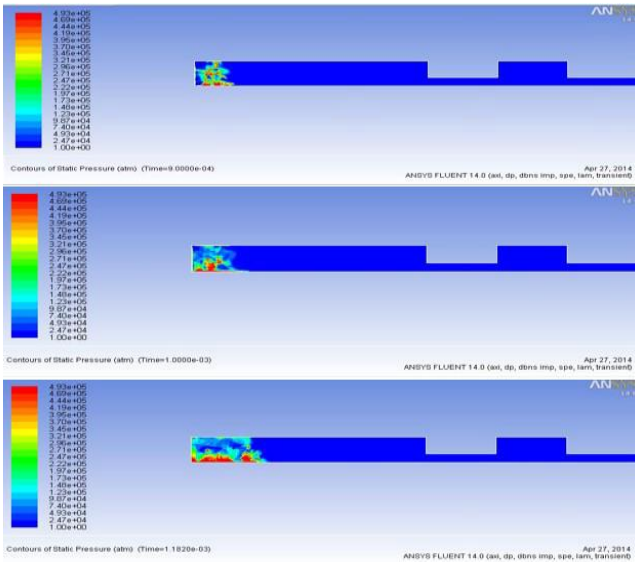

Figure 5: Propagation of Detonation wave.

By observing these figures, physical phenomenon of detonation inside the pre detonation chamber has been achieved.

Table 3: Properties at Three Different Time Steps

Average Pressure at Initiation Point (KPa)	Average Velocity Before First Disturbance (m/s)	Velocity at the entry of CD nozzle (m/s)
1422	33.8	795
1518	32.36	898
1615.72	25.32	982

After the initiation process, waves were travelling at some speeds and disturbances in the form of Shchelkin spiral were available in the path of wave and due to these disturbances most of the waves have been accelerated while some were decelerated too.

At the end of these disturbances waves have been accelerated to supersonic speeds. CD nozzle at the end of pre-detonator has been used to accelerate this supersonic wave to hypersonic wave. Flow has been accelerated to supersonic level in pre-detonator.

Table 4: Properties Obtained for PDE tube at Three Different Times–Steps

Average Static Pressure at the exit of PDE (MPa)	Average Exit Velocity of PDE (m/s)
2.3762	1694
2.6315	1758
2.690	1865

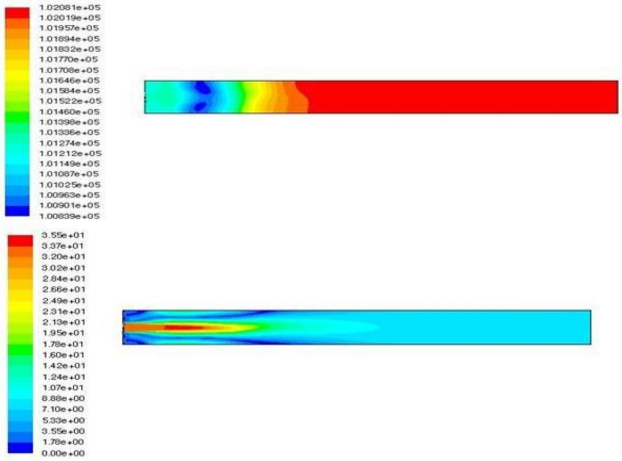

Figure 6: 2D pressure and Velocity contours at t=0.18 sec.

Due to the presence of converging-diverging nozzle velocity of the detonation has been reached to hypersonic level and also there was sharp increment in pressure ratio which resulted in the sharp increment in static pressure ratio.

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In the Table 5 average exit static pressure and exit velocity of pulse detonation engine has been shown.

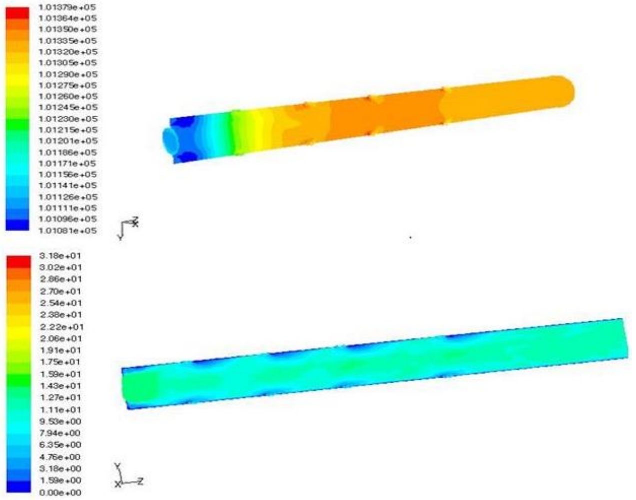

Figure 7: Isometric view of Pressure and Velocity Contours at t=0.009 sec.

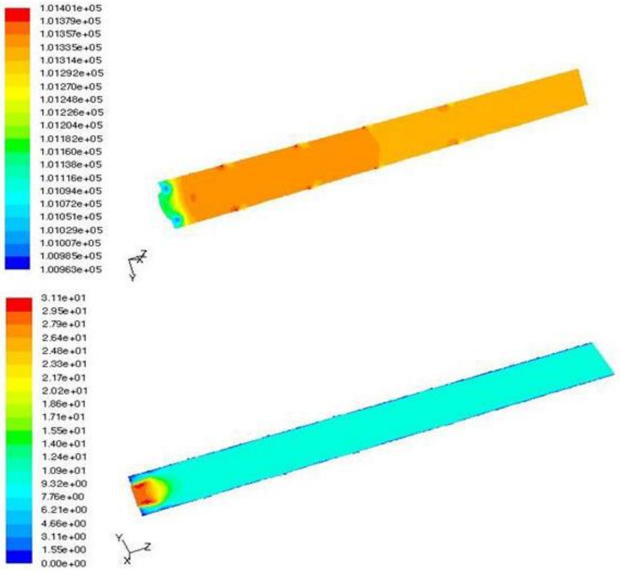

Figure 8: Isometric view of Pressure and Velocity contours at t=0.035 sec.

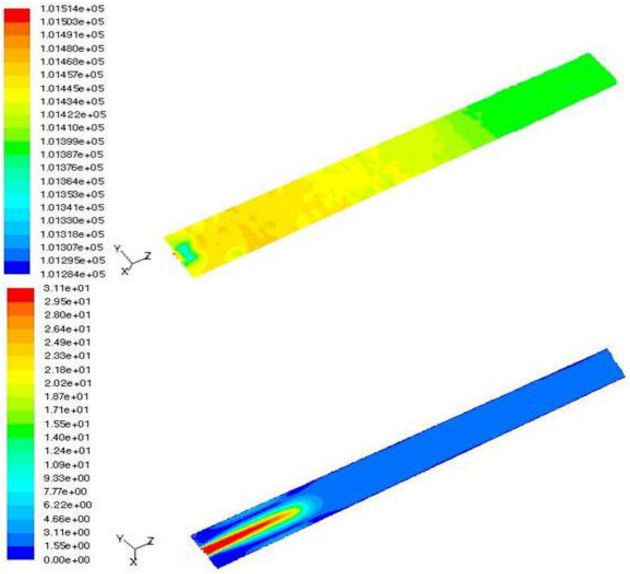

Figure 9: Isometric view of pressure and Velocity Contours at t=0.18 sec.

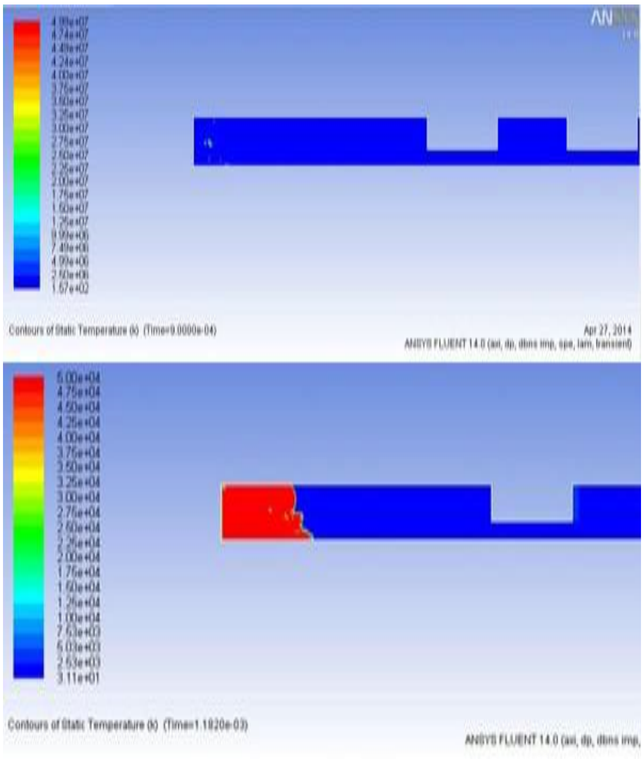

Figure 10: Temperature plots at different time steps.

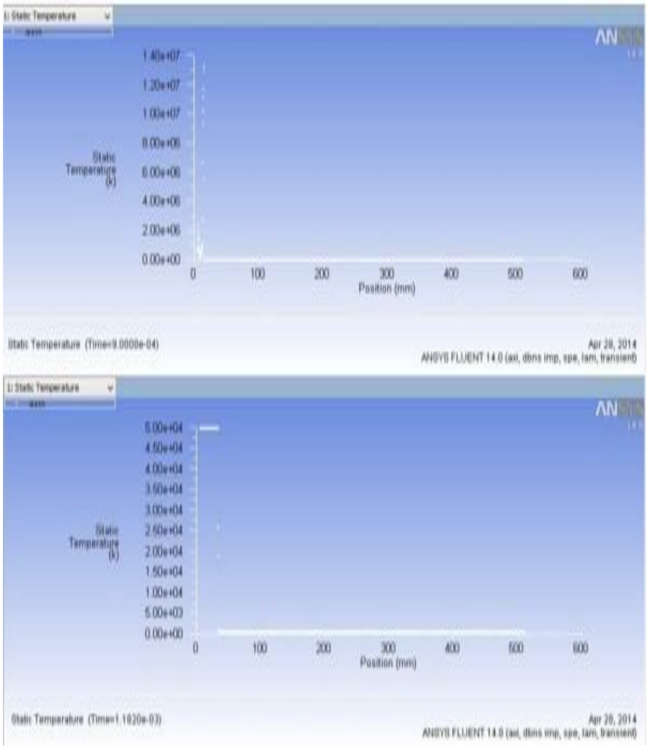

Figure 11: Static Temperature (K) variation at different time steps.

IV. CONCLUSION

- For pure Liquid kerosene/air mixture, predetonator of length 420mm and OD of 30mm and detonation frequency of 5 Hz was successfully realized and this was an important step for the decrement of overall PDE tube length.

- Numerical analysis has been done for predetonator and variation of pressure, Temperature and Velocity with respect to change in position have been plotted at different time steps. 2-D plots of temperature, pressure and velocity has been processed which was clearly indicating the initiation and propagation of detonation wave.
- Numerical simulations are equally important to visualize the detonation combustion phenomena in PDE combustor. The PDE combustor with obstacles having kerosene-air mixture has been simulated using CFD code FLUENT. It has been observed that obstacles of BR 0.43 were useful for PDE combustor design and development and CFD results also indicated that converging-diverging nozzles were not more effective at low ambient pressure.
- CFD results also indicated that converging-diverging nozzles were not more effective at low ambient pressure.
- Use of pre detonator resulted in reduction of the total length of pulse detonation engine tube.
- Static pressure and detonation wave velocity obtained through numerical analysis were 2.65 MPa and 1865 m/s respectively. Results obtained in both the case were comparable and computational result differs from the theoretical NASA CEA code result due to method chosen for analysis and some human error.
- Results obtained in Numerical analysis were 65 percent approx. of results calculated through NASA CEA code

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Appendix "A"

This model has been solved using the above mentioned initial conditions, boundary conditions and a simplest k-" turbulence model, using the Navier-Stokes equations.[10; 7] The general form of conservation equations, neglecting the body force has given.

$$\frac{\partial\rho}{\partial t} + div\,(\rho V) = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ (1)\ \{\text{Continuity}\}$$

$$\frac{\partial(\rho u)}{\partial t} + div\,(\rho u V) = -\frac{\partial p}{\partial x} + div\,(\mu\, grad\,(u)) \ldots\ldots\ldots\ (2)\ \{\text{X-momentum}\}$$

$$\frac{\partial(\rho v)}{\partial t} + div\,(\rho v V) = -\frac{\partial p}{\partial y} + div\,(\mu\, grad\,(v)) \ldots\ldots\ldots\ (3)\ \{\text{Y-momentum}\}$$

$$\frac{\partial(\rho w)}{\partial t} + div\,(\rho w V) = -\frac{\partial p}{\partial z} + div\,(\mu\, grad\,(w)) \ldots\ldots\ldots\ (4)\ \{\text{Z-momentum}\}$$

$$\frac{\partial(\rho e)}{\partial t} + div\,(\rho e V) = -div\,(V) + div\,(k\, grad\,(T)) + \Phi \ldots\ldots\ (5)\ \{\text{Energy}\}$$

Where ρ is the density, μ is the dynamic viscosity, T is the temperature and Φ is the dissipation function. The two dimensional form of the equation can be obtained by dropping the parameters relevant to third dimension. The realizable k-ε model is defined by the following two transport equations,[13; 10].

one for the turbulent kinetic energy (k) and second for the rate of dissipation of turbulent kinetic energy.

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]}{\partial x_j} + G_k + G_b - \rho e - Y_M + S_k \;\ldots\ldots\ldots\ldots \;(6)$$

{Turbulent Kinetic Energy (k)}

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial \varepsilon}{\partial x_j}\right]}{\partial x_j} + C_{\varepsilon 1}\frac{\varepsilon}{k_M}\left(G_k + C_{\varepsilon 3}G_b\right) - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} + S_\varepsilon \ldots\ldots \;(7)$$

{Rate of Dissipation of T.K.E}

In these equations, $G_(k)$represents the generation of turbulence kinetic energy due to the mean velocity gradients; G_b is the generation of turbulence kinetic energy due to the buoyancy; Y_M represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate;[10; 13] $C_{\varepsilon 1}$,$C_{\varepsilon 2}$ and $C_{\varepsilon 3}$ are constants; and are the turbulent Prandtl numbers for k and , respectively.

The values of the constants can be listed as:

$$C_{\varepsilon 1} = 1.45, C_{\varepsilon 2} = 1.91, C_{\varepsilon 3} = 0.07, \sigma_k = 1.0, \sigma_\varepsilon = 1.25$$

Above default values have been observed from the experiments with water and air for fundamental turbulent shear flows. Decaying isotropic grid turbulence and homogeneous shear flows have been included in this fundamental turbulent shear flow experiment and it was found that this experiment was working fairly well for wide range of wall – bounded and free shear flows.