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CFD Analysis of Premixed Methane-Air Combustionusing Laser Ignition

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Abstract

In this work Computational fluid dynamics (CFD)model is developed for analysis of premixed methane-air combustion in constant volume combustion chamber. First CFD model was implemented for natural gas –air mixture and validated with experimental results for pressure-time history from literature. Then CFD model is implemented for analysis of methane-air mixture.For ignition of premixed mixture laser ignition method is used. In this study the variation of pressure versus time is investigated to study the combustion characteristics. Also variation of mass fractions for reactants and products with respect to time was found out from CFD analysis. For CFD analysis commercial CFD solver STAR CCM+ is used.

Keywords:*STAR CCM+, Premixed, Laser ignition, methane-air mixture.*

1. Introduction

The research is going in the area of alternative fuels for improvement in efficiency and reduction in pollutant emissions compared to conventional fuels. Gaseous fuels are attractive as used in internal combustion engines, since they have wide ignition limits and capability to form homogeneous mixtures. Amonggaseous fuels, Compressed Natural Gas (CNG) contains approximately 96% of methane. Methane has wide flammability limits and better anti-knock characteristics as compared to gasoline. Methane has higher octane number as well as higher spontaneous combustion temperature, thus methane fuelled engines can lead to higher thermal efficiencies by operated at relatively higher compression ratios. In addition to this, formation of pollutants and fuel consumption can be further decreased by igniting lean methane-air mixtures.
To ignite the air-fuel mixture under extreme conditions like lean combustible mixture and high initial pressure requires high voltage when using conventional spark plug. Life time of spark plugs is significantly reduces by providing the necessary spark energy to operate these engine conditions. An alternative solution to standard spark plug is the use of pulsed laser which is focused to create plasma, called as laser ignition. Laser ignition also has the advantage ofgiving lower emissions. Interest in laser ignition has increased in recent years because of its many potential benefits over conventional ignition system.

Hassan Mohamed et al.(1999)worked on laser induced spark ignition of methane-air mixture in a constant volume combustion chamber to study the combustion characteristics. They varied initial pressure, equivalence ratio and spark energy to explore flame behavior. Shrivastava et.al (2011)experimentally investigated the flame kernel characterization of natural gas-air mixture, in this research work they used Nd-YAG 1064 nm laser to ignite the natural gas-air mixture. (Tran X. Phuoc) studied Single-Point Versus Multi-Point Laser Ignition. He investigated the experimental Measurements of combustion times and pressures for single point and two point laser ignitions of methane-air and H_2-air mixtures. Also Tran X. Phuoc (2000) measured laser-induced breakdown thresholds of combustion gases. He experimentally found breakdown threshold laser intensities of air, O_2, N_2, H_2 and CH_4 using a Q-switched Nd–YAG laser operating at 532 nm and 1064 nm. Robert Doddet.al (2007) work on the laser ignition of IC test engine. They studied thecombustion parameters by varying the several laser parameters mainly, pulse energies, pulse lengths and their effect on the engine performance.

2. Geometry and materials

In this analysis, methane is used as fuel and air is used as oxidizing agent. In constant volume combustion chamber premixed mixture of fuel and air is already present. To ignite the premixed mixture present in combustion chamber Q-Switched Nd-YAG laser is used. The pulse duration for this laser is 6-9 ns.

Geometry used in this simulation is shown in figure 1. The constant volume combustion chamber has the total length of 180 mm and the diameter of 80 mm. As the fuel methane and oxidizing agent air is already mixed before entering the constant volume combustion chamber, hence combustion chamber is closed from all sides. The combustion chamber is made up of steel and has maximum pressure capacity of 250bar.

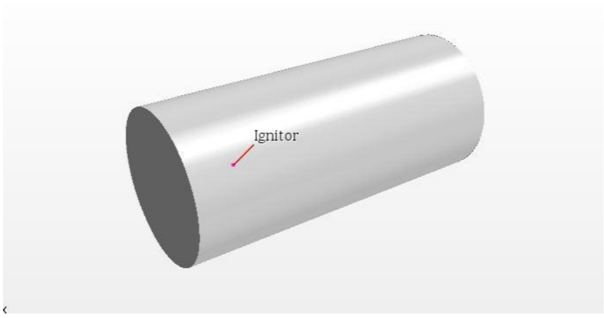


Fig.1 Geometry of combustion chamber

3. Meshing

Meshing plays vital role towards the exact solution of the problem. Meshing should be fine enough to get the more accurate results. A mesh is descretized representation of the computational domain. The mesh is used by physics solver to provide numerical solution. In this work Star CCM+ mesher is used to generate meshing. Models used for meshing are surface remesher, polyhedral mesher, and prism layer mesher. Surface mesher is used to improve overall quality of existing surface and optimized it for volume mesh model. It is used to retriangulate the surface. For volume meshing polyhedral mesh model is used because it is easy and efficient to build. Also in terms of solution quality polyhedral mesh gives more accurate result as compare to tetrahedral mesh but it uses more computational time. In these present work two dimensional meshes is used to solve the numerical equations. The following meshingconditions and sizes were applied to obtain the required meshing of constant volume combustion chamber which is a computational domain for CFD analysis,

Table 1 Mesh details

Base Size	1 mm
Relative Minimum Size	10 % of Base Size
Relative Target Size	50% of Base Size
Surface Growth Rate	1.2
No. Of Prism Layer	3
Prism Layer Thickness	33.33% of Base Size
No. of Cells	58041

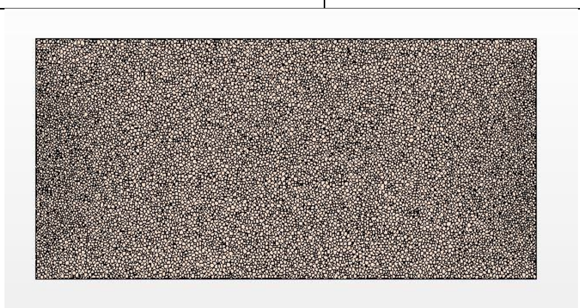


Fig. 2 (a) Two dimensional mesh view of combustion chamber

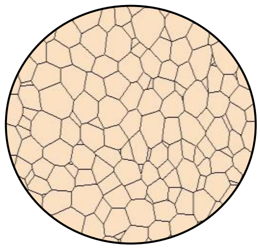


Fig.2 (b) Polyhedral mesh

Mesh sensitivity is checked with three different mesh having 2mm, 1.5mm and 1mm base size for fined mesh. To check mesh sensitivity simulation is run with different mesh sizes. Detailed of mesh sensitivity is given in table 2.

Table 2 Mesh Sensitivity

	MESH 1	MESH 2	MESH 3
Base Size	2 mm	1.5 mm	1 mm
No. of Cells	14621	26215	58041
Maximum Pressure (bar)	41.215	42.447	43.057

From mesh sensitivity it is clear that meshing with 1 mm base size gives better results and large number of cell count than the other base sizes for mesh. Hence, to avoid extra computational time we select mesh of 1 mm base size for mesh.

4. Model description and simulation method

Present work deals with the study of combustion in constant volume combustion chamber. In this study we assumed that homogeneous mixture of fuel and air is already present in computational domain. As fuel methane and oxidizing agent air is already mixed before entering the combustion chamber hence reactive flow can be modeled as premixed combustion. To solve the premixed combustion as reacting flow regime coherent flame model is used. The mean species concentration are obtained as a function of mean fuel mass fraction and one step global reaction scheme, which is internally calculated based on unburnt gas composition. In this model, a fuel mass fraction on grid is tracked through transport equations.

Segregated flow method is used to solve the governing equations. To model the turbulence, standard K-ε model is implemented. In this CFD analysis equivalence ratio of mixture is varied as a function of laminar flame speed.

For CFD analysis the focused point of laser is modeled as ignitor. For ignition of the premixed mixture in computational domain ignitor is required.This ignitor is set in computational domain to ignite the premixed mixture which is activated for particular pulse duration.The ignitor is located at some distance from wall in computational domain.In this pulse this ignitor delivers sufficient energy to ignite the mixture.

5. Governing Equations

The basic set of conservation equations, describing a general case of multicomponent, chemically reacting, ideal gas mixture, includes the Navier-stokes, energy and species transport equations are given below.

These equations are formulated with the following assumptions:
1. External forces in the form of gravity and electro-magnetic field are negligible.
2. The fluid is assumed to be a perfect gas mixture.
3. The radiation heat transfer is neglected.

Continuity Equation:

$$\frac{\partial P}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0$$

Momentum Equation:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

Energy Equation:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u_j h)}{\partial x_j} = \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial h}{\partial x_j}\right) - \sum_{i=1}^{N} h_i \frac{\partial}{\partial x_j}\left[\left(\frac{\lambda}{C_p} - \rho D_i\right)\frac{\partial Y_i}{\partial x_j}\right]$$

Species Transport Equation:

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_j Y_k)}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\rho D_k \frac{\partial Y_k}{\partial x_j}\right) + \dot{\omega}_k$$

Turbulence model equation :

1. Turbulent kinetic energy equation:

$$\rho \frac{D}{Dt}(K) = -\frac{\partial}{\partial x_j}\left(u_j\left[P' + \rho\frac{u_i u_i}{2}\right]\right) + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial k}{\partial x_j}\right) + P_k - \rho\varepsilon$$

2. Turbulent Dissipation rate equation :

$$\rho \frac{D}{Dt}(\varepsilon) = \frac{\partial}{\partial x_j}\left(\left[\mu + \frac{\mu_t}{\sigma_\varepsilon}\right]\frac{\partial \varepsilon}{\partial x_j}\right) + \frac{\varepsilon}{k}(C_{\epsilon 1} P_k - \rho\epsilon)$$

6. Numerical Scheme

For solving the governing equations on grid initial conditions and boundary conditions are required. As we considered the homogeneous mixture of fuel and air is present in combustion chamber, the boundaries of combustion chamber are modeled as wall for CFD analysis. Initial and boundary conditions used for this problem are specified as below.

Table 3 Initial Conditions

Pressure	5 bar
Static Temperature	373K
Equivalence ratio	1
Progress Variable	0
Species Mass Fraction	CH_4 = 0.055 O_2 = 0.22 N_2 = 0.725

Table 4 Boundary Conditions

Wall	Adiabatic
Ignitor shape	Spherical
Ignitor variable value	1
Activator	Pulse (Time)
Pulse Duration	Start= 0 End= 6e-9

7. Experimental validation

In this study to validate the CFD model, experimental data from literature is used. Particularly experimental work done by (Shrivastava et.al) is used to validate the CFD model for premixed combustion.

Shrivastava et.al had done the experimental study of flame kernel characterization of laser ignition of natural gas-air mixture in constant volume combustion chamber. In this work they used the premixed mixture of natural gas-air and Q-switched Nd-YAG 1064 nm laser is used to ignite the mixture present in constant volume combustion chamber. For their experimental research work initial pressure and initial temperature conditions are 10 bar and 373 K as mentioned in research paper.

To validate our CFD model with experimental results pressure-time history is considered from research paper. CFD model is implemented for natural-gas air mixture with geometry mentioned in research paper. In research paper pressure-time history for equivalence ratios are mentioned, but for validation purpose we considered only one equivalence ratio i.e. 0.833.

Fig.3 shows the variation of pressure vs. time in constant volume combustion chamber by experimentally and by results from CFD analysis.

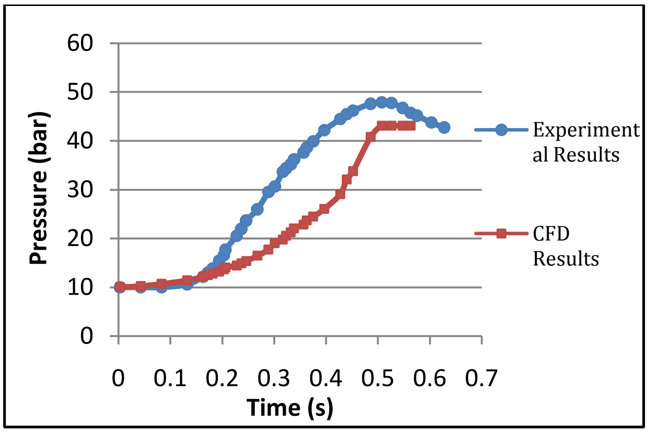


Fig.3 Experimental validation with CFD results

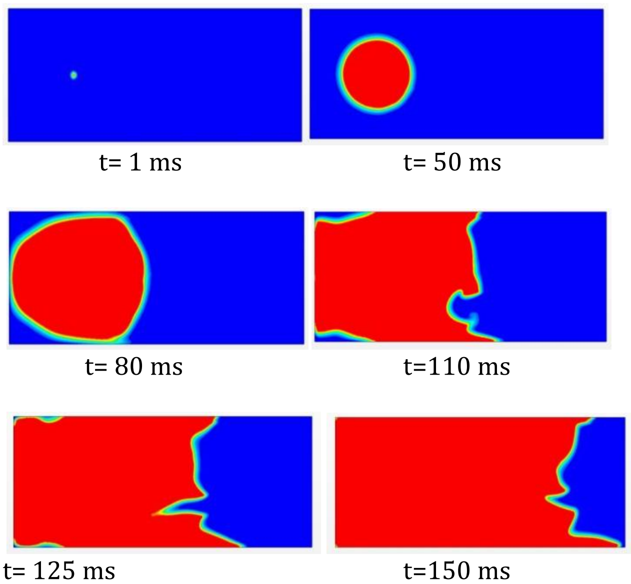
From Fig.3 we can observed that CFD model shows the closest result with experimental results. Percentage error for between CFD results and experimental results is approximately 10-20%.

8. Results and discussion:

In this work CFD model is implemented for combustion of premixed mixture of methane-air with equivalence ratio one. Figure 5 shows the variation of pressure with respect to time in constant volume combustion chamber. For CFD analysis only two-dimensional domain is considered.

Figure 4 shows the flame kernel development and flame propagation in premixed mixture of methane and air for different time durations.

As soon as ignition occurs, initial plasma is formed near the focusing point of laser in the mixture. The gas which is in the surrounding of this plasma gets heated and ionized.As laser is focused at some distance from wall in the mixture, laser generated flame kernel exhibits elongation and after some time duration two separate flame fronts are formed. One of which is moving forward and another is moving backward with respect to ignition point.



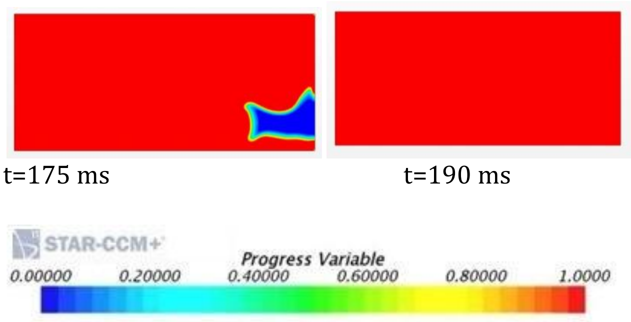


Fig. 4 Flame propagationwith time in combustion chamber.

Fig.5 shows the pressure-time history in constant volume combustion chamber due to combustion from CFD analysis. From figure it is observed that maximum pressure attained in cylinder is 25.3 bar.

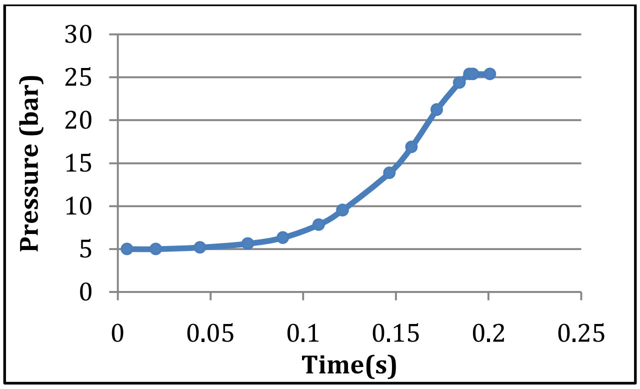


Fig.5 Pressure variation in combustion chamber

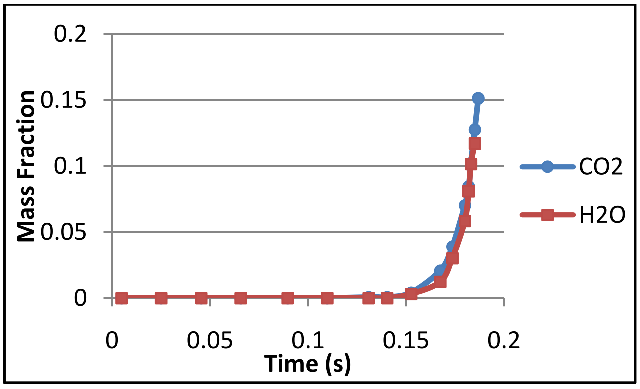


Fig.6 Mass fraction of Products

Above figure shows the variation of mass fraction of products (i.e., CO_2&H_2O) with respect to time. From figure it is observed that at the beginning, CO_2 formation is very negligible, because of in CFD analysis we considered only one step global reaction for methane oxidation, but in actual there are large number of reactions are involved due to which intermediate species are formed and we does not considered these intermediate species in CFD analysis. From figure we can observed that formation of CO_2 goes on increasing with respect to time up to 15.088%.

Also from figure it is observed that H_2O formation is increases with respect to time as reaction proceeds and the final mass fraction of H_2O in the mixture is 12.41%.

Initially the combustion chamber is filled with air and methane mixture. As laser is focused at a point in mixture, ignition is started and the reaction initiates. By stoichiometric calculation initial mass fraction of oxygen and nitrogen in mixture is 22% and 72.50% respectively for stoichiometric fuel-air ratio. As reaction initiates the oxygen in the mixture is gets consumed to react with methane. Hence the oxygen content in the mixture gets reduced with respect to time.

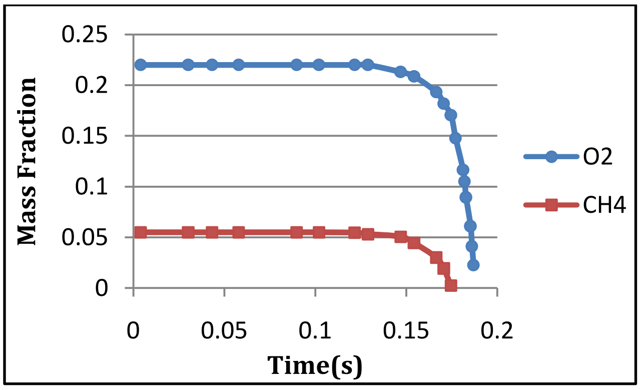


Fig.7 Mass fraction of Reactants

Mass fraction of methane in the mixture is 5.5% initially. After ignition the mass fraction in mixture gets gradually reduced because methane is consumed in methane oxidation reaction.

Conclusion:

In this study, CFD model for laser induced ignition of methane–air mixture is successfully implemented by commercial CFD solver STAR CCM+. Developed CFD model in STAR CCM+ is first validated with experimental data in research work done by Shrivastava et.al (2011).For validation purpose, pressure-time history from experimental work is compared with results from CFD analysis for natural gas-air mixture ignited with laser ignition. Further for CFD analysis of methane-air premixed mixture, a constant volume combustion chamber is considered as computational domain in which homogeneous mixture of methane and air is already present. For ignition of mixture energy pulse from Nd-YAG 1064 nm laser is used.
Flame kernel development and its growth with respect to time in combustion chamber are shown for methane air mixture. Also in this study pressure-time history is investigated, pressure-time history shows that leaner methane-air mixture takes longer combustion duration. In addition, the variation of mass fraction of reactants and products with respect to time are studied for premixed methane-air mixture.

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