Diesel engine CFD simulations: investigation of time step on the combustion phenomena

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Abstract –*Increasing thermal efficiency of internal combustion engines in addition to stringent emission regulations cause researchers to study different phenomena during combustion of fuels inside the cylinder. These research efforts can help to understand fundamental reasons of production of pollutants and reduce emissions due to combustion of hydrocarbons. Therefore, they can be utilized to reduce the emissions of engines and protect the environment. The primary objectives of the present work are development of a CFD model to simulate combustion of diesel (n-Heptane) during Top Dead Center (TDC) of a single cylinder research engine and study the effect of time step on combustion characteristics of n-Heptane and production of emissions. The results showed that heat transfer from the piston and head affected significantly the combustion of diesel in the chamber due to reduction of the temperature of mixture.*

Key Words: Diesel engine, CFD, combustion, emission, time step, turbulent

1. INTRODUCTION

Increasing consumption of fossil fuels for various type of engine applications and environmental concerns regarding both pollutant and greenhouse gas emissions have led to an increasing demand for improving the fuel conversion efficiency (FCE) of internal combustion (IC) engines. Various researchers have investigated different aspects of IC engines to devise strategies for reducing fuel consumption and for increasing engine efficiency. The biggest challenges in achieving more efficient IC engines are abnormal combustion and increased emissions [1]. IC engines are studied for decades to increase their efficiencies and reduce their emissions [2-6]. In spark ignition (SI) engines, increasing compression ratio (which increases fuel conversion efficiency) is limited by knock occurrence due to auto ignition of the end gas mixture which causes the engine damage while in compression ignition (CI) engines full load operation is limited by onset of black smoke in the exhaust gas.

There are different ways to investigate IC engines. Some researchers studied second law of thermodynamics for analysing IC engines and addressing sources of irreversibilities [7-10]. By considering first law and second law of thermodynamics, Caton [11] studied the effects of high compression ratios, lean operation and high exhaust gas recirculation (EGR), on engine processes using a spark-ignition engine simulation. He reported that the gas temperature during combustion can affect entropy generation during combustion. Mahabadipour et. al. [12] introduced two new engine-size-independent performance metrics called the lost available indicated mean effective pressure (LAIMEP) and the fuel conversion irreversibility (FCI) based on second law of thermodynamics. These parameters can be applied to engines with different sizes and different combustion strategies to compare their irreversibilities.

Computational Fluid Dynamics (CFD) is a powerful method to study fluid behaviour in different applications [13-16]. Since experimental methods can be more expensive than numerical methods, thus a lot of researchers applied CFD in different types of IC engines [17-20]. CFD simulations of diesel engine combustion has performed by Huang et. al. [21], using the commercially-available CONVERGE software package by focusing on the prediction of ignition timing. An unsteady RANS approach with available sub-models has used to describe spray breakup physics. Chemistry is treated with a reduced global reaction model that incorporates parameters to describe fuel variability and can represent a range of real diesel and jet fuels. For fuel reactivity, the derived cetane number (DCN) is used as a metric and a means to define rate parameters within the global reaction model. The relative importance of chemistry, spray breakup, and turbulence in predicting ignition delay and the importance of chemistry in governing fuel ignition variability were shown with sensitivity analyses.

A new modelling methodology over a wide range of Diesel engine combustion strategies (such as conventional single-injection and multiple injection) and a number of engine-related experiments was developed and validated with Senecal et. al. [22], using MoSES CFD code. The code included sub-models for simulating the complex physical and chemical processes that occur in engines. It used a modified cut-cell Cartesian technique and included state-of-the-art numerical techniques. For efficient and accurate simulations, the authors used advanced features (e.g., shared and distributed memory parallelization, user-specified grid embedding, a multigrid pressure solver, and a new adaptive grid embedding technique). In order to reduce the CPU time needed for each case simplified models were employed in the present study for the engine simulations. A multistep kinetics model based on the Shell model has been implemented in the code to simulate Diesel ignition delay. Characteristic Time Combustion (CTC) model has used to model cells that are in the combustion phase. The CTC model considered chemical and mixing timescales and simulates the rate of change of concentration of species based on the local and instantaneous thermodynamic equilibrium

concentration value. They addressed that the MoSES CFD code was a powerful tool for internal combustion engine simulations because of its combination of rapid grid generation, modern numerical methods and state-of-the art sub-models.

The primary objectives of the present work are development of a CFD model to simulate combustion of diesel during TDC of a single cylinder research engine and study the effect of time step on combustion characteristics of n-Heptane and production of emissions. The detailed investigation of combustion of diesel inside the engine is provided in the following sections.

2. ENGINE SPECIFICATION AND INPUT DATA

The engine specifications, model and operating conditions examined in the present study are provided in Table 1. The engine was operated at medium load for every operational condition at a constant speed of 1200 rev/min, while the n-Heptane injected quantity was fixed at 0.001 kg/s, boost pressure was fixed at 1.2 bar. Wall temperature of chamber i.e. engine head, piston and liner is considered 500 K. Nozzle angle for spraying n-Heptane is considered 30 degrees.

Table -1: Engine Specifications

Number of Cylinders	1
Compression Ratio	19
Displacement	2.1 liter
Valve Train	2 Intake, 2 Exhaust
Bore x Stroke	132 x 152 mm
IVO	5 CAD
IVC	175 CAD
EVO	495 CAD
EVC	715 CAD

Since the piston movement around TDC is negligible, a constant volume combustion chamber was considered to model combustion process with injection of n-Heptane. Figure 1 shows the cylinder, piston and engine head as the combustion chamber in addition to location of injector:

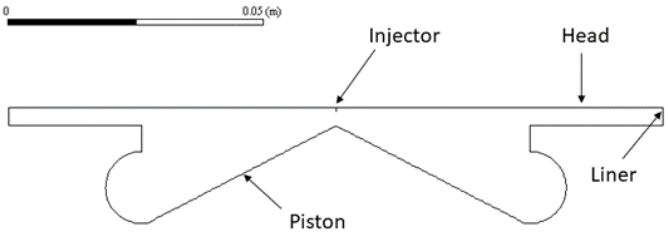

Fig -1: Combustion Chamber of single cylinder research engine at TDC

3. CFD SIMULATION

3.1 General procedure

The numerical model was established for a 2.1 Liter single cylinder research engine operating in DI diesel mode with the specifications listed in Table 1. For simplicity of calculation and due to symmetric combustion chamber, half of the chamber is considered for CFD simulation. The calculations for unsteady equations of mixtures on closed system were carried out around TDC by injection of vapor n-Heptane for 0.0005 s which is corresponding to 5 CAD for and engine operating at 1200 rpm. The turbulent flows within the combustion chamber were simulated using the RNG k–omega turbulence model.

Using ANSYS-Fluent to solve CFD equations, the local mass fraction of each species, Yi, through the solution of a convection-diffusion equation for the ith species was predicted according to the following equation:

$$\frac{\partial(\rho Yi)}{\partial t} + \nabla(\rho v Yi) = -\nabla(Ji) + Ri + Si \quad (1)$$

where Ri is the net rate of production of species by chemical reaction and Si is the rate of creation by addition from the dispersed phase plus any user-defined sources, and Ji is diffusion flux of species i.

$$Ji = -\rho * Di,m * \nabla(Yi) - D_{T,i}\frac{\nabla T}{T} \quad (2)$$

where, Di,m is the mass diffusion coefficient for species in the mixture, and $D_{T,i}$ is the thermal diffusion coefficient. In the current study, Eddy-Dissipation Model was considered to correlate between turbulence and chemistry. Therefore, in certain premixed flames, the turbulence slowly mixes cold reactants and hot products into the reaction zones, where reaction occurs rapidly, which can assume the combustion is mixing-limited, allowing neglect of the complex chemical kinetic rates.

3.2 Overall Mesh Resolution

To have a reliable solution in a CFD code, grid of the geometry should be resolute enough to demonstrate the results are independent of the grid size. In the current study, the combustion chamber included more than 100000 nodes. Therefore, it consists the highest resolution in solving the problem. The numerical grid of combustion chamber in this case is shown in Fig. 2 as follows:

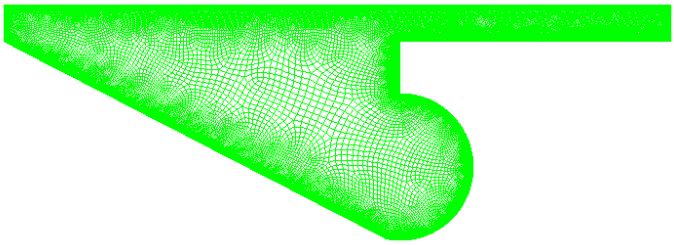

Fig -2: mesh diagram of the combustion chamber for highest resolution

4. RESULTS

Considering the mentioned parameters for initial condition and according to CFD simulation, in this section, transient results of 0.001 kg/s n-Heptane injection at TDC of a single cylinder research engine are studied at TDC of an engine running at 1200 rpm. Different time steps for the current study are 0.0001 s (0.1 ms), 0.0003 s (0.3 ms), 0.0005 s (0.5 ms), 0.001 s (1 ms). For better interpreting the sequential effects, some of the important results were reported., the following results are obtained for temperature, turbulent kinetic energy and CO_2 mole fraction distribution in the combustion chamber:

4.1 Temperature

Fig -3: Temperature distribution in the combustion chamber (0.1 ms)

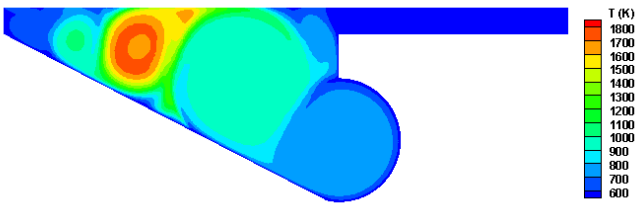

Fig -4: Temperature distribution in the combustion chamber (0.3 ms)

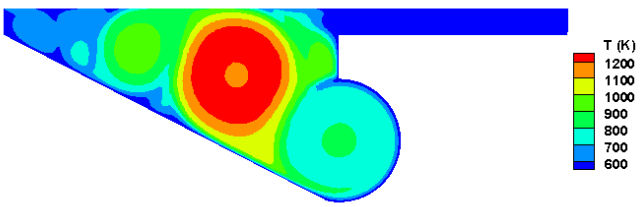

Fig -5: Temperature distribution in the combustion chamber (0.5 ms)

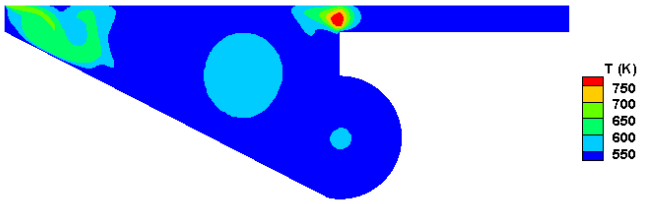

Fig -6: Temperature distribution in the combustion chamber (1 ms)

4.2 Turbulent kinetic energy

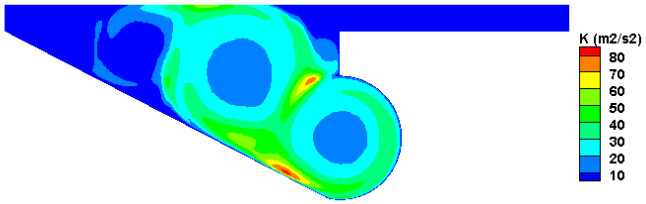

Fig -7: Turbulent kinetic energy distribution in the combustion chamber (0.1 ms)

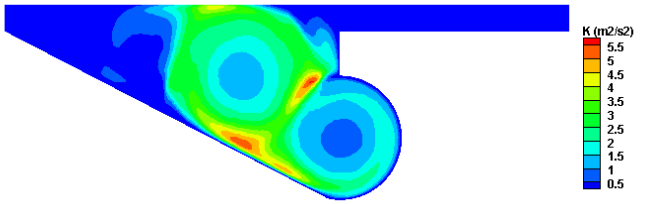

Fig -8: Turbulent kinetic energy distribution in the combustion chamber (0.3 ms)

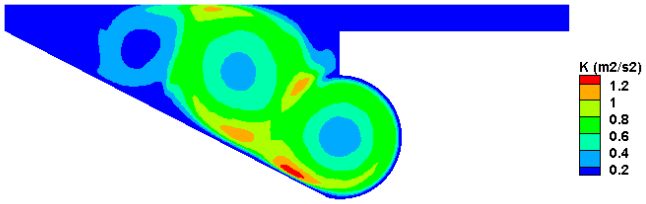

Fig -9: Turbulent kinetic energy distribution in the combustion chamber (0.5 ms)

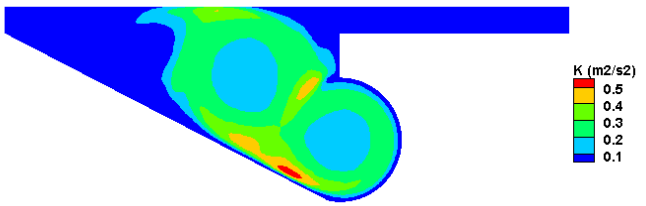

Fig -10: Turbulent kinetic energy distribution in the combustion chamber (1 ms)

4.3 CO_2 mole fraction

Fig -11: CO_2 mole fraction distribution in the combustion chamber (0.1 ms)

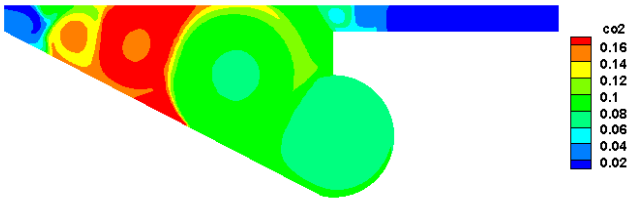

Fig -12: CO_2 mole fraction distribution in the combustion chamber (0.3 ms)

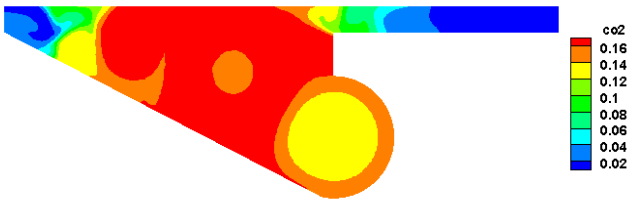

Fig -13: CO_2 mole fraction distribution in the combustion chamber (0.5 ms)

Fig -14: CO_2 mole fraction distribution in the combustion chamber (1 ms)

3. CONCLUSIONS

According to the results of CFD simulation, when time step changed from 0.1 ms to 1 ms, the maximum temperature inside the chamber was obtained which was more than 1800 K. The maximum temperature occurred for the fastest time step. Considering the turbulent kinetic energy contour for 0.1 ms, it showed that the entire combustion chamber had high enough turbulence which causes the mixing to be maximum. Therefore, since the combustion model is based on turbulent behavior of the fluid, therefore, having the maxim temperature in this timestep seems logical. The highest temperature moved further inside the chamber for 0.3 ms timestep which showed an Eddy with maximum temperature of 1800 K. For 0.5 ms time step, the maximum eddy temperature reduced to 1200 K but the size of Eddy increased significantly. Thus, heat transfer effect is dominant from this time step which can be recognize from the reduced averaged of temperature inside the chamber. Finally, for the 1 ms time step, combustion is almost finished inside the chamber and heat transfer from the piston, head and liner caused the chamber to cool rapidly. Investigation of velocity vector and turbulent kinetic energy contours inside the chamber shows that the maximum mixing occurred inside the circle of piston. The level of turbulent is maximum in the lowest time step and significantly decreased with increasing time steps.

Study the results of species inside the chamber shows that n-Heptane is the only species that existed next to the site of injection within the combustion chamber. Therefore, there should not be any combustion within this area which is compatible with the temperature contour. However, heat transfer from the piston and head reduced the temperature of mixture (which is mostly fuel) significantly. Also, next to the site of injection, there is not sufficient mixing between the fuel and the oxidizer for higher time step due to consumption of oxygen. Therefore, the dominant species at the outlet of injector was n-Heptane. Looking at the oxygen mole fraction contour, it is shown that it was consumed in the direction of fuel injection with increasing the time steps. Thus, it can be interpreted that the diffusion flame propagated in the direction of flame and quench at the narrow part of chamber at TDC. It is also evident by considering the mass fraction of CO2 in the chamber. For the 0.1 ms, after fuel rich area, next to the site of injector, co2 is maximum which shows the products of combustion. With increasing the time step to the 0.3 ms and combustion of more fuel in addition to movement of mixtures inside the chamber, co2 peak concentration reached to the center of chamber and subsequently closed to the circle of piston. Finally, at the maximum time step of 1 ms, product of combustion reached to the circle of the piston while at the narrow part of chamber the amount of CO2 is negligible because there is not any combust in this area.

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