



Numerical Investigation on Performance Improvement of Hydrogen-diesel Fuelled Engine with Various Charge Induction Strategies

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ABSTRACT

In this work, effects of various H_2 charge induction strategies on the performance and emissions of H_2 -diesel dual fuel engine have been studied through numerical analysis using a high-fidelity computational fluid dynamics tool-Converge. A 120° three-dimensional (3D) sector model was created for the engine (port fuel injected H_2 and direct injected diesel dual fuel) under study. Closed cycle simulations have been carried out to understand the in-cylinder combustion and emission formation processes. Results of the study showed that an addition of H_2 at lower loads deterred the performance of the engine due to the lower combustion temperatures, but at higher loads H_2 starts actively participating in combustion, thus improving the performance. It has been noticed that combustion efficiency of H_2 fuel at lower loads is poor due to lower in-cylinder temperature and charge dilution effect. Other than this, at lower H_2 substitution levels, lean H_2 -air mixture outside the diesel spray plume zone caused poor combustion efficiency of H_2 fuel. Because of replacement of carbon-based fuel with H_2 , a reduction in carbon dioxide, carbon monoxide emissions have been observed with increased HES. While at higher loads, the combustion performance is found better than that of the lower loads due to the increased temperature leading to improved combustion participation of hydrogen. The NO_x emissions were found to be high at higher loads with high HES.

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1. Introduction

Without the internal combustion (IC) engine, a single day is unimaginable as it has become an indispensable part of our daily life. Most of the IC engines in the market now use fossil fuels as the power source, and the fossil fuels are not renewable by nature, and they are not environment-friendly owing to the emissions from their combustion. Various alternate fuels have been proposed to replace the fossil fuel-based energy model. However, most proposed alternate fuels are carbon-based. These commercially available carbon-based energy carriers (fossil fuels) damage the environment as they release higher amount of carbon dioxide (CO_2) and carbon monoxide (CO) during the combustion. Renewable fuels based on biomass can cut down carbon emissions but scaling up to the requirement is the major issue with the biomass-based energy carriers. Hydrogen has also been proposed as an alternative to the existing fossil fuels, and it is a non-carbon-based fuel, boasting the cleanest combustion properties. Hence, hydrogen is a promising fuel for the reduction in emissions of the greenhouse gases (mainly CO_2) when produced from renewable sources, during the combustion [Heywood, 1988; Sharma and Dhar, 2018a].

The pioneers of IC engines have tried to use hydrogen in engines as early as 1810. De-Rivaz in the year 1810 developed an engine that operated on hydrogen. But, with the arrival of petrol and diesel fuels and their secure handling processes, hydrogen was put aside at that time [Ratiu,

2003]. With the emission norms getting stringent by time, the search for clean fuel took a turn towards hydrogen and researchers started experimenting with hydrogen to use it as a fuel in IC engines. Since, it is challenging to convert the current fleet of engines to run on pure hydrogen, the experiments have been done using dual-fuel engines where hydrogen is premixed with air and pilot injection of diesel attempts to control the start of ignite the fuel.

Dimitriou and Tsujimura [Dimitriou and Tsujimura, 2017] investigated the possibilities to run compression ignition (CI) engine using hydrogen. Hydrogen supplementation in CI engine showed a significant reduction in hydrocarbon (HC), CO, CO_2 and smoke emissions. Moreover, high hydrogen rates have positive effects on the combustion process, increasing the heat release rate and brake thermal efficiency (BTE). Sandalcı and Karagöz [Sandalcı and Karagöz, 2014] modified an existing diesel engine with liquefied petroleum gas (LPG)-compressed natural gas (CNG) injector to inject hydrogen in the intake manifold of the engine. The study showed that the thermal efficiency was reduced with increasing hydrogen percentage. Also, with the addition of hydrogen, an increase of the HC was observed because of the incomplete combustion of diesel fuel in the presence of hydrogen. Similar study was carried out by Karagöz et al. by enriching diesel combustion with hydrogen and studied the effects of various hydrogen energy shares (HES) on the engine performance. The hydrogen was inducted using LPG/CNG gas injector at the manifold. The hydrogen induction at higher loads helped in improvement of in-cylinder peak pressure and heat release rates (HRR) with increasing HES.

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Lilik et al. [Lilik et al., 2010] studied hydrogen assisted combustion on a 2.5 litre, 4-cylinder, turbocharged, common rail direct injection (CRDI) light-duty diesel engine. HES of 0%, 2.5%, 5%, 7.5%, 10% and 15% were inducted into the engine replacing diesel through port-based induction strategy. It has been observed in the study that with fixed injection timings, hydrogen-diesel combustion produced higher oxides of nitrogen (NO_x) emissions (decreased NO emissions and increased NO_2 emissions) and also it was observed that retardation in injection timing resulted in reduced NO_x emissions. Results of their study also showed that in-cylinder hydroperoxyl radical (HO_2) levels were increased with increasing hydrogen, resulting in increased conversion of NO into NO_2 [Lilik et al., 2010]. It was also observed that CO and CO_2 emissions were reduced with the increased HES. It was observed that the hydrogen induction decreased fuel economy because the volumetric efficiency was lowered with hydrogen in port, which displaced the intake air. Debet al. [Debet et al., 2015] studied the dual fuel mode operation with hydrogen-diesel fueled engine at various HES (0%, 11%, 17%, and 30% and 42%). The study has shown that increasing HES decreased CO, CO_2 , HC and smoke emissions while increasing the NO_x emissions. Sharma et al., summarized the effectiveness of Hydrogen enrichment on particulate matter reduction in a review article [Sharma and Dhar, 2019a].

Yang et al. [An et al., 2013] investigated the various characteristics of hydrogen-diesel combustion with the help of multi-dimensional KIVA-4 software and CHEMKIN. The base model was validated against the results from experiments at 0% HES. The study found that increasing HES at lower engine speeds had increased indicated thermal efficiency (ITE), in-cylinder pressure and HRR. However, in contrary at higher loads and speeds, with increasing HES, no significant changes were observed. Sharma and Dhar [Sharma and Dhar, 2018b] had investigated the effects of HES on the performance of the port fueled hydrogen and direct injection (DI) dual fuel CI engine experimentally. The tests were done at 25%, 50% and 75% loads and at HES of 0%, 5%, 10% and 20%. They found that CO_2 and CO were decreased up to 17% and 21% respectively at the HES of 20%. They also reported that NO_x was decreased at lower loads and increased at the higher loads when HES was increased because of the in-cylinder temperatures, which were low at lower loads and high at higher loads. Sharma and Dhar [Sharma and Dhar, 2018c] also studied the effects of increasing HES and compression ratio (CR) variation on engine emissions and found that with increasing the HES, CO and HC emissions were reduced while NO_x emissions were increased. However increasing the HES beyond 30%, increased NO_x , HC and CO and decreased soot emissions. The study investigated the influence of CR and HES on knocking limit of the engine at CR of 14.5, 16.5 and 19.5 at various HES from 0% to 55%. The study showed that there exists a tradeoff between knock from increasing HES to CR and found that knock limit of HES increased from 20% to 45% in lower CR. Szwaja and Rogalinski [Szwaja and Grab-Rogalinski, 2009] studied homogeneous charge compression ignition (HCCI) operation of hydrogen on a two-cylinder engine at various CR and have found that there is a trade-off between knocking and efficiency of combustion. The level of trade off varied with the compression ratio. Sharma and Dhar [Sharma and Dhar, 2016] also studied the hydrogen-based homogeneous charge compression ignition (HCCI) engine numerically. The study involved developing a stochastic multi-zone chemical kinetics-based model to study the HCCI model with varying parameters. The results were validated against the experimental results from a hydrogen HCCI engine. Equivalence ratio, intake temperature and charge quality were varied to study their effects on the engine output characteristics. The factors affecting the start of combustion were also studied as it is difficult in HCCI engines to control the start of combustion. The investigations showed that combustion was sustainable even at lean equivalence ratio up to 0.20 with intake temperature of 383 K. The low-temperature lean combustion resulted in reduced levels of NO_x emissions.

Bose and Maji [Bose and Maji, 2009] studied the effects of exhaust gas recirculation (EGR) on dual fuel (port fueled hydrogen and DI diesel) engine. It has been observed that adding EGR in dual fuel mode helped to lower the smoke, particulate matter (PM) and NO_x emissions coming out from the engine. The NO_x emissions from the engine started increasing with hydrogen addition due to the higher temperatures in the combustion chamber. However, temperature and hence NO_x emissions started gradually decreasing with increased in EGR rate.

The literature study had shown that increasing the energy share of hydrogen in diesel in general reduces the performance and increases NO_x emissions from the engine and the compression ratio plays an important role in enabling combustion. With the inputs from the literature, the behavior of the hydrogen-diesel fuel mixture in the engine is understood and based on the previous works the current work was

planned. Previous works have limited the HES to 30% because the combustion did not sustain at higher HES [Sharma and Dhar, 2019b]. The goal of this study was to investigate the various effects of increasing the hydrogen energy share (HES) over the diesel on the performance and emissions characteristics of the engine in dual fuel mode and the effects of various parameters on the same. The main goal is to understand the effects on the engine characteristics at higher HES using simulation tools, since the use of higher HES is limited in experimentation.

2. Methodology

The numerical simulations were carried out with CONVERGE, a 3-dimensional simulation tool. CONVERGE make surface utility was used to create the simulation geometry of the engine. Results from the experiments performed by Sharma and Dhar [Sharma and Dhar, 2018b] using timed manifold injection of hydrogen and direct injection of diesel in a CI engine, were used to validate the simulation model. The experimental study was performed using a Kirloskar TV1 engine, which is a single cylinder 661 cubic centimeter (cc) capacity-diesel engine modified for the dual fuel operation. The validated model was made as the base for investigating the effects of various parameters (One at a time) on the combustion and emissions characteristics of the engine. The input energy supplied to the engine was kept constant with respect to base loads of 25% and 75% for the parametric investigations. The effects of varying HES on the performance and emissions were analyzed in the study.

The CONVERGE CFD software used in these simulations, has multiple advantages over competing software, amongst which adaptive mesh refinement (AMR) and fixed embedding (denser grid regions) sets is out drastically. AMR brings down the mesh processing time considerably, while the fixed embedding improves accuracy of the simulations in physics extensive regions like spray and fluid structure interaction zone. The simulations were carried out using a 120° sector model of the Kirloskar TV1 Engine (the engine has a three-holed injector— hence three sectors) as shown in Figure 1. The engine and injector specifications required for simulation are given in Table 1.

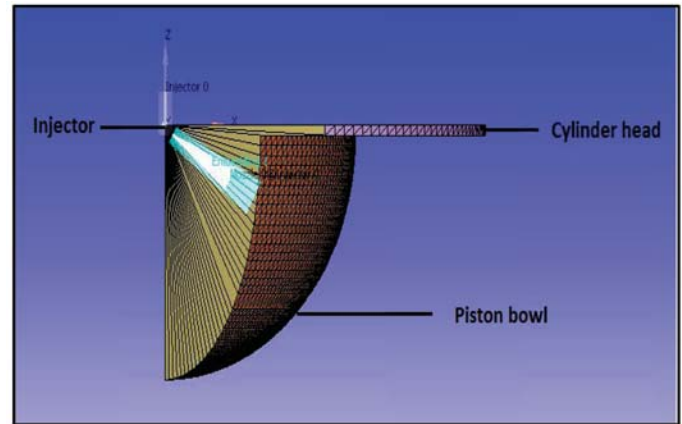


Figure 1 Sector model of the engine in CONVERGE

Table 1 Engine and injector specifications

Parameters	Specifications
Make and model	Kirloskar, TV1
Engine type	Single-cylinder, 4-stroke, water cooled, CI engine
Rated power	5.2 kW @1500 rpm
Swept volume	661 cc
Bore × Stroke	87.5 mm × 110 mm
Clearance volume	40.1 cc
Compression ratio	17.5:1
Injection pressure	270 bar at full load
Intake valve close (IVO)	-144.5° aTDC
Exhaust valve open (EVO)	144.5° aTDC
Number of nozzles	3
Diameter of nozzleFuel	0.288 mm Diesel & Hydrogen
Injector angle	15° with vertical axis
Nozzle tip protrusion	1 mm

Closed cycle simulations were carried out on the engine from the close of both the valves to the opening of the exhaust valve. In this case, the time the run started from -144 degrees to 144 degrees. The condition of port fueled hydrogen was simulated with initializing hydrogen in the boundary conditions.

SAGE chemistry solver was used for solving the combustion process [Senecal et al., 2003]. SAGE calculates the reaction rates for each elementary reaction while the CFD solver solves the transport equations. Converge uses PISO algorithm for pressure-velocity coupling. The PISO algorithm as implemented in CONVERGE starts with a predictor step where the momentum equation is solved. After the predictor, a pressure equation is derived and solved, which leads to a correction, which is applied to the momentum equation. This process of correcting the momentum equation and re-solving can be repeated as many times as necessary to achieve the desired accuracy. Converge uses the STL file to load surface data in the simulations. The model uses 1.4 mm cells as base grid and 200000 cells in AMR which comes into action when specified conditions are exceeded during simulation... The reaction mechanism, optimised for dual fuel combustion: includes 464 reactions of 76 chemical species, is used for the validation and parametric investigation [Rahimi et al., 2010]. The spray parameters such as injection timings, injection duration, injection pressure, nozzle configuration etc. were defined in the spray modeling. Heptane was used as surrogate for diesel fuel in the simulation.

The spray is modeled using KH-RT Breakup Model [Reitz and V. Bracco, 1986; Ricart et al., 1997]. A Modified KH-RT model simulates the primary, secondary and combined breakup of the spray. The turbulence in the cylinder was modeled using Reynolds-Averaged Navier-Stokes (RANS) of RNG (Renormalization Group) $k-\epsilon$ [Han and Reitz, 1995]. The CO and CO₂ emissions are obtained from the coupled CFD and chemical kinetic solution produced by the SAGE solver. While NO_x is predicted using the extended Zeldovich mechanism.

3. Validation of the Model

The results from simulations were compared with the results of the experiments carried out by Sharma and Dhar [Sharma and Dhar, 2018b] for the validation of the created model. The model was tuned by changing various parameters such as inlet charge pressure, inlet charge temperature, temperatures of various components such as piston, cylinder wall and cylinder head. By changing these values, a match in the results between the experimental and simulated trends of in-cylinder pressure and HRR can be seen in Figure 2.

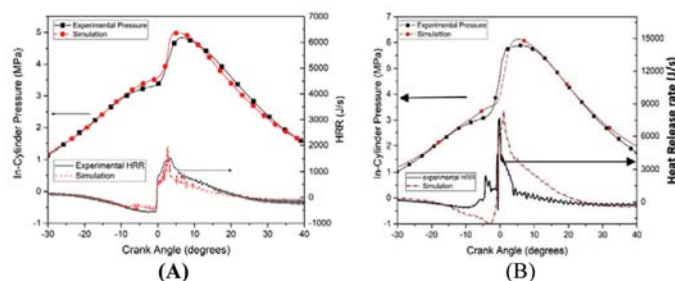


Figure 2 Validation of in-cylinder pressure and HRR traces at equal energy input of 25% load with 0% HES and 75% load and HES of 10%

By changing these values, a match in the results between the experimental and simulated trends of in-cylinder pressure and HRR can be seen in (Figure 2) for various load and HES. The simulation validated at the energy input same as that of 25% load (603.5 J/cycle) and 0% of HES is shown in Figure 2-A. It can be seen from Figure 2 that matching between experimental and simulation for both in-cylinder pressure and HRR trends is very good. Model validation with the energy input same as that of 75% load (1001.646 J/cycle) and 10% of HES is also carried out, as can be seen in Figure 2-B, to make model more robust. The Figure 2 shows that there is a good match in results between the predicted values from simulation and results from experimentation.

The emission result from the simulation was validated using NO_x levels measured in ppm from the experiments [Sharma and Dhar, 2018b] at the same energy input as that of 75% load (1001.646 J/cycle) and 10% of HES. As tabulated in Table 2, simulated NO_x value is very close with the experimentally reported data. Based on all these comparisons (in-cylinder pressure, HRR, NO_x), it can be concluded that model is validated well and can be used for further study.

Table 2 validation of emissions at equal energy input of 75% load and HES of 10%

Emission	Experimental	Simulation
NO _x (PPM)	1086	1163

4. Results and Discussion

The parametric investigation was done in two phases. In the first phase, the effects of increasing HES (with fixed injection conditions on diesel injection) on combustion at the energy input equal to 25% and 75% loads were studied. The results were compared with each other to understand the effects on emissions and performance. The effects of increasing HES (with matched performances of that of the base diesel condition on energy input equal to 75% load –within 10% gross mean effective pressure -GMEP) on the NO_x emissions were studied in the second phase. The load conditions were studied by keeping the total energy shares of the mixture same as that of the points where base measurements were taken.

5. Effect of Increasing HES on Engine Performance

The simulations were done by keeping the total energy input of the mixture equal to that of base 25% and 75% loading conditions and the HES of 0%, 20%, 70% and 90% were investigated. The injection conditions such as injection time and duration in the simulations were kept constant as in the base conditions of both 25% and 75% loads. The results of the simulation are represented in Figure 3 and Figure 4.

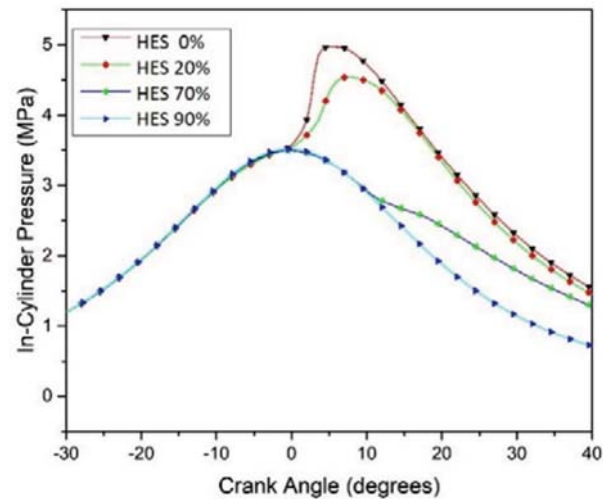


Figure 3 Effect of increasing HES on in-cylinder pressures with energy input equal to 25% load

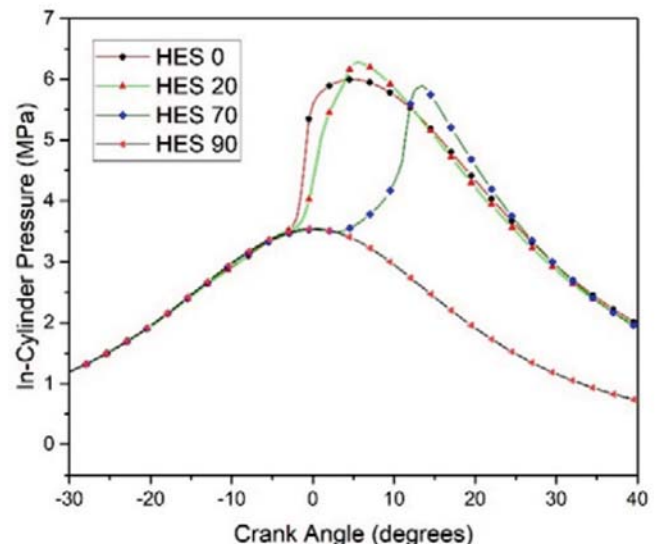


Figure 4 Effect of increasing HES on in-cylinder pressures with energy input equal to 75% load

At 25% loading conditions, as can be seen in Figure 3, increasing HES deterred the performance of the engine. With lower loads, the combustion did not sustain at higher HES (~ 70% and above). The pilot diesel was not able to ignite the hydrogen mixture enough to sustain combustion. However, at 75% load condition, the hydrogen starts actively participating in combustion at even higher HES, thus improving the performance of the engine (Figure 4, HES 70%). However, the performance started deteriorating with HES 90% with higher load too. The engine was able to sustain combustion at 75% load with higher HES. This is due to the higher in-cylinder temperatures at higher engine load.

Figure 5 shows the comparison between in-cylinder mean gas temperature at 25% and 75% loading conditions at HES 0% and 20%. At the lower loads, increasing the HES has reduced the mean temperature of the engine. At the lower loading condition (25% load), the deterioration of performance with increasing HES is due to the incomplete combustion of hydrogen and due to the lower combustion temperatures as reported by Sharma and Dhar[Sharma and Dhar, 2018c]. At higher loads, the higher cylinder temperature has resulted in better combustion of the mixture. The hydrogen has actively taken part in the combustion, which lead to increase in-cylinder temperature. From Figure 5, the mean temperature of hydrogen- diesel mixture at 20% HES is greater than that of base diesel operation.

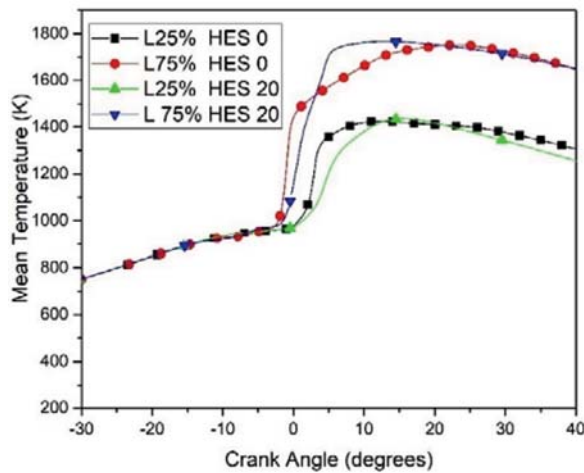


Figure 5 In-cylinder mean gas temperature comparison between 25% and 75% loading with various HES

6. Effect of Injection Timing on Performance

Following the preliminary investigation, this part of the study was aimed at improving the combustion performance by optimizing the gross mean effective pressure (GMEP) with respect to injection timing. It was observed that advancing the diesel fuel injection with increased HES had helped in improving the GMEP (Figure 6).

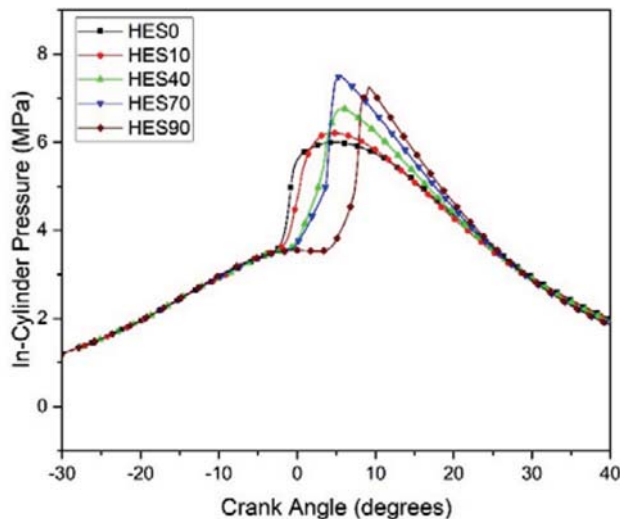


Figure 6 Pressure traces with improved performance within 10% GMEP of base 75% load

The diesel injection parameters such as start of injection (Figure 7) and duration were varied in the simulations with 75% loading conditions at HES of 10%, 40%, 70% and 90% to obtain the GMEP within 10% of the base engine (HES 0%) performance on diesel at energy input equal to 75% load. Results of pressure traces corresponding to these optimized injection timings are presented in Figure 6. The diesel fuel injection timings were varied (advanced with increase HES) to obtain the equal GMEP (within 10% variation).

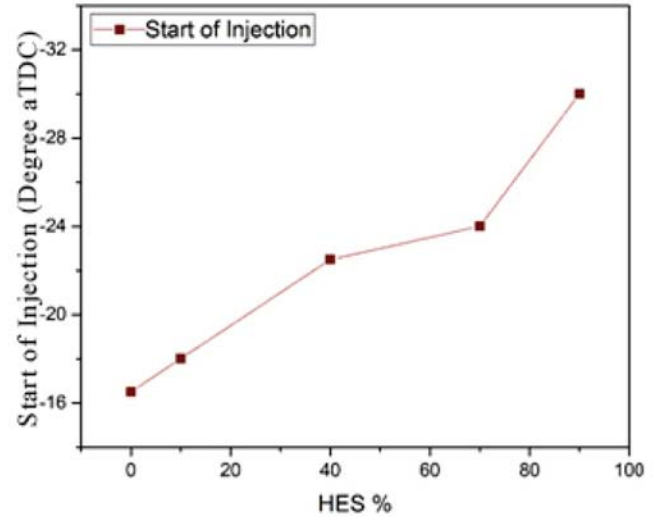


Figure 7 HES Vs SOI at energy input equal to 75% load to match the GMEP

Figure 8 presents the comparison between the temperature contours of the pressure trace of HES 70 from Figure 4 and Figure 6. The contours presented are from the start of injection (SOI) (a) and 5 crank angle degrees after SOI (b). The diesel fuel start of injection has been varied in two cases. Temperature contour corresponding to figure 6 has start of injection advanced by 8 crank angles to ensure that enough time is available for the mixture to combust. The diffusion front needs time to ignite the premixed mixture, hence the advanced injection timings are helpful in burning the charge with higher hydrogen energy share.

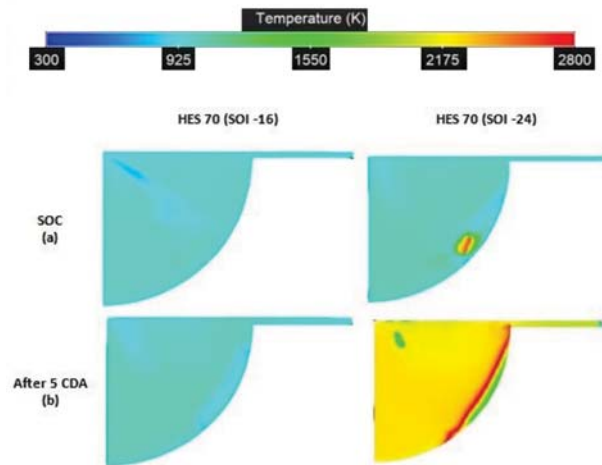


Figure 8 Comparison of temperature contours of two different SOI of diesel at fuel input equal to 75% load

7. Effect of Increasing HES on Emissions

Figure 9 presents the comparison of NO_x emissions and the in-cylinder temperature profile during combustion with increasing HES, while the GMEP is within the range 10% of the base diesel engine (HES0%) corresponding to optimized injection timings of cases shown in Figure 6. Figure 9 infers that NO_x emissions increase with increasing HES for the same performance as that of diesel (HES 0%). The increased NO_x formation is due to the higher in-cylinder temperature, which gives rise to the thermal NO_x , the predominant form of NO_x in IC engines.

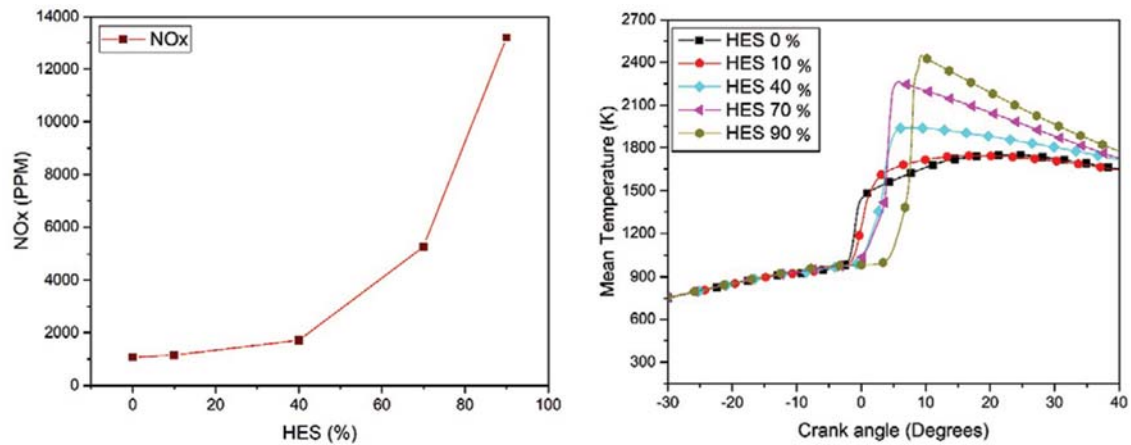


Figure 9 NO_x emissions and temperature profiles with increased HES with advanced injection timings (as described in Figure 8) at energy input equal to 75% load

Comparisons of in-cylinder temperature at the top dead center (TDC), start of combustion (SOC) and end of combustion (EOC) of the simulations at the HES of 0% and 90% at energy input equal to 75% load are shown in Figure 10. It can be understood that the temperature in the cylinder increases with increased HES. The in-cylinder temperature is very high in the higher (HES 90%) due to the higher burning rate of hydrogen in comparison to that of diesel while the performance is same as that of base diesel. The temperature of the pure diesel combustion is much lower than the hydrogen supplemented combustion at the same level of performance. With higher concentrations of the hydrogen, the temperature of the cylinder is higher due to the high diffusivity and high adiabatic flame temperature of hydrogen, which resulted in higher NO_x emissions (for equal GMEP performance).

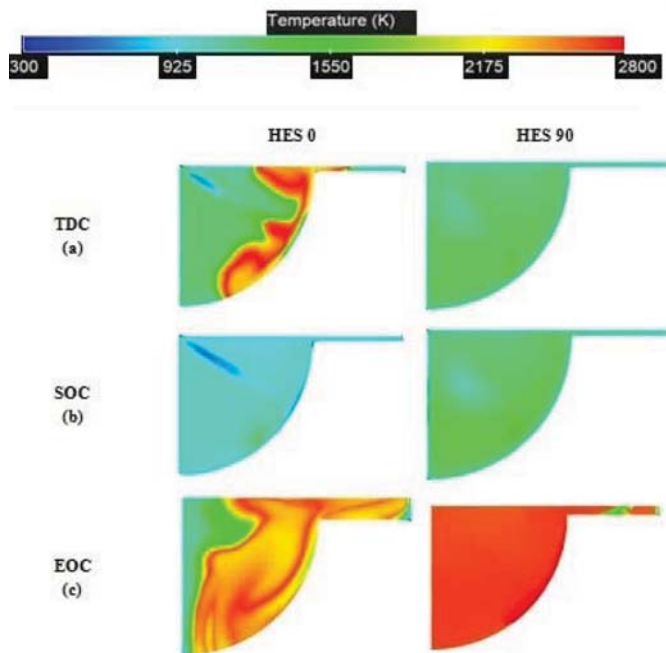


Figure 10 In-cylinder temperature contours for HES 0% and 90% at energy input equal to 75% load

Figures 11 and 12 give the comparison between CO₂ and CO emissions respectively with various HES (with equal GMEP of the base diesel engine) at the energy input equal to 75% load. Figures 11 and Figure 12 show that the CO₂ and CO emissions get reduced with the increase in HES at the same level of performance (within range of 10% GMEP) as that of base diesel (HES 0%). This is due to the supplementation of

carbon-based diesel fuel with the hydrogen fuel and better combustion of injected diesel (remaining share) from the high temperature of hydrogen combustion.

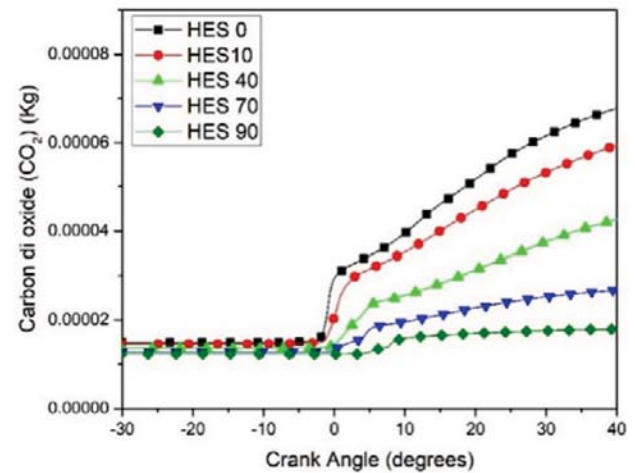


Figure 11 CO₂ emissions with various HES percentages at the energy input equal to 75% load

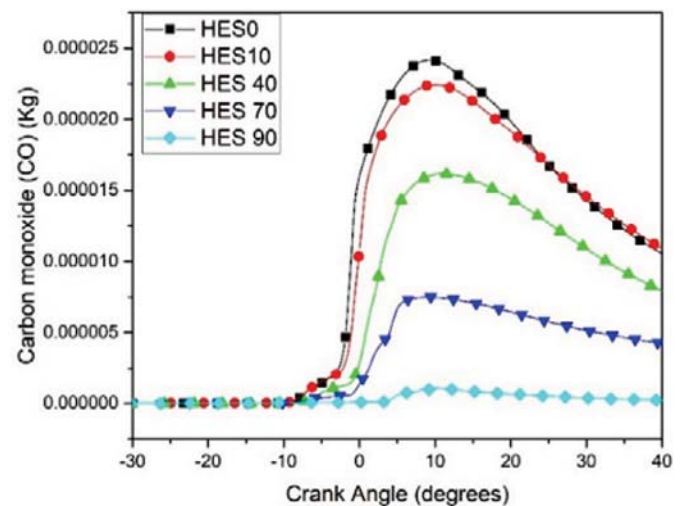


Figure 12 CO emissions with various HES percentages at the energy input equal to 75% load

8. Conclusions

In this work, a CONVERGE, CFD closed cycle model with sector of 120° has been validated against the experimental results. The effects of higher HES percentages on the combustion performance and emissions were studied. Following conclusions are drawn from the study.

- Combustion can be sustained at higher substitution of diesel by hydrogen up to 90% with closer performance to that of base diesel engine (GMEP variation within 10%)
- The higher substitution of diesel by hydrogen requires advancement of the start of injection of diesel fuel to meet equal engine GMEP (within 10%).
- The NO_x emissions are very high as the HES gets higher in the same level of performance of the mixture because of increased in-cylinder temperature with increase in HES percentages.
- Increase in HES reduces the CO₂ and CO emissions considerably as compared to the diesel only operation.

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