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CFD-3D analysis of a light duty Dual Fuel (Diesel/Natural Gas) combustion engine

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Abstract

Nowadays, the most critical issues concerning internal combustion engines are the reduction of the pollutant emissions, in particular of CO_2, and the replacement of fossil fuels with renewable sources. An interesting proposition for Diesel engines is the Dual Fuel (DF) combustion, consisting in the ignition of a premixed charge of gaseous fuel (typically natural gas) by means of a pilot injection of Diesel Fuel.

Dual fuel combustion is a quite complex process to model, since it includes the injection of liquid fuel, superimposed with a premixed combustion. However, CFD simulation is fundamental to address a number of practical issues, such as the setting of the liquid injection parameters and of the gaseous fuel metering, as well as to get the maximum benefit from the DF technique.

In this paper, a customized version of the KIVA-3V Computational Fluid Dynamic (CFD) code was adopted to analyze the combustion process of a 4-cylinder, 2.8 l, turbocharged HSDI Diesel engine, operating in both Diesel and DF (Diesel and Natural Gas) modes.

Starting from a previously validated diesel combustion model, a natural gas combustion model was implemented and added to simulate the DF operations. Available engine test data were used for validation of the diesel-only operation regimes. Using the calibrated model, the influence of the premixed charge composition was investigated, along with the effect of the diesel injection advance angle, at a few characteristic operating conditions. An optimum setting was eventually found, allowing the DF engine to deliver the same brake power of the original Diesel unit, yielding the same maximum in-cylinder pressure.

It was found that DF combustion is soot-less, yields a strong reduction of CO and CO2, but also an increase of NO.

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Keywords: Dual fuel, Diesel, Natural Gas, CFD

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1. Introduction

Nowadays, the most critical issues concerning internal combustion engines are the reduction of the pollutant emissions, in particular of CO_2, and the replacement of fossil fuels with renewable sources. An interesting proposition for Diesel engines is the use of natural gas in combination with the conventional liquid fuel[1]. This technology, known as Dual Fuel (DF) combustion, consists in the ignition of a premixed charge of gaseous fuel by means of a pilot injection of Diesel Fuel. With a proper control of the premixed charge composition and of the injection advance, it is possible to achieve a smoke-less combustion, reduce CO and CO_2, and get acceptable levels of nitrogen oxides [2-11].

In this paper, the KIVA-3V Computational Fluid Dynamic (CFD) code was implemented and used to analyze the combustion process of a 4-cylinder, 2.8 l, turbocharged HSDI Diesel engine, operating in both Diesel and DF modes. Dual fuel combustion is a quite complex process to model, since it includes liquid injection, atomization, vaporization, mixing and ignition, superimposed with a premixed natural gas combustion. However, the combustion process detailed analysis is crucial for engine performance optimization, hence for getting the maximum advantage from the dual fuel technique. In particular, the effective reduction of specific CO_2 emissions, is related to the global fuel conversion efficiency. If this parameter is reduced, passing from Diesel-only to dual fuel operations, the potential advantage of natural gas (-20% of brake specific CO_2, considering typical fuels composition) may be spoiled. Furthermore, the presence of methane in the exhaust gas, as a result of incomplete combustion, has a negative impact on the Greenhouse effect, as well as on fuel efficiency. However, from the pollutant emissions' point of view, the most critical exhaust component is NO: in fact, nitrogen oxides are very difficult to control, because of the high temperatures and the availability of oxygen.

Combustion simulation is also fundamental to prevent mechanical failures, a quite real risk, as reported in many papers reviewing conversions from Diesel to Natural Gas. The most important reasons of these failures are:

- Auto-ignition or even knocking, generally associated to lean operations
- High combustion temperatures and pressures, typical of stoichiometric or rich operations

For achieving efficient and clean and reliable operations on a dual fuel engine, it is necessary to assess the influence of the premixed charge composition, as well as of the injection advance.

Starting from a previously validated diesel combustion model, a natural gas combustion model was implemented and added to simulate the ignition and combustion process in a dual fuel light duty engine. Available engine test data were used for validation of the diesel-only operation regimes. Using the calibrated model, the influence of the premixed charge composition was analyzed, along with the effect of the diesel injection advance angle. An optimum setting was eventually found, allowing the dual fuel engine to deliver the same power of the original Diesel unit, while yielding the same maximum in-cylinder pressure.

2. 3D CFD Models

A full engine cycle CFD model based on a customized version of the KIVA-3V [12] codes coupled with detailed combustion chemical kinetics was used to investigate DF engine operations. The sub-models implemented into the customized version of the KIVA 3V code are listed in Table 1.

Table 1 Computational Models

Turbulence model	RNG k-ε model
Breakup model	Hybrid KH-RT model
Droplet collision model	Droplet trajectories
Evaporation model	Single component, KIVA-3V
Diesel Combustion	PaSR / coupled chemical kinetics
Flame Propagation	TFC / Premix code for aspirated fuel
Fuel compositions	Natural gas/DOS

These sub-models were previously implemented by the authors in the framework of the KIVA-3V and KIVA-4 codes and they are fully described in [13-17]. Thus, in the present paper, only a brief description of DF combustion model is provided.

The model of DF combustion involves two coupled modes: the "conventional" partially premixed reactor spray combustion mode, PaSR, [14] and the flame propagation mode. For the latter, a new expression for the reaction rate based on the flame speed was derived. The development and validation of the chemical kinetic mechanisms for natural gas/diesel oil compositions were carried out according to measurements of ignition delay times in shock tube experiments and flame propagation data for constituent components of natural gas. Since the best approach for the validation of the reduced mechanisms was based on both laminar flame speeds and ignition delay times, natural gas ignition delay calculations were also performed. The mechanism tuning methodology used in this study was based on a sensitivity analysis of complex mechanisms and is fully described in [18]. In the model, since temperature and reaction rate sensitivities are higher at the moment of ignition, the reaction rate coefficients of the most sensitive reactions were modified within limits given in literature to improve the agreement with the ignition delay experimental data. The SENKIN [19] code was used to calculate ignition delay times under constant volume conditions.

The natural gas was selected as a four-component mixture of methane (>90%), ethane, propane and n-butane, whereas diesel oil was represented by the Diesel Oil Surrogate (DOS) model, in which liquid fuel properties are the same of real diesel oil, while fuel vapor is made up of a blend of n-heptane and toluene [12]. The integrated combustion mechanism includes 81 species, 421 reactions for natural gas/diesel oil mixture. The PREMIX code [20] was used to calculate the laminar flame propagation speeds and the comparison results between predictions and experimental data are presented in Fig. 1 illustrating good agreement at atmospheric conditions.

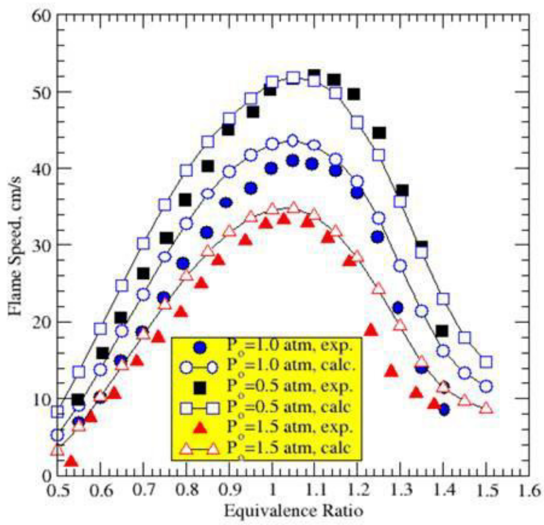

Fig. 1 Simulated and experimental flame propagation velocities for NG/air mixtures

3. CFD Engine Modeling

The base engine that has been selected to investigate DF combustion is a 4-cylinder, 2.8 L HSDI turbocharged Diesel unit, manufactured by VM Motori (Cento, Italy). The main features of the engine are listed in Table 2.

Before the investigation on the dual fuel application, a 3D model of the engine has been built and validated by comparison with a set of experimental data, for Diesel-only combustion (normal Diesel operations). The computational grid for combustion simulation has been constructed using the K3prep preprocessor, included in KIVA-3V package [12]. Because of the axial-symmetric nature of the combustion chamber and injection system, a 60° sector grids has been considered, imposing proper cyclic boundary conditions. In designing the grid, particular care has been devoted to get a good aspect ratio of cells and to correctly reproduce the actual compression ratio of the engine. A minimum of 4 cell layers has been enforced in the squish region at Top Dead Center, while the typical cell size is about 0.5-1.0 mm. As found in previous analyses [13,17], these meshing criteria guarantee a good compromise between accuracy and computational demand. The computational grid is shown in Fig. 2 and consists of about 110.000 cells at TDC and of about 25.000 at BDC.

Table 2 Main features of the base engine

Number of cylinders	4 in-line
Total displacement [cm^3]	2776
Bore [mm] x Stroke [mm]	94 x 100
Compression ratio	17.5:1
Valves per cylinder	4
Air metering	VGT, Intercooler
Injection system / Max injection pressure [bar]	Common rail / 1600

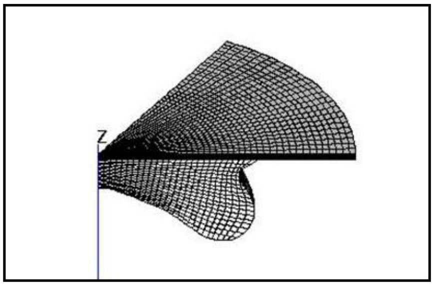

Fig. 2. Views of the computational grid at TDC

Initial conditions for combustion simulations, such as pressure, temperature, trapped mass and charge composition, have been obtained from experimental data, while the intensity of the initial swirl flow has been derived from previous CFD simulations [20].

Combustion simulations have been carried out at full load and at 3 different rotational speeds of the engine (2000, 3000 and 4000 rpm). In order to assess the accuracy of the CFD model, figure 3 shows a comparison between predicted and measured in-cylinder pressure and Rate of Heat Release curves, for the 3 simulated operating points in normal Diesel operation. As visible, a good agreement with experiments has been found.

As far as emissions are concerned, the comparison between experiments and simulation is presented in figure 4. Only CO and NO are considered, since it is well known that the emissions of soot are negligible in DF operations. Again, a good agreement between simulation and testing is found. CO_2 measures were not available for this Diesel engine, however the satisfactory agreement found for the other exhaust components, as well as for the combustion and in-cylinder parameters visible in figure 3, supports the confidence also in the numerical prediction of Carbon Dioxide.

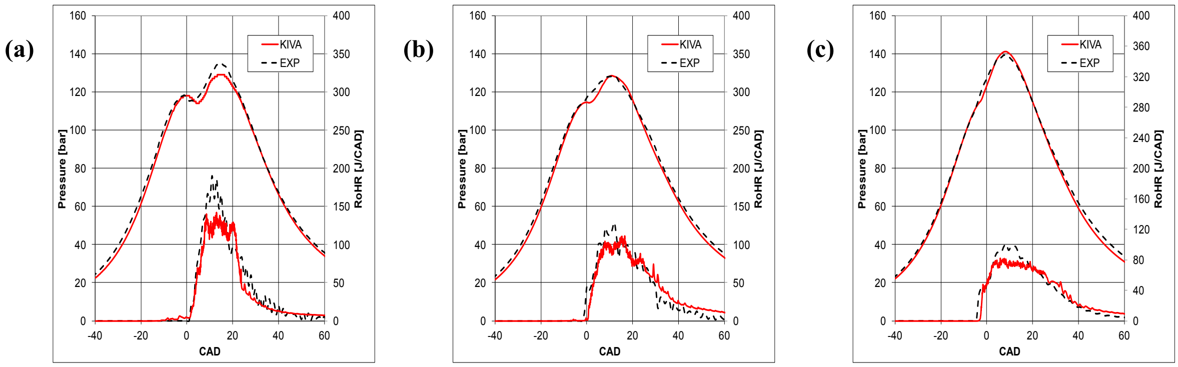

Fig. 3. Comparison between experiments and KIVA simulation (normal Diesel operation): in-cylinder pressure and Rate of Heat Release, at (a) 2000 rpm, (b) 3000 rpm, and (c) 4000 rpm, full load.

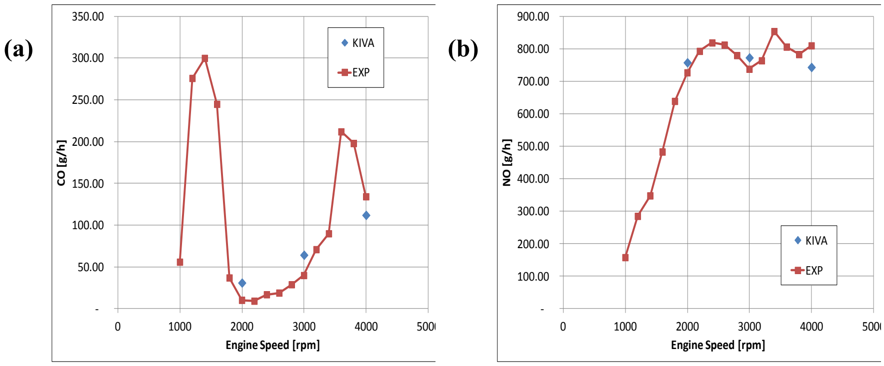

Fig. 4. Comparison between experiments and KIVA simulation (normal Diesel operation): (a) CO emissions, (b) NO emissions

4. Dual Fuel operations

The DF combustion in the VM engine has been carried out keeping the same initial and boundary conditions as in normal Diesel operations, to isolate the effect of the combustion process. The injection strategy for DF operations consists in a pilot injection, that contributes only for a small fraction to the engine power output: the amount of liquid fuel that is injected is 10% of the fuel injected in the corresponding normal Diesel operation.

A set of simulations has been performed for each of the 3 investigated cases (2000, 3000 and 4000 rpm) varying both premixed natural gas concentration and start of injection. The total fuel used in DF operations has been compared to the one consumed under normal Diesel (ND) operations by means of the parameter:

$$Xcng = \frac{m_{nat.gas,DF} + m_{Diesel,DF}}{m_{Diesel,ND}} \quad (1)$$

In order to evaluate the indicated work, directly related to the engine power output, a Gross Indicated Mean Effective Pressure (IMEP*), is calculated as the pressure-volume integral from 40° BTDC to 110° ATDC, divided by the engine unit displacement.

Figure 5 plots IMEP* as a function of both Xcng and start of pilot injection (SOI) for (a) 2000, (b) 3000 and (c) 4000 rpm. The dashed lines indicate the maximum in-cylinder pressure reached in DF operation, for each combination of Xcng and SOI. For each engine speed, the values of IMEP* and maximum in-cylinder pressure obtained under ND operation are highlighted using, respectively, a bold solid line and a bold dashed line.

As expected, Fig. 5 shows that the IMEP* corresponding to ND operations can be reached in DF combustion with a lower amount of fuel (about 80% at 2000 and 3000 rpm and about 90% at 4000%), thanks to the higher heating value of Natural gas. It is interesting to note that adopting a proper combination of premixed Natural Gas concentration and SOI, both the IMEP* and the peak of in-cylinder pressure can be kept constant from ND to DF operations, for all the considered cases. Table 3 shows the values of Xcng and SOI meeting the constraint of constant IMEP* and maximum in-cylinder pressure.

Fig. 5 shows also that the target IMEP* can be obtained at smaller Xcng, when accepting higher in-cylinder peak pressures. On the one hand, this setting can further reduce the CO2 emissions and the fuel consumption; on the other hand, NO emissions become higher, as well as the peak temperatures and the risk of knocking.

Figure 5 also provides a guideline to address the DF engine setting at partial load.

Table 3 Optimum setting for DF operations

rpm	Operation	SOI [° ATDC]	m_{Diesel}[mg/stroke]	M_{NG}[mg/stroke]	Xcng
2000	Normal Diesel	3*	84.10	0	-
	Dual Fuel	0	8.41	57.6	78.5%
3000	Normal Diesel	-3.9*	78.70	0	-
	Dual Fuel	-2	7.78	57.2	82.6%
4000	Normal Diesel	-9.1	69.70	0	-
	Dual Fuel	-8	6.97	56.2	90.1%

* main injection

Fig. 6 provides a comparison among the cases listed in Table 3 in terms of: in-cylinder pressure, in-cylinder temperature and rate of heat release. It can be observed that pressure traces are almost identical, while some difference can be found in combustion development and temperatures. DF operations always correspond to higher peak temperatures. Burn rates are comparable at 2000 and 3000 rpm, but at 4000 rpm DF combustion is smoother. Finally, it is observed that the slightly lower cylinder pressures and temperatures visible during the compression stroke of DF configuration are due to the higher specific heat capacity of the Natural Gas/air mixture.

Figure 6 finally shows the comparison between optimized DF and ND operations. The following considerations are made: a) besides the elimination of smoke, DF combustion yields an average 20% reduction of CO_2 and an even larger abatement of CO (from 40 to 80%); b) fuel economy is improved by 20%, on average; c)the only drawback appears the increase of NO.

The last issue can be reduced, or even canceled, by means of a different setting of X_{cng} and SOI. This new setting should slightly reduce, but not cancel, the advantages in terms of fuel economy and CO2.

(a)

(b)

(c)

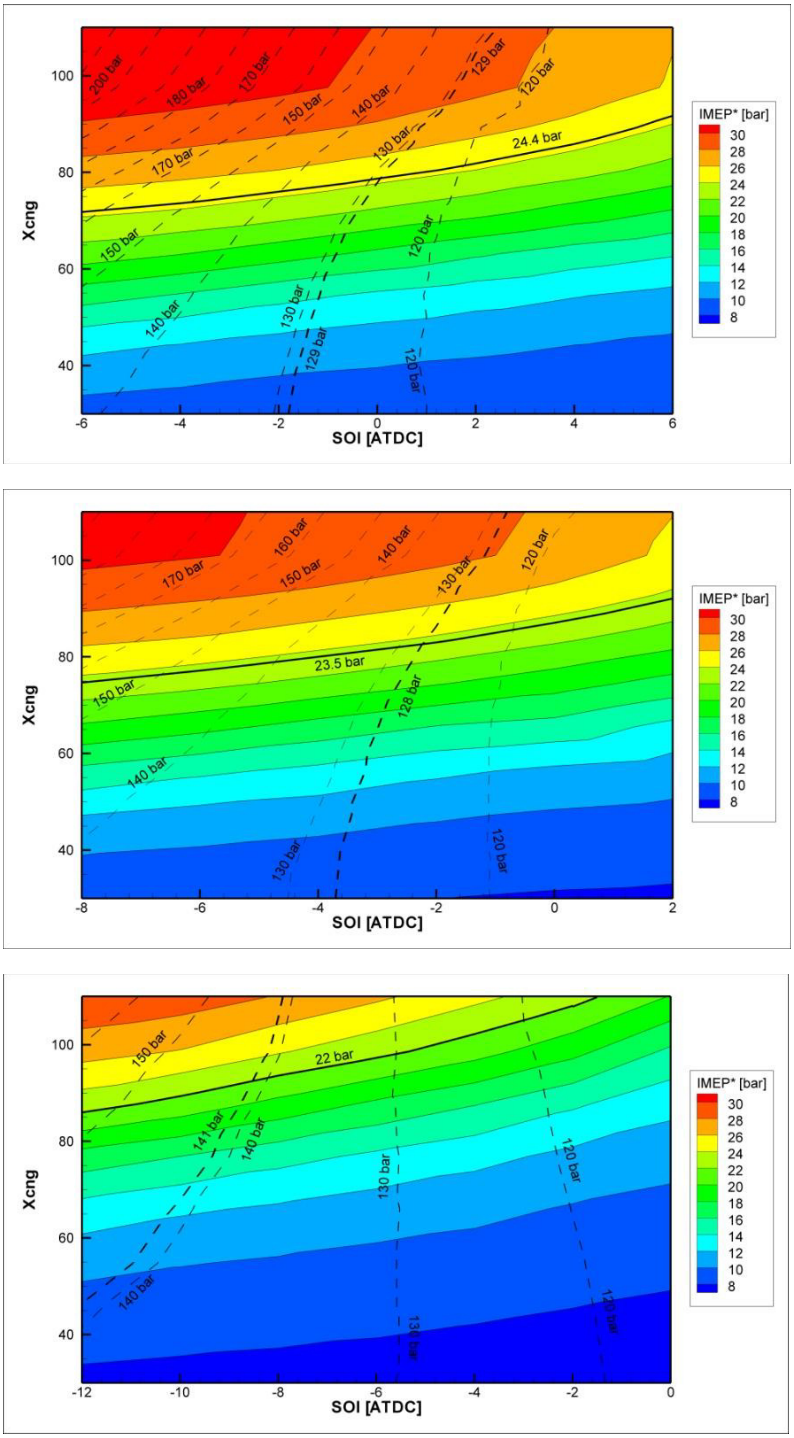

Fig. 5. Contours plot of Indicated Mean Effective Pressure calculated from 40° BTDC to 110° ATDC (IMEP*) as a function of Start of Injection angle (SOI) and ratio between fuel mass (gas and liquid) in DF operation and liquid fuel mass in corresponding normal Diesel operation (Xcng) for (a) 2000 rpm, (b) 3000 rpm and (c) 4000 rpm.

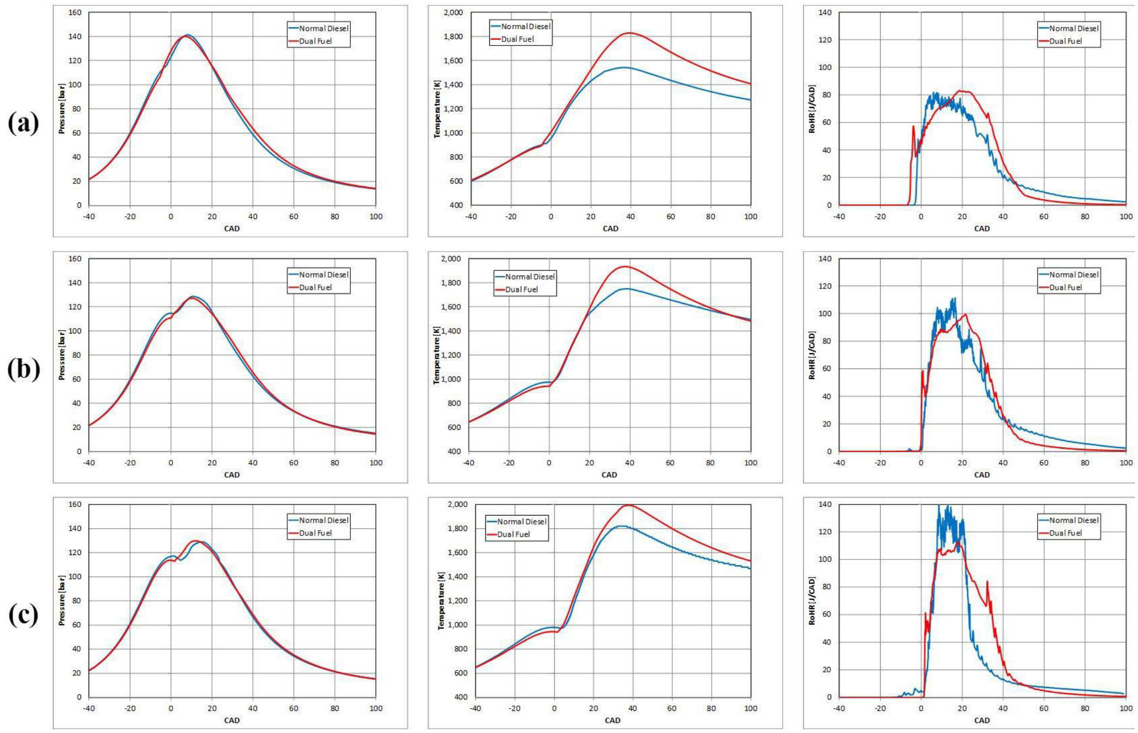

Fig. 6. Comparison between normal Diesel and Dual Fuel operation in terms of in-cylinder pressure, temperature and Rate of Heat Release, at (a) 2000 rpm, (b) 3000 rpm, and (c) 4000 rpm.

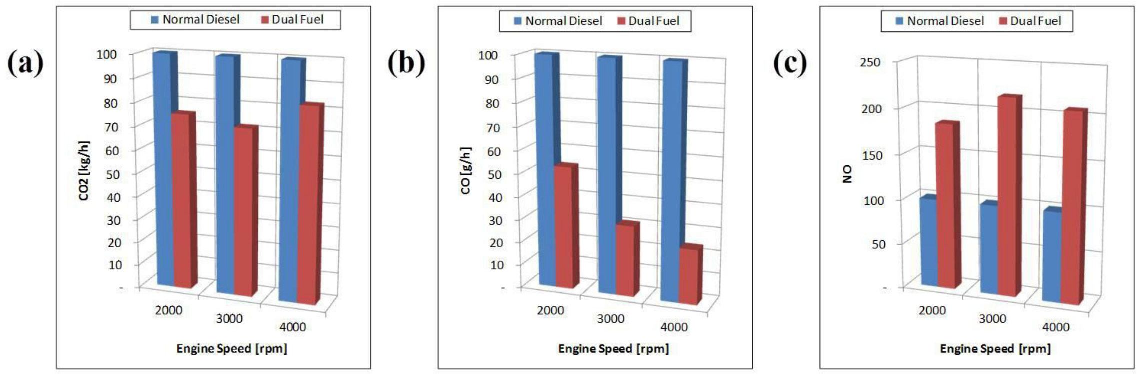

Fig. 7. Comparison between normal Diesel and Dual Fuel operation in terms of (a) CO2 emissions, (b) CO emissions, (c) NO emissions

Conclusion

In the paper the Natural Gas/Diesel Dual Fuel (DF) combustion was investigated in order to explore one promising solution to reduce the emissions of conventional Diesel engines. A 4-cylinder, 2.8 l, turbocharged HSDI Diesel engine was selected and Normal Diesel (ND) operation was simulated using a customized version of the CFD code KIVA 3V that includes a previously validated combustion model comprising both partially premix reactor and flame propagation modes. The results of ND combustion have been calibrated against experimental data in terms of in-pressure pressure and pollutant emissions.

A set of simulations has been then performed for DF combustion at 3 different engine speed, varying both premixed natural gas concentration and start of pilot injection. Simulations demonstrate that Gross Indicated Mean Effective Pressure of ND operation can be reached with DF combustion keeping the same in-cylinder pressure and with a with a lower amount of fuel. It was also observed that DF, in addition to the elimination of smoke, allows the reduction of CO_2 (about 20%) and CO (from 40 to 80%) emissions. The only drawback appears the increase of NO that can be reduced, or even canceled, by means of a different setting of premixed Natual gas concentration and SOI. This new setting should slightly reduce, but not cancel, the advantages in terms of fuel economy and CO2 emission reduction.

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