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Research Article
Modeling of a Spray of Diesel Fuel with Dissolved Liquefied Natural Gas

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Abstract
Background and Objective: Using Natural Gas (NG) for combustion process modification in compression ignition engines is considered to be a promising method due to its high volumetric efficiency, high thermal efficiency and low emissions. However, the natural gas has a penalty in terms of how to be involved in a combustion process due to its high auto-ignition temperature and lower cetane number. This study is a numerical investigation of the steady spray characteristics of diesel fuel containing dissolved natural gas. **Materials and Methods:** The simulation was carried out using ANSYS fluent software and a standard k-ε model was chosen with heat transfer condition at 300 K. The effect of natural gas concentration of 0, 5, 10 and 15% by mass in the diesel fuel on the spray characteristics for a typical diesel engine was studied numerically. A high pressure common rail injector with pressure of 200, 500 and 600 bar was investigated. **Results:** The results showed that the spray tip velocities increased with the increase in the natural gas concentration and injection pressure, while the spray cone angle of diesel-NG were smaller compared to that of pure diesel at the same conditions. **Conclusion:** The K-ε model of turbulence was successfully used to evaluate the spray characteristics and the results were compared to the some of the experimental data.

Key words: Fuel technology, diesel engine, liquid-gas spray, fuel injection, computational fluid dynamic

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Data Availability: All relevant data are within the paper and its supporting information files.

INTRODUCTION

In recent years, Natural Gas (NG) is being used increasingly in internal combustion diesel engines due to the lower costs compared to petroleum. There are different principal methods for NG to be used in compression ignition engines; the first one, the natural gas is injected into the inlet manifold, mixes naturally with the air and forms a fully pre-mixed fuel-air mixture in the combustion chamber. Thus a mixture of gas and air is compressed during the compression stroke and before the end of the stroke; a pilot quantity of diesel fuel is injected to initiate combustion[1]. This kind of operating condition produces a none-uniform mixture distribution of the natural gas inside the engine. In addition, this system does not favour the two-stroke engine due to the escape of some of the natural gas fuel into the exhaust. The second method of using natural gas in diesel engines is the direct injection of natural gas near to the diesel fuel spray into the combustion chamber[2]. Thus a full stratification of the fuel-air mixture can be obtained with good flammability over the entire load range. Recently, successful operation has been demonstrated by applying this method using a prototype co-injector[3], resulting in diesel-gas two phase mixtures which were then injected into the chamber. A new idea of pre-mixing diesel and Compressed Natural Gas (CNG) was suggested to increase the air quantity inside the cylinder more than if a mixture of CNG-air is injected in the engine which may result is a rich mixture[4,5]. This mixture required a study of macroscopic parameters through the injector such as spray tip penetration, spray cone angle, spray velocity and spray impingement (spray travel along the wall, radial penetration and spray height). Zhang *et al.*[6] studied the steady spray characteristics of kerosene and diesel fuel containing dissolved methane (NG), the spray pattern images were captured using a digital camera at the nozzle exit and six types of the straight-hole nozzles with different length/diameter ratios (L/D) were employed in the study. Ismael *et al.*[7] showed the jet penetration rate was observed to be higher in the diesel-CNG dual-fuel case than that of the pure diesel spray, while the spray cone angle was found to be lower. Brown *et al.*[8] used three injectors and their result showed that co-injection of dual-fuel (diesel-CNG) was better. They simplified a representation of two methods of diesel-gas mixing within a co-inject gas plenum as shown in Fig. 1. The spray characteristics such as spray penetration rate, spray cone angle, spray velocity, droplet size and droplet atomization were largely dependent upon the injection pressure, chamber pressure and temperature[9].

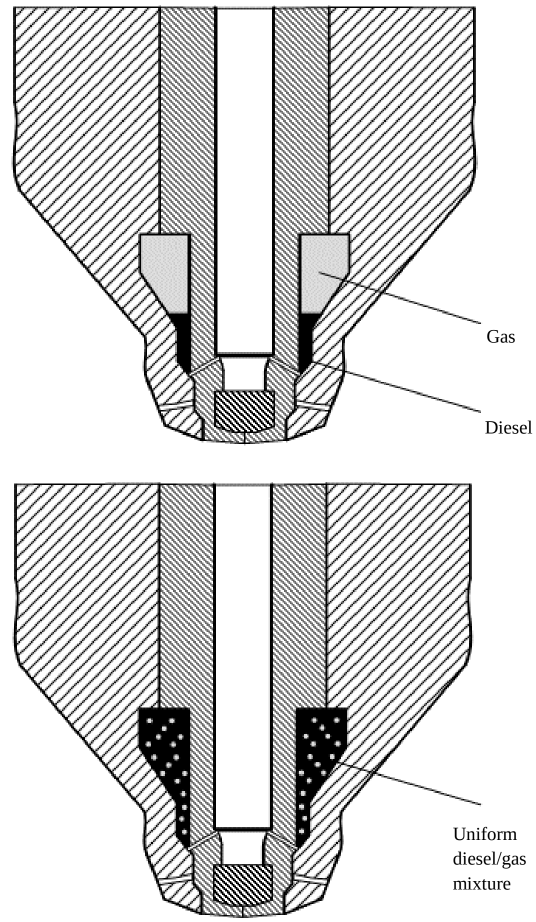

Fig. 1: A simplified representation of two methods of diesel-gas mixing within a co-injector gas plenum[8]

On the other hand, the transient nature of the flow through injector systems and their small sizes makes it very difficult to analyze them experimentally. Numerical analysis is often used to analyze the flow inside the injectors and provide the physical flow processes visibility that occurs in them and the entire fuel system[10-13]. Because of that, Computational Flow Dynamics (CFD) analysis of flow through the injector was performed. In the past, most of the fuel injector CFD analysis was limited to the steady state time conditions. This approach is simplistic and does not fully reflect the actual state occurring in the spray process, while the unsteady analysis conditions will be accurately predict spray-combustion in engine cylinder. In order to improve computation processing, a moving mesh is used nowadays. Depending on the computing solver, there are many ways to simulate the movement of the elements. Lee and Reitz[14] used a special algorithm of needle movement, which contained a structural grid consisting of hexahedral elements. Certainly, the development of model discretization methods and movement simulation increase the design options. Injector designing is still challenged by constant striving to improve economic and ecological aspects in combustion engines, alternative-fuel supply and varied injection pressure.

In this study, activities were first simulated to determine the influence of dissolved Natural Gas (NG) in diesel fuels on the atomization of a steady spray through six-hole nozzle using an injector of diesel engine (Denso) under actual conditions of the diesel cylinder. Spray characteristics such as spray tip penetration, cone angle and spray velocity were investigated for different amounts of NG dissolved in the diesel fuel at different injection pressures.

MATERIALS AND METHODS

Research methodology: The methodology adopted for the present study is as follows; the main parameters of the engine are given in Table 1. The crank angle for the calculation is from intake valve close to exhaust open[15].

A detailed understanding of the fuel injection, spray characteristics and the dissolving processes of the Natural Gas (NG) in diesel fuel before injection is required in order to enhance the combustion within the engine cylinders, while not compromising the engine fuel economy. The former involved spray tip penetration, spray cone-angle and the derivatives of them such as spray tip velocity and spray volume as shown in Fig. 2.

Before measuring the spray characteristics of diesel fuel containing dissolved NG. The concentration of dissolved NG was set at 5, 10 and 15% by mass. The concentration (C) of NG dissolved in diesel fuel was defined as following in Eq 1::

$$C = \frac{M_{NG}}{M_{Diesel}} \quad (1)$$

where, M_{NG} is the mass of dissolved NG and M_{Diesel} is the mass of diesel fuel in which the natural gas was dissolved. The solubilities of natural gas in diesel fuels increase with the increased of the dissolving pressure, so the concentration could be controlled by the dissolving pressure, the material algorithm for mixing two different fuel properties and under high pressure has been re-programmed based on the critical pressure for liquefied natural gas, which is higher than 100 bar. Enough time was needed for reaching a uniform mixture of diesel fuel and NG. In this study, the range of injecting pressure was set at 200, 500 and 600 bar.

Simulation model: The Computational Fluid Dynamics (CFD) is based on the numerical solutions of the fundamental governing equations of fluid dynamics namely the continuity, momentum, energy, species and turbulent equations, two phase flow. The FLUENT software package was used to accomplish this job, a standard k-ε model was chosen with ambient temperature condition at 300 K for a mixture. The assumptions of a geometric numerical model were based on real geometry and experimental studies of diesel engine, the combustion chamber is axisymmetric. In order to save calculation time, the simulation area is one sixth of the combustion chamber because the number of spray hole is 6 at 0.3 mm diameter as shown in Fig. 3. The number of cells

Table 1: Diesel engine's parameters[15]

Parameters	Values
Cylinder diameter × stroke (mm)	96×92.4
Connecting rod (mm)	153
Compression ratio	16.2
Number of spray hole	6
Injected fuel per cycle (mg)	54.9
Start of injection (°CN)	15°(BTDC)
End of injection (°CN)	13°(ATDC)
Swirl ratio	1.7

BTDC: Before top dead centre, ATDC: After top dead centre, CN: Crank angle

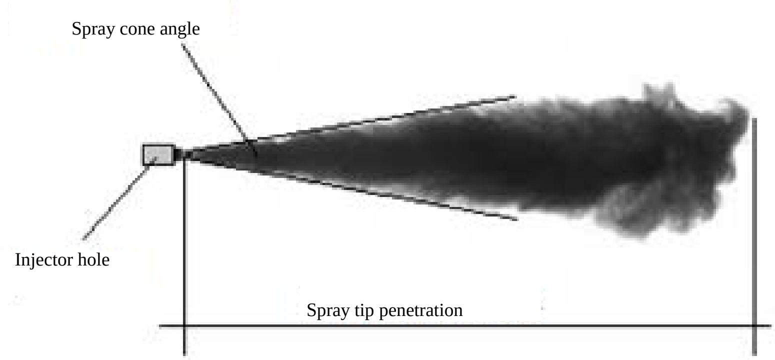

Fig. 2: Spray parameters

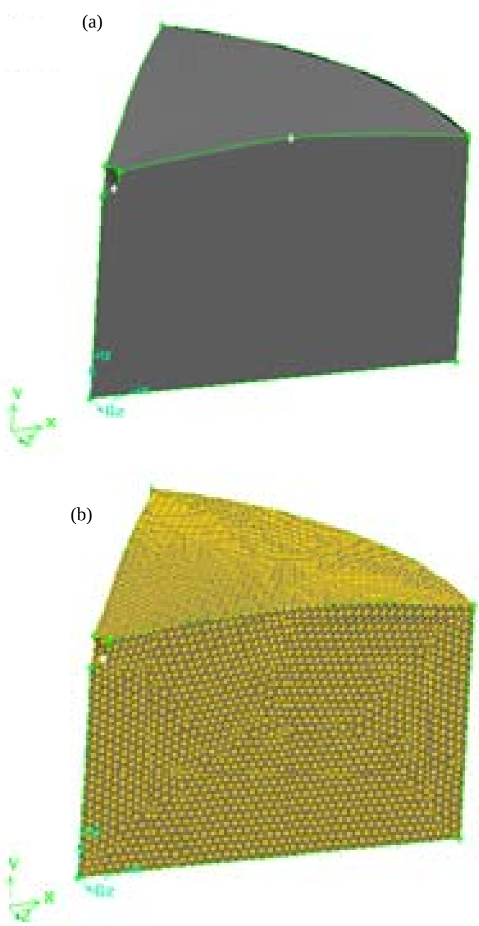

Fig. 3(a-b): (a) Solid modeling and (b) Mesh for case under study

used in this model was 786,277. Mesh refinement investigation has been carried out to optimize the number of cells used. It has been found that increasing the number of cells to 957,697 and 1,211,045 has no effect on the results accuracy. Hence, 786,277 was selected to be the optimum number of cells that can be used in the simulation.

Governing equation: Turbulence consists of fluctuations in the spray flow field in time and space and can have a significant effect on the characteristics of the spray. The k-ε model of turbulence is widely chosen for fluid flow analysis where, k is the turbulence kinetic energy and is defined as the variance of the fluctuations in velocity and ε is the turbulence eddy dissipation (the rate at which the velocity fluctuations dissipate). To simulate the turbulence parameters and spray analysis, a standard k-ε model was chosen with isothermal heat transfer condition at 300 K. The solver uses this model with two new variables: transient term B and diffusive term G and the equations as follows:

The continuity equation is defined in Eq. 2:

$$\frac{\partial}{\partial z_j}\left(\rho\bar{\mu}_j\right)=0 \tag{2}$$

The momentum equation as shown in Eq. 3:

$$\bar{\mu}_j\frac{\partial}{\partial z_j}\left(\rho\bar{\mu}_i\right)=B-\frac{\partial\bar{p}}{\partial z_i}+\frac{\partial}{\partial z_j}\left(\mu\left(\frac{\partial\bar{\mu}_j}{\partial z_i}+\frac{\partial\bar{\mu}_i}{\partial z_j}\right)+\rho\bar{\mu}_i\bar{\mu}_j\right) \tag{3}$$

The energy equation as shown in Eq. 4:

$$\bar{\mu}_j\frac{\partial}{\partial z_j}\left(\rho cp\bar{T}\right)=H+\frac{\partial}{\partial z_j}\left(\rho cp\alpha\frac{\partial\bar{T}}{\partial z_j}-\rho cp\bar{\mu}_j\bar{T}\right) \tag{4}$$

The model with two new variables: first, this study has been performed by use of the implicit unsteady solver with a first order temporal discretization scheme. The first order temporal scheme is known as Euler implicit and discretize the unsteady term using the solution at the current time level. Second, the diffusive term from Eq. 5-7:

$$\bar{\mu}_j\frac{\partial}{\partial z_j}\left(\rho\bar{c}\right)=R+\frac{\partial}{\partial z_j}\left(\rho D\frac{\partial\bar{c}}{\partial z_j}-\rho\bar{\mu}_j\bar{c}\right) \tag{5}$$

$$\rho\frac{\partial k}{\partial t}+\rho\bar{\mu}_j k_{1,j}=\left(\mu+\frac{\mu_t}{\partial_k}k_{1,j}\right)_{1,j}+G+B-\rho\varepsilon \tag{6}$$

$$\rho\frac{\partial\varepsilon}{\partial t}+\rho\bar{\mu}_j\varepsilon_{1,j}=\left(\mu+\frac{\mu_t}{\partial_\varepsilon}\varepsilon_{1,j}\right)_{1,j}+c_1\frac{\varepsilon}{k}G+c_1\left(1-c_3\right)\frac{\varepsilon}{k}B-c_2\rho\frac{\varepsilon^2}{k} \tag{7}$$

where, j = 1, 2, 3, which are refereeing to three axis.

Boundary conditions: Since the dissolved NG in diesel does not change its state during or after the injection, its introduction into the computational domain is through a simple "Mass-flow" inlet. In fluent, parameters for such inlets include the actual mass-flow of the fluid as well as the fluid's stagnation temperature. In this study, the injection is taken to be choked at a mass-flow of 4.43 g sec^{-1} and thus the stagnation temperature has been set at 300 K and the spray tip velocity equal zero when t = 0 (in injection time), while the concentration of dissolved LNG was adjust at 5, 10 and 15. Table 2 shows properties of diesel fuel and liquefied natural gas.

RESULTS AND DISCUSSION

Spray tip velocity: The spray tip velocity contours of the diesel (C = 0%) and diesel-NG (C = 15%) at 500 bar injection pressure at different elapsed time are shown in Fig. 4. While, Fig. 5 shows the comparison between the tip velocities of the mixture at different concentrations at C = 0, 5, 10 and 15%. It can be seen that, at the early stage (t = 0.2 msec), all the spray tip velocities were higher compared to the pure diesel spray. While in the second stage (t = 0.4 msec), the differences in the velocity of diesel-NG become significant compared to the pure diesel (C = 0%). At this stage, the NG dissolved with C = 15% showed a higher tip velocity (138 m sec^{-1}), compared to the pure diesel spray (64 m sec^{-1}). The reason for this phenomenon can be explained by an expansion and evaporation of the NG[16]. In other words, the diesel spray droplets momentum enhanced the NG in the axial direction caused an increase in the velocity as their kinetic energy increased. The density and viscosity are completely affecting on the droplet velocity, which is very high initially, decreases slowly at the tip of the spray[17].

The phenomena of diesel and diesel-CNG velocity profile was studied by Ismael *et al.*[7] who noticed that, both the droplets velocities and diameters of the liquid were largely influenced by the flow momentum, where the droplets diameter were small with the high momentum. These results are contradicting with the findings of present study. This is because the researchers used two injectors. At the last stage (t = 0.6 msec), the pure diesel spray showed the highest velocity where the mixtures lost their momentum and became slower.

Spray cone angle: The development of the spray cone angle with time for different NG concentration at injection pressure 500 bar is shown in Fig. 6. At the initial stages, all the spray cone angles decreased before reaching a constant fully developed value as in agreement with results in the study of Xie *et al.*[18]. The results also showed that the spray cone angle of the pure diesel C = 0 was greater compared to those for the diesel (C = 5, 10 and 15%). With increasing the concentration C, the cone angle becomes lower. This was thought to be due to the effect of the LNG dissolved in the diesel spray resulting in an increase the spray momentum in the axial direction. Also this finding in agreement with Huo *et al.*[19] who showed that with the increase of water content on the emulsion showed wider spray cone angle and shortened initial tip penetration in the first couple of snapshots.

Table 2: Properties of diesel fuel and liquefied NG

Parameters	Diesel	LNG
Density (kg m^{-3})	840	450
Viscosity (Nsec m^{-2})	0.0024	7.8×10^{-3}
Carbon (%, w/w)	86.83	73.3
Hydrogen (%, w/w)	12.72	23.9
Oxygen (%, w/w)	1.19	0.4
Sulphur (%, w/w)	0.25	-

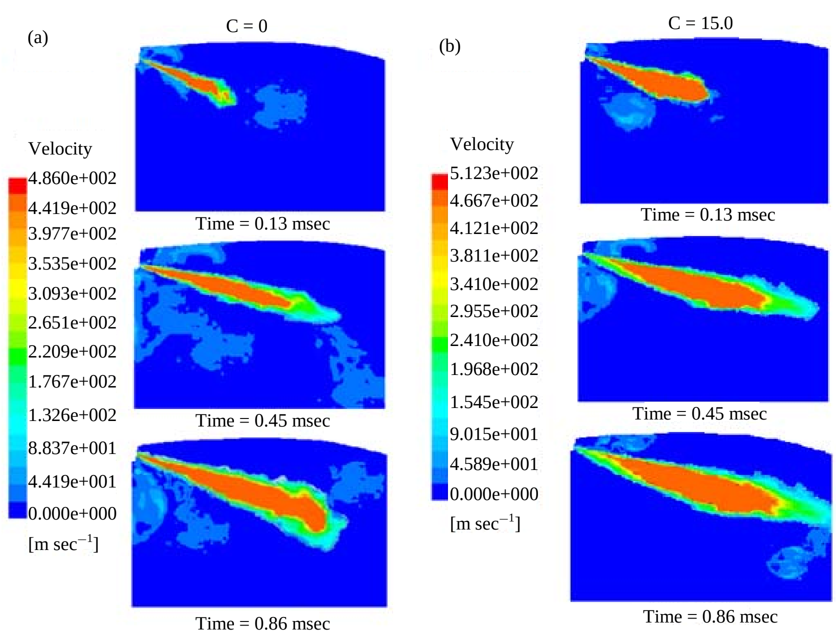

Fig. 4(a-b): (a) Contours of the spray tip velocity for the concentration ratios C = 0 and (b) 15% at different times after start of injection

Effect of injection pressure on spray penetration: To go further in the comparison between sprays of pure diesel and LNG diesel the fuel injection pressure was varied to 200, 500 and 600 bar as shown in Fig. 7 and 8. The results showed that the highest spray tip velocity was found to occur with the highest injection pressures which is in agreement with the findings of previous study of Ismael *et al.*[2]. The results also showed that the pure diesel spray (C = 0) started to diverge earlier than that of the diesel-NG with at all NG concentrations. This was probably caused by the differences in the spray momentum of single fuel compared to the mixtures. Also it can be noticed that the differences in the spray tip velocity between injection pressures 200, 500 and 600 bar in diesel at C = 15% was greater in comparison with the differences between the same pressures in the diesel at C = 0, 5 and 10%. It is believed that the main reason for the influence of the injection pressure on the percentage of NG in the mixture, as the percentages of the mixture increased, the droplets penetrated faster. The increased viscosity makes the anti-shear capacity of the spray droplet greater, which in turn makes the spray more difficult to break up[20,21].

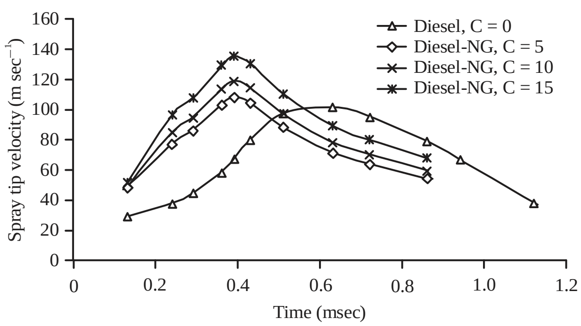

Fig. 5: Spray tip velocity of diesel and diesel-NG when the concentration of NG dissolved in diesel at C = 0, 5, 10 and 15%

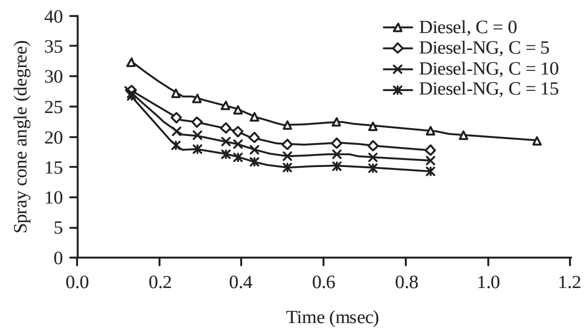

Fig. 6: Spray cone angle of diesel and diesel-NG at injection pressure: 500 bar of diesel-NG at C = 0, 5, 10 and 15%

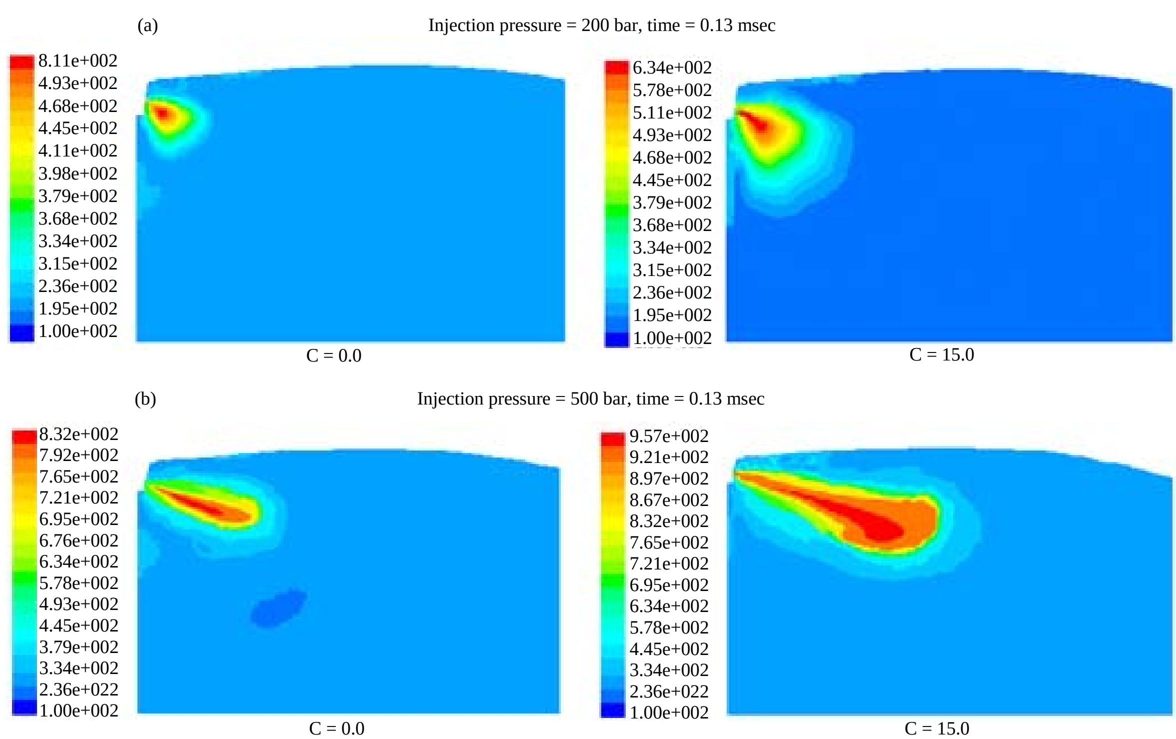

Fig. 7(a-b): (a) Contours of the diesel and diesel-NG dissolved at C = 0.0 and (b) 15 at injection pressure 500 bar

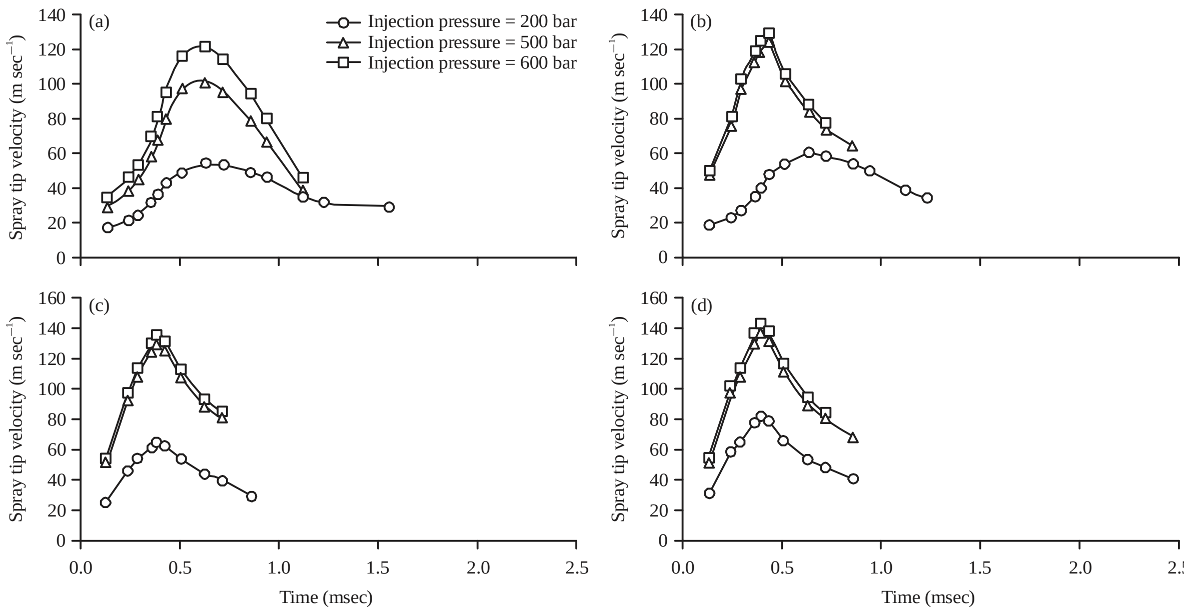

Fig. 8(a-d): Effect of different injection pressures (200, 500 and 600 bar) on spray tip velocity (a) C = 0, (b) C = 5.0%, (c) C = 10.0% and (d) C = 15%

This finding is in agreement with the previous studies by Ismael *et al.*[7] who compared the diesel spray (single fuel) and diesel-CNG dual fuel spray. They observed that the higher injection pressures generated small droplets and increased the rate of fuel delivery time. The diesel-CNG dual fuel also showed a higher penetration rate with lower jet cone angle than that of the pure diesel spray.

CONCLUSION

The spray characteristics of liquefied natural gas dissolved in diesel fuel at different concentration i.e. 0, 5, 10 and 15% by volume were investigated using ANSYS fluent software. The K-ε model of turbulence was successfully used to evaluate the spray characteristics such as spray velocity, tip penetration and cone angle under different injection pressures. A comparison between the computational results and the experimental data from the literature were discussed. The results showed that with increasing the concentration of LNG, the spray tip velocities increased particular with increasing the NG concentration. Also with increasing the injection pressure, the spray tip velocities increased particular with increasing the NG concentration.

SIGNIFICANCE STATEMENTS

- This study modifies of the idea of pre-mixing diesel and gas, it was suggested in study to increase the air quantity inside the cylinder more than if a mixture of fuel gas-air is injected in the engine which may result in a rich mixture
- Results from the validated simulation, presents clear prediction of the spray characteristics such as spray tip penetration, cone angle and spray velocity
- User design function code has been developed to solve the mixing of liquid-gas dissolved fuel boundary problem during the spray process

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