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> ISSN 1333-1124 eISSN 1849-1391

# LARGE EDDY SIMULATION OF ULTRA-HIGH INJECTION PRESSURE DIESEL SPRAY IN MARINE DIESEL ENGINES

UDC 621.43:519.6

## **Summary**

Large Eddy Simulation (LES) scheme and a new modified breakup model have been implemented in the OpenFOAM freeware for simulating ultra-high injection pressure diesel and Marine Diesel Fuel (MDF) sprays. Also, the dynamic of dispersed droplet has been modelled by the Lagrangian Particle Tracking (LPT) scheme. The proposed LES/LPT method has been validated by matching it against published experimental data and numerical results of Fluent software under different injection pressures of up to 300 MPa. Furthermore, comparisons have been drawn with Reynolds Averaged Navier-Stokes (RANS) simulations. Spray shape and geometry, droplet penetration and size as well as equivalent ratio are compared with experimental data. Based on the obtained numerical results, main spray characteristics have been simulated accurately by LES and RANS, but the LES results display greater precision in transient conditions. Later, numerical sensitivity of the LES results to the mesh resolution is discussed. Finally, it is found that the proposed LPT/LES scheme along with the advanced breakup model gives more accurate results than the conventional RANS model under ultra-high injection pressures. This advanced scheme has been implemented to investigate the influence of Marine Fuel on spray characteristics.

Key words: Large Eddy Simulation (LES), Ultra-high injection pressure, Marine diesel engine, OpenFOAM

## 1. Introduction

Because of a unique combination of efficiency, power, reliability, and durability, diesel technology plays a vital role in many important industries such as power generation and land and marine transport. Technologies and actions which promote performance and emission reductions have been increasingly attractive in the recent decades. Improved fuel atomization and air-fuel mixture are among the most effective solutions for diesel engine applications. In the meantime, increasing injection pressure is the optimal solution that provides a better air-fuel mixture [1]. Increasing the injection pressure is the best remedy that generates a small droplet size for high-viscosity marine fuels.

Recently, the diesel engine injection pressure has reached more than 300 MPa and many studies have been conducted on the effects of high injection pressure on engine performance.

Kato et al. [2] and Yokota et al. [3] experimentally examined the effects of injection pressure of up to 250 MPa. They concluded that the droplet size is correlated to the average injection pressure and also to the change in injection pressure over time. Lee et al. [4] experimentally and numerically investigated the ultra-high injection pressure in the range 150 to 355 MPa. The effects of nozzle geometry and injection timing on the diesel spray have been studied experimentally by Kastengren et al. [5]. A detailed experimental inspection of diesel and biodiesel spray characteristics under three injection pressures (100, 200 and 300 MPa) has been reported by Wang et al. [6].

CFD-based computer simulations have become standard tools for investigating flow, spray and combustion phenomena in engines. One of the key related issues is an exact description of turbulence. RANS methods solve the time-averaged conservation equations for mass, species, momentum and energy, while LES solves their space-averaged (filtered) counterparts. The main advantage of the LES technique over the computationally more efficient RANS approach is the increased level of detail it can provide [7].

In recent years, many researches have performed simulations of the diesel spray. Most of them have focused on the breakup, atomization and turbulence modelling as the main phenomena of the spray. Effects of the breakup model on spray characteristics were investigated by Som et al. [8] and Hosseinpour et al. [9]. Turner at al. [10] presented a new breakup model and implemented it in the Kiva software. A numerical simulation was also carried out on the effect of injection pressure on spray characteristics by Shervani-Tabar et al. [11]. Open source softwares are effective tools for the simulation of diesel spray and have been used by many researchers. For example, Kadocsa et al. [12], Gjesing et al. [13], Kassem et al. [14], Vuorinen et al. [15], Nowruzi et al. [16] and Yousefifard et al. [17] used either the KIVA or the OpenFoam code to simulate the diesel spray.

The important role of marine diesel engines has led to many specific researches on this field ([18], [19]). In more recent years, other researchers like Goldsworthy [20], Ushakov et al. [21], and Sigurdsson et al. [22] also studied marine diesel engines. On the other hand, Marine Diesel Fuels (MDF) have also been the focus of many studies and researches. Kyriakides et al. [23] developed a model with the thermophysical properties of Heavy Fuel Oil, typically used in marine diesel engines and implemented in the KIVA CFD code. Prucole et al. [24] presented a study on combustion quality of biodiesel and marine fuel blends.

Most of the existing CFD (Computational Fluid Dynamics) researches on fuel spray simulations have been carried out using the RANS method [25]. In the past few years, Large Eddy Simulations have become increasingly popular in CFD because of the increasing computational power of the new computers. Rutland [26] reviewed the large-eddy simulation research for internal combustion engines. Zhou et al. [27] reported a comparison between the RANS and the LES simulation used for modelling the diesel spray. They found that the LES approach predicts spray characteristics more exactly, especially in the highly transient flow field. The LES turbulence model was implemented by Karrio et al. [28] to investigate the effects of gas density on fuel sprays. Jones and Lettieri [29] also developed a stochastic sub-grid model for the droplet breakup in Large Eddy Simulation. Hori et al. [30] showed that the mesh density has an important role for LES/LPT spray simulations. Recently, Irannejad and Jaberi [31] presented a Large Eddy Simulation study on the turbulent spray breakup and evaporation.

In this paper, the potential of the LES/LPT framework for ultra-high diesel injection pressure modelling is investigated. For this purpose, non-evaporating and non-reacting sprays under three injection pressures (100, 200 and 300 MPa) are studied using the OpenFOAM code. An advanced KH-RT (Kelvin-Helmholtz/Rayleigh-Taylor) breakup model based on a new scheme that was presented by Sazhin et al. [32] has been implemented in the OpenFOAM software. Fuel droplet penetration, spray angle and volume, Sauter Mean Diameter (SMD) and equivalent ratios have been computed and compared with experimental

data. Also, numerical results of the RANS modelling have been presented and compared with the LES results. Finally, Marine Diesel Fuel is used under these conditions and spray characteristics are compared with kerosene as a normal diesel fuel.

#### 2. Governing equations

Governing equations of the fluid phase together with the description of motion of the dispersed particle/droplet phase are full Navier–Stokes equations as in

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_i} = 0, \qquad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( -p \delta_{ij} + \tau_{ij} \right) + M, \qquad (2)$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial (\rho u_j h)}{\partial x_j} = \frac{\partial}{\partial x_j} (\sigma_{ij} u_i) + \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} \right), \tag{3}$$

where M is the momentum source term exerted from droplets to gas phase. The viscous stress tensor is defined as

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \mu \frac{2}{3} \frac{\partial u_k}{x_k} \delta_{ij} \,. \tag{4}$$

These equations have been filtered spatially. The filtered form of nonlinear term leads to similar terms with an additional sub-grid scale (SGS) term [33]. The sub-grid stress tensor  $\tau_{ij}^{sgs}$  is modelled using the Boussinesq type assumption as in

$$\tau_{ij}^{sgs} = \frac{2}{3} k^{sgs} \delta_{ij} - 2\upsilon_t \left(\overline{S}_{ij} - \frac{1}{3} \overline{S}_{kk} \delta_{ij}\right), \tag{5}$$

where  $\mathcal{U}_t$  is the turbulent kinematic viscosity given by

$$\nu_t = C_k \overline{\Delta} \sqrt{k^{sgs}} . \tag{6}$$

Here,  $\overline{\Delta}$  is the characteristic grid length scale,  $k^{sgs}$  is the sub-grid scale kinetic energy and  $C_k$  is the adjustable model parameter [34].

The Lagrangian Particle Tracking (LPT) technique is usually employed for spray simulation. In the current study, simulations of particles are done using the equation of motion which assumes that that force acting on a droplet is due to the drag as in

$$\frac{1}{6}\rho_{p}\pi d^{3}\frac{\mathrm{d}u_{p}}{\mathrm{d}t} = \frac{1}{2}(u_{g}-u_{p})|u_{g}-u_{p}|\rho_{g}C_{D}\frac{\pi d^{2}}{4},$$
(7)

Where  $u_p$  is the particle velocity,  $u_g$  is the gas velocity that is interpolated to the particle position from the adjacent cells and  $C_p$  is the droplet drag coefficient that is defined by

$$C_{D} = \begin{cases} \frac{24}{\text{Re}_{p}} \left( 1 + \frac{1}{6} \text{Re}_{p}^{\frac{2}{3}} \right), & \text{Re}_{p} < 1000\\ 0.424, & \text{Re}_{p} \ge 1000 \end{cases}$$
(8)

The droplet Reynolds number is given by 
$$\operatorname{Re}_p = \frac{|u_g - u_p|d}{\upsilon_g}$$
.

Atomization modelling is one of the most important processes in the spray CFD simulation. The breakup process is caused by the aerodynamic stripping of smaller droplets from larger droplets (Kelvin-Helmholtz instability) or by the disintegration of larger droplets into smaller ones due to the effect of normal stresses (Rayleigh-Taylor instability). The KH-RT instability model is a combination of the Kelvin-Helmholtz (KH) instability and Reyleigh-Taylor (RT) instability models. The KH-RT model, known as a hybrid model, is favoured in the high speed and high Weber number spray model [35].

The source of Kelvin-Helmholtz wave is induced by aerodynamic forces between gas liquid phases, whereas the Rayleigh-Taylor wave is a result of the acceleration of shed droplet ejected into free-stream conditions. This hybrid model combines the effects of Kelvin-Helmholtz waves driven by aerodynamic forces with Rayleigh-Taylor instabilities due to the acceleration of shed drops ejected into free-stream conditions [36]. In the KH-RT model, the aerodynamic force acting on the drop flattens it into the shape of a liquid sheet, and the decelerating sheet breaks into large-scale fragments by means of the RT instability. KH waves with much shorter wavelengths originate at the edges of fragments, and these waves break up into micrometer-size drops.

The growth of KH instabilities on the liquid surface at the interface of the two phases that have different densities causes "child" droplets to be stripped from the liquid core of the jet, which is approximated by "parent" droplets. The radius,  $r_d$ , of the injected droplet is assumed to continuously decrease in size during the breakup process, as described by equation

$$\frac{\mathrm{d}r_d}{\mathrm{d}t} = -\frac{r_d - r_s}{\tau_{bu}},\tag{9}$$

where  $\tau_{bu}$  is the characteristic breakup time of the droplet, and  $r_s$  is the radius of stable droplets, given by

$$r_{s} = \begin{cases} B_{0}\Lambda & B_{0}\Lambda \le r_{d} \\ \min\left(\frac{(3\pi r_{d}^{2}U_{m}/2\Omega)^{0.33}}{(3r_{d}^{2}\Lambda/4)^{0.33}}\right) & B_{0}\Lambda > r_{d} \end{cases},$$
(10)

where  $B_0 = 0.61$  is the model constant and  $\Lambda$ ,  $\Omega$  are the wave-length and the growth rate, respectively, of the fastest growing wave on the surface of the liquid jet, given by

$$\Omega_{KH} = \sqrt{\frac{\sigma}{\rho_l r_0^3}} \cdot \frac{0.34 + 0.38W e_g^{1.5}}{(1 + Oh)(1 + 1.4Ta^{0.6})},$$
(11)

$$\Lambda_{KH} = 9.02r_0 \cdot \frac{(1+0.45\sqrt{Oh})(1+1.4Ta^{0.7})}{(1+0.865We_g^{1.67})^{0.6}},$$
(12)

where the non-dimensional numbers are as follows:

$$Oh = \frac{\sqrt{We_l}}{\operatorname{Re}_l}, \ Ta = Oh\sqrt{We_g}, \ We_g = \frac{\rho_g r_0 u_{rel}^2}{\sigma}, \ We_l = \frac{\rho_l r_0 u_{rel}^2}{\sigma}, \ \operatorname{Re}_l = \frac{\rho_l r_0 u_{rel}}{\mu_l}$$
(13)

 $r_0$  is the droplet radius before breakup,  $u_{rel} = |u_d - u|$  is the relative velocity between a droplet and the surrounding gas, *Oh* is the Ohnesorge number, *Ta* is the Taylor number,  $We_g$  and  $We_l$  are the Weber numbers for the liquid and the gas, respectively, and  $Re_l$  is the Reynolds number for the liquid.

Also, the breakup time is given by

$$\tau_{bu} = 3.7626 \frac{B_1 R}{\Lambda \Omega},\tag{14}$$

where  $B_1$  is the adjustable model constant which varies approximately between  $\sqrt{3}$  and [36] 60, depending on the injector type. This model was modified by Sazhin et al. [32] and Turner et al. [10] to incorporate transient effects. Based on the new modified model in the previous equation, the model constant ( $B_1$ ) has been changed to

$$B_{1}^{\text{mod}} = B_{1} \left( 1 + C_{1} \left( a^{+} \right)^{C_{2}} \right), \tag{15}$$

where

$$a^{+} = 2\sqrt{\operatorname{Re}_{2}} \frac{r_{d}}{U_{inj}^{2}} \frac{\mathrm{d}U_{inj}}{\mathrm{d}t}$$
(16)

is the acceleration parameter,  $C_1$  and  $C_2$  are the adjustable model constants and Re<sub>2</sub> is the gas Reynolds number.

Similar to KH instabilities, the wavelength and the growth rate of the fastest growing wave in the RT breakup model can be obtained through the linear stability analysis. The fastest growing wave growth rate and the corresponding wave length of the Rayleigh-Taylor model are given by Bellman and Pennington [37].

In the current study, the LPT/LES approach is adopted and the modified breakup time (Eq. 14) is implemented. Also, a new advanced KH-RT breakup model is developed to simulate the ultra-high pressure diesel injection.

## 3. Simulation Set up

Simulations were carried out using the SprayFOAM solver of OpenFOAM 2.1.1 code. A simple grading structured mesh has been utilized in a constant volume chamber. The injector diameter is considered to be 160  $\mu$ m, and surrounding gas properties are set as  $T_{amb} = 295$ K and  $P_{amb} = 1.27$  MPa. The simulation domain is a rectangular cube of size  $50 \times 50 \times 100$  mm. Fuel properties of kerosene are presented in Table 1 according to the experimental data of Wang et al. [6].

Density / kg/m <sup>3</sup>	830
Viscosity / mm <sup>2</sup> /s	3.36
Surface tension / mN/m	25.5
Nozzle diameter / µm	160
Injection duration / ms	1.5
Ambient gas temp. / K	295

Table 1	Fuel	properties
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In addition, the fuel mass flow rate is calculated based on the Payri et al. [38] method using the injection pressure and the ambient pressure. This inflow velocity profile has been used as an initial condition for the spray. Also, velocity vectors of the gas field have been set to zero. The Gauss upwind method is utilized as a convection scheme.

Selection of a proper grid size is important for the RANS and LES approaches, especially for the LES. Therefore, grid sensitivity studies have been carried out for three different mesh sizes. A coarse mesh contains  $0.5 \times 10^5$  and  $1.0 \times 10^6$  cells for the RANS and the LES, respectively. These numbers are  $1.0 \times 10^6$  and  $2.0 \times 10^6$  for fine meshes. Droplet penetration, as the key parameter of the diesel spray, is used as a basis for comparison and results are presented in Fig.1. The LES scheme requires a finer mesh resolution than the RANS, and  $0.7 \times 10^5$  cells were selected for the RANS simulation while  $1.5 \times 10^6$  cells were assumed for the LES.



Fig. 1 Droplet penetration for various grid sizes (a: RANS simulation, b: LES simulation).

## 4. Results and discussion

Capability of the LPT/LES model as well as the modified breakup model for predicting the spray characteristics under ultra-high-pressure has been investigated and compared with the experimental results presented by Wang et al. [6]. Figure 2 shows the spray images of experimental data [6] and the numerical results of the RANS and LES approaches at t=0.5ms for various injection pressures. As observed in this figure, RANS and LES can produce an acceptable general spray shape. However, small scale phenomena, especially at the boundary edge of the spray have been simulated more realistically by the LES method.



Fig. 2 Comparison of the spray shapes under various injection pressures (a: Exp. [6], b: RANS, c: LES).

Spray tip penetration is the most important parameter in characterizing the spray. Computationally, the penetration length is defined as a distance between the nozzle and the farthest axial location of the spray boundary. Computational and experimental results for the spray tip penetration are displayed in Figs. 3-5. Numerical results of the current advanced KH-RT model have been compared with the default KH-RT model of the OpenFOAM code. Also, numerical results of the Fluent software that were presented by Ghasemi et al. [39] have been presented for each injection pressure. It is evident from these figures that the current simulation has given more accurate results for the spray penetration.







Fig. 4 Spray tip penetration vs. time (Pinj=200 MPa).



Fig. 5 Spray tip penetration vs. time (Pinj=300 MPa).

The spray opening angle is another parameter that defines the spray shape. The spray angle is measured based on the radial distance at axial location of 40 mm. Computational and experimental spray angles are shown in Fig.6. It is concluded that the injection pressure and the turbulence modelling method seem to have a small influence on the diesel spray angle.



Fig. 6 Spray opening angle.

To better understand the spray morphology, the spray volume is numerically estimated. Results of the LES approach are presented for various injection pressures in Figs.7-9. As evidenced in these figures, numerical results have displayed good agreement with the experimental data of Wang et al. [6].



Fig. 8 Spray volume vs. spray penetration (Pinj=200 MPa).



Fig. 9 Spray volume vs. spray penetration (Pinj=300 MPa).

The quality of spray mixing is described by the droplet size. The Sauter Mean Diameter (SMD) is defined as the diameter of a sphere that has the same volume/surface area ratio as the entire spray. The SMD correlation was presented by Ejim et al. [40] as follows:

$$SMD = 6156\nu^{0.385}\sigma^{0.737}\rho_f^{0.737}\rho_a^{0.06}\Delta P^{-0.54},$$
(17)

where  $\nu$  and  $\sigma$  are the viscosity and the surface tension, and  $\Delta P$  is the pressure difference between the injection and ambient pressures. The effect of injection pressure on the SMD for Pinj=100 MPa is presented in Fig.10.



Fig. 10 Effect of injection pressure on the SMD (Pinj=100 MPa).

After the start of injection, the high SMD value means that the blob size is equal to the injector diameter. Also, the SMD value decreases due to the atomization process of droplets. The atomization rate is increased at a high injection pressure. Compared to the LES cases, the droplet sizes of the RANS cases are always larger.

Another case of simulation is related to the Marine Diesel Fuel (MDF) spray under ultra-high injection pressure. Physical properties of MDF are used from the ASTM standard D-2069 [41]. Fuel density and viscosity have been set to 890.0 kg/m<sup>3</sup> and 6.00 mm<sup>2</sup>/s, respectively. Other thermophysical properties are used according to the ASTM D-2069 standard. OpenFOAM liquid properties have been updated and simulations have been performed under three injection pressures. Spray penetration, spray volume and SMD of the Marine Diesel Fuel are illustrated in Figs.11-13, respectively. Higher viscosity and surface tension of MDF lead to high penetration and great/large droplet sizes. However, the spray volume shows a very small change.



Fig. 13 Comparison of SMD values for the MDF and the Kerosene fuel (Pinj=100 MPa).

## 5. Conclusions

The current study is focused on the differences between the LES and RANS approaches towards spray characteristics of non-evaporating and non-reacting Kerosene and Marine Diesel Fuel (MDF) diesel sprays under ultra-high injection pressure. The LPT/LES model and the modified KH-RT breakup model are implemented using the OpenFOAM code. Furthermore, the grid incipiency analysis has been done using three different mesh resolutions for the LES and RANS schemes. Computational results are compared with the published experimental data. Spray penetration, spray angle, spray volume, Sauter Mean Diameter (SMD), and equivalent ratio are the main parameters whose results are compared with experimental data. Current simulations have been performed under three injection pressures of up to 300 MPa. Injection pressure is the main parameter affecting the spray characteristics.

Injection pressure was found to have a significant effect on spray penetration. Accuracy of spray parameters was displayed by good agreement between numerical results and experimental data. Higher density, viscosity and surface tension of MDF lead to different spray characteristics. At ultra-high injection pressure, the Marine Diesel spray shape and the droplet size are more satisfactory. This implies that the combustion process of the Marine Diesel Fuel could be improved by using the ultra-high injection pressure.

The obtained numerical results demonstrated that the LES and RANS schemes can capture the general spray shape reasonably. This basically implies that large-scale quantities display a similar behaviour for both turbulence modelling. On the other hand, LES provides more reliable results in highly transient sprays. Particularly, at the ultra-high injection pressure, the LES results are more accurate than the RANS results.

Based on the reported findings, one may conclude that under the ultra-high injection pressure the LES scheme should be preferably used for predicting detailed characteristics of the fuel-air mixture, albeit the SprayFoam solver of the OpenFOAM software produce acceptable results for both the RANS and LES methods.

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Submitted: 04.4.2014

Accepted: 10.12.2014

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