Large Eddy Simulation of GDI Spray Evolution in a Realistic IC-Engine

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Abstract

In the present study, an effort is made to numerically investigate the real unsteady behavior of evaporating GDI spray in a realistic engine configuration by applying Large Eddy Simulation together with a spray module using KIVA-4mpi Code. A comprehensive model set is integrated in a Eulerian-Lagrangian framework allowing to describe the spray evolving from the injector nozzle and propagating within the engine combustion chamber. It includes sub-models to account for various relevant sub-processes. The atomization is described using combined primary and secondary atomization sub-models. Instead of performing costly level set method or volume of fluid (VOF) technique a Linear Instability Sheet Atomization (LISA)-based sub-model is applied for the primary atomization. The secondary atomization is modeled by a Taylor Analogy Break-up (TAB) model. The novelty of the proposed methodology is to include droplet-droplet interaction processes via an appropriate collision sub-model that is independent of mesh size and type. Thereby, it takes into account different regimes, such as, bouncing, separation, stretching separation, reflective separation and coalescence of droplets. A resulting droplet distribution is then tracked in Lagrangian way. The droplet evaporation is described by an appropriate evaporation model and the turbulent dispersion by the filtered velocity only. The spray module is coupled to LES of the carrier phase in which a Smagorinsky model is used for the filtered flow field. An appropriate approach is used to describe the moving boundary conditions for the piston and valves movement. The fuel is injected during the air intake stroke. The results show a strong effect of the incoming air stream on the spray evolution properties along with the mass fraction distribution. The model is also able to predict the formation of wall film on the piston surface. In the context of IC-engine, the predictive capability of the RANS and LES turbulence model is evaluated.

Introduction

In recent time, the rising fuel cost, depleting fuel reserve together with strict environmental regulation has put great thrust on research activity on internal combustion engines (ICE). It is a complex trade among the stringent regulations concerning pollutants, fuel consumption, engine thermal efficiency and wheel power output. To meet these requirements an understanding of the salient features of all the engine processes are very important. In the case of gasoline direct injection (GDI) engines, mixture formation pattern varies from the lean to reach mixture and stratified to homogeneous mixture depending upon different engine status and loading conditions. The fuel injection is a vital process for air-fuel mixture preparation under such varied engine conditions. Very often during the intake charge of fresh air, fuel is injected, which gets evaporated and prepares air-fuel mixture for subsequent combustion in power stroke. Therefore, it is worth mentioning that, being the primitive process of engine operations, it influences whole engine cycle via air-fuel mixture preparation, thereby the combustion behavior and subsequently its emission performance. The fuel spray investigation is generally carried out for stationary case (no moving piston and valves) with varying cylinder conditions due to slight convenience in measurement technique [1]. In real configuration when the piston and valves are in motion, the spray dynamics change considerably, while the high speed intake air interact with the evolving jets, and often the experimental investigation becomes complex and expensive. On the contrary CFD based investigations provide comprehensive insight about in-cylinder flow field, spray injection phenomena and subsequent processes such as droplet dispersion, evaporation, mixture formation and combustion. Thereby the accuracy of the numerical results and their contribution to the design analysis and optimization tasks strongly depend on the predictive capabilities of the physical processes. A reliable CFD model should be able to predict and resolve reasonably all relevant physical phenomena involved, that occur in a highly unsteady manner making steady state computations, at best, an approximation.[2]-[12]

The two-phase flow as encountered in IC engines are very complex. To resolve all the scales involved in the atomization process, the direct numerical simulation (DNS) remains the only candidate, but its prohibitive computational cost restricts its use primarily to academic applications. The coupled large eddy simulation (LES)/DNS technique has also been proposed [2, 3, 4] with slight reduction in computational cost, but is still expensive as

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pointed out in [5]. To carry out parametric studies or incorporate simulations into a design optimization process, it is essential to implement a model capable of providing quick and reasonably good results. Therefore, numerical studies are usually carried out for selected spray phenomena only using Reynolds-averaged Navier-Stokes (RANS) [6, 7]. However, such highly unsteady turbulent flows required unsteady calculation techniques [8, 9]. However, unsteady RANS models the turbulence and only resolves unsteady mean flow structures. Recent innovative concepts appear promising, even though they are not yet mature [8]. The LES has proven to be an appropriate technique to treat unsteady phenomena occurring in ICE by requiring less computational cost compared to DNS or DNS/LES. It is able to well capture intrinsically time and space dependent phenomena. It computes the large scale flow and mixing process accurately, thereby providing a valuable platform for small scale models that describe the micro-mixing and combustion process [10, 11]. The most LES work on two-phase flows reported in the literature are rather achieved by an assumption of predefined dispersed droplets of fuel spray, while atomization processes are neglected (see, [12, 4]). Few LES studies have been reported which comprise relevant spray models for injection process applicable to IC engines [2, 4, 13, 14]. A recent review is provided by Rutland [7]. Comparative studies of the effect of different turbulence models on spray evolution were carried out for non evaporating spray in [15]. In [16, 17] a comprehensive modeling and simulation of gasoline direct injection (GDI) using LES with KIVA-4mpi has been validated for both evaporating and non-evaporating sprays.

In the present work, a CFD study is carried out for a realistic engine configuration with moving piston and valves to study the evaporating fuel spray and subsequent mixture formation inside the engine cylinder. This is achieved by means of the KIVA-4mpi code [18, 19]. The fuel injector is considered as gasoline direct injection (GDI), for which a comprehensive model has been already developed. The spray module to be applied takes into account all relevant and important physical phenomena (atomization, collision, turbulence, drag, and evaporation) as suggested in [16, 17]. The paper is organized as follows. In the next section, the mathematical models are described and computational details are provided. The results are presented an discussed before concluding.

Mathematical Models

The numerical modeling is carried out using KIVA-4mpi CFD code, which is based on finite volume formulation, especially designed for the engine simulations. It is a structured/unstructured CFD code for compressible flow and is appropriate for IC engine simulations following an arbitrary Eulerian-Lagrangian (ALE) approach. The KIVA-4mpi code has feasibility to solve with parallel processors using Open-MPI. For the dispersed phase, droplets are considered as parcels and tracked in time-accurate manner in a Lagrangian reference frame by solving their evolution equation, i.e. equations for droplet position, velocity components, diameter (evaporation, collision, & break-up) and temperature (heating). In particular equation of droplet motions include the drag and gravitation according to particle loading conditions under consideration. An appropriate methodology for moving mesh and mesh rezoning is chosen for the piston and valve movements. The detailed formulations of the governing equations for gas phase solver and ALE description for spray are provided in [18]. To avoid repetition, these are not discussed here. Rather a description of the comprehensive spray module suggested is provided. It consists of many sub-models such as primary and secondary atomization model, collision/coalescence model, turbulence, evaporation and dispersion models.

Atomization Model:

The atomization is described as consisting of primary and secondary atomization mechanisms, that are described by standard models, namely the linear instability sheet atomization (LISA) model [20] for primary atomization and Taylor-analogy breakup (TAB) model for the secondary atomization [21].

Primary atomization:

The injector modeled is a Continental piezoinjector with outwardly opening nozzle, which represents one of the available GDI piezoinjector. In the Lagrange particle tracking framework as stated before, there is not a universally applicable model available for primary atomization process. For GDI the primary atomization is modeled with the linear instability sheet atomization (LISA) model suggested by Senecal et al. [20]. It was derived primarily for the hollow cone spray as encountered in case of GDI. The model is based on the assumption that, hollow liquid sheet is formed near the nozzle exit; the unstable liquid sheet breaks into ligaments, and ligament breaks to form primary droplets. .

Secondary atomization:

The Taylor-analogy breakup (TAB) suggested by O'Rourke et al. [21] is used for secondary atomization of droplets formed during primary atomization. The model is based on the assumption of competitive contribution from viscous, surface tension, and aerodynamics forces. The droplet undergoes deformation similar to linear spring mass-damped system. When the deformation is sufficiently high, it results in droplet breakup.

The model constant for both the primary and secondary atomization model are kept constant as suggested in literature. The model has been validated extensively for various operating parameters (chamber pressure, and temperature) in the previous works [15, 16, 17], so that the deficiencies are known.

Table 1. Engine parameters

Parameter	Value	Parameter	Value
Bore	86 mm	Fuel	Gasoline
Stroke	92 mm	Fuel mass	8.0 mg
Engine RPM	1200	P_{inj}	100 bar
Compression ratio	10	T_{inj}	333 K
Intake valve open	Intake-BTDC 18°	Start of Injection	53° ATDC
Intake valve close	Intake-ATDC 240°	Duration of Injection	10° CA
Exhaust valve open	Intake-BTDC 148°	Injector slit thickness	25 μm
Exhaust valve close	Intake-ATDC 28°	Spray cone angle	95°

Collision/coalescence model:

In general, the fuel injection processes involve dense flow. Therefore, the probability for the droplet-droplet interactions is very high. This ultimately influences final droplet distribution and spray profile. The collision models are commonly based on the model proposed by O'Rourke [23], a two regimes binary collision model, but it is computationally expensive when large number of parcels are used. Schmidt and Rutland [25] proposed a NTC (No Time Counter) method, that has linear dependency in computational cost with number of parcels. This method only considers a randomly chosen subset of candidate pairs after scaling up the collision probability by the estimated maximum probability. The numerical issue associated with this method is reported by Hieber [26], Nordin [28], Aneja and Abraham [29]. The collision model is still very sensitive to grid size and its type. This issue is also confirmed by Schmidt and Rutland [30], who suggested that, this dependency may be linked to the mesh used for the gas phase solver. Apart from, mesh dependency, these models only account for stretching separation and permanent coalescence. Due to this fact, it over-predicts the droplet coalescence process. A comprehensive four regime (i.e. coalescence, stretching separation, reflexive separation and collision) collision model has been proposed by Munnannur et al. [24]. This was further modified to take into account the exact momentum exchange during the collision by Pischke et. al. [6]. However, the model is based on binary collision of droplets in given control volume (CV). Therefore it becomes highly sensitive to control volume size and types (e.g. structure/unstructured). This grid dependency has been reduced by incorporating additional mesh for spray calculation other than regular mesh for gas phase solver [27]. Nevertheless, this becomes impracticable, when multiple injection points are defined, as it is very common in modern IC engine applications. In the present work, the collision model based on the Munnannur et al. [24] model is modified to make it independent of mesh size and type as proposed by Nishad et al. [16]. It is then used together with an evaporation model, that accounts for the convective flow environments, to better retrieve the evaporating spray properties. For this purpose, an accurate description of the turbulence of the gas phase is required.

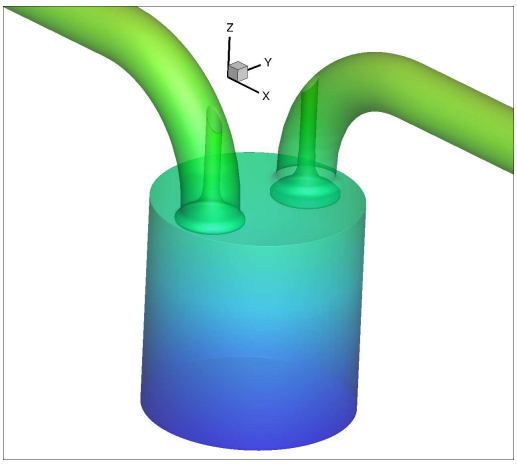


Figure 1. Engine geometry showing cylinder squish, intake/exhaust valves and ports [37].

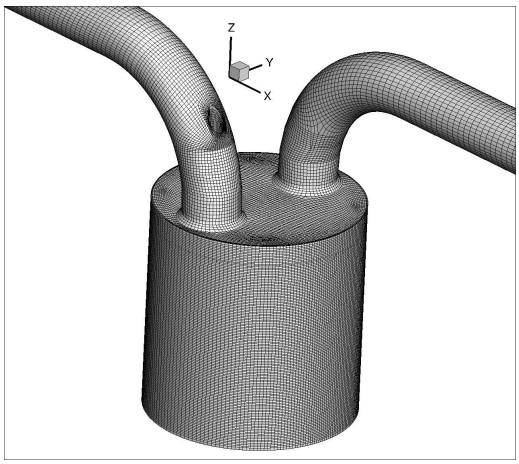


Figure 2. Hexa-hedral mesh for engine geometry generated in ICEM-CFD [37].

Carrier Gas Phase Description: Flow turbulence via LES model:

For the description of the Eulerian carrier phase, KIVA-4mpi that originally offers simple RANS models to account for turbulence effects has been extended to an LES solver including the classical Smagorinsky model [31] to close the sub-grid scale (sgs) stress tensor τ_{ij} in the Navier-Stokes equation.

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\nu_t \overline{S}_{ij} \tag{1}$$

where

$$\nu_t = (C_s\Delta_g)^2 \sqrt{2\overline{S}_{ij}\overline{S}_{ij}} = (C_s\Delta_g)^2 |S| \,, \overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \tag{2}$$

Δ_g is the filter width representing the model length scale and C_s the model parameter. In the current study it is taken as 0.1. The filtered governing equations (continuity, Navier-Stokes, energy, mass fraction of vapor) include source terms for phase exchange and phase transition processes. These additional source terms characterize the direct interaction between the two-phases and account for a simple two-way coupling between the fluid turbulence and evaporating droplets. More details can be found in [12, 32, 33].

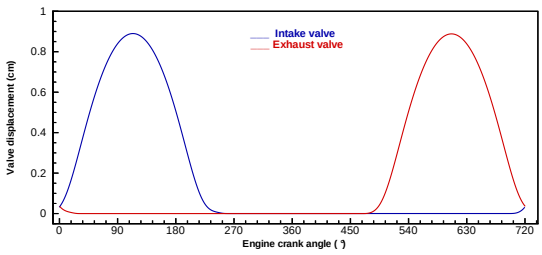


Figure 3. Intake/exhaust valve displacement with engine crank angle

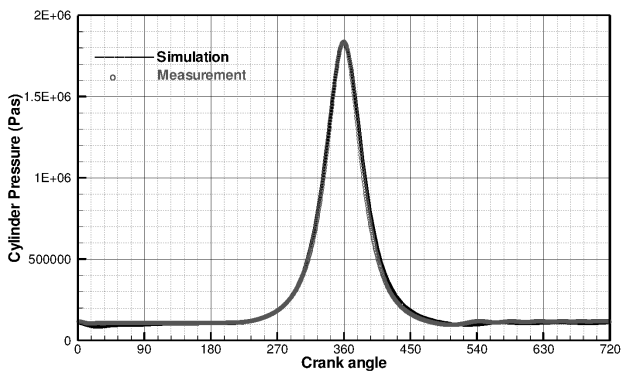
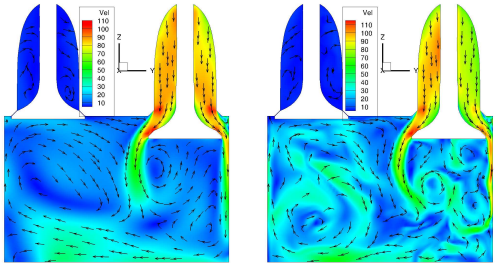


Figure 4. Comparison of pressure curve: simulated (black line), experimental (gray circle [37])

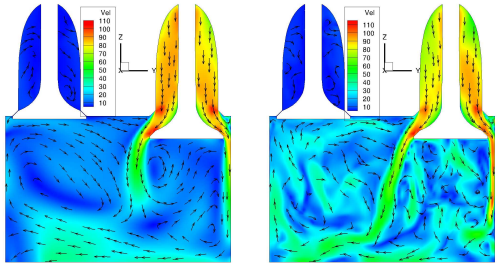
Droplet evaporation Model

In the KIVA-4mpi code the evaporation behavior of the fuel spray is described by a detailed multi-component evaporation model [18] with possibility to solve for 100 fuel components. As the fuel used in iso-octane, a multi



(a) (b)

Figure 5. Comparison of velocity profile at 90° ATDC for 2nd engine cycle, (a) RANS (b) LES



(a) (b)

Figure 6. Comparison of velocity profile at 90° ATDC for 3rd engine cycle (a) RANS, (b) LES

component model is suitable. To reduce the complexity of the calculations, in the recent approach a single component evaporation model based on the lumped-body theory is chosen [19]. The application of the complex model is work in progress. In the model used the energy balance on the droplet surface due to heat transfer from the surrounding and latent heat evolution due to evaporation, can be formulated as Eqn. (3).

$$Q_t = \dot{m}_f L + \dot{Q}_i \, , \dot{Q}_i = 4\pi r^2 h_c (T_\infty - T_s) \tag{3}$$

where, the quantity L is the latent heat of liquid droplets and $\dot{Q}_i$ the heat conduction rate from the droplet surface into the droplet interior, r expressing the droplet radius, T_∞ and T_s the ambient and droplet surface temperature, respectively. The heat transfer coefficient h_c is dependent on the Nusselt number given by

$$Nu = \left(2.0 + 0.6 Re^{\frac{1}{2}} Pr^{\frac{1}{2}}\right) \frac{ln\left(1 + B_T\right)}{B_T} \tag{4}$$

where the Reynold's number $Re = 2\rho_g U r/\mu_g$, the Prandtl number $Pr = \mu_g C_p / K_g$, and ρ_g, μ_g, C_p, K_g being the air density, viscosity, heat capacity and heat conductivity, respectively. B_T expresses the Spalding heat transfer number given by $B_T = C_p \left(T_\infty - T_s\right)/L + \left(Q_i/\dot{m}_f\right)$. The mass transfer from the droplet in Eqn. (3) is given by the correlation suggested by the Frossling correlation [19].

$$\dot{m}_f = 2\pi r (\rho D)_g B_m Sh_d \tag{5}$$

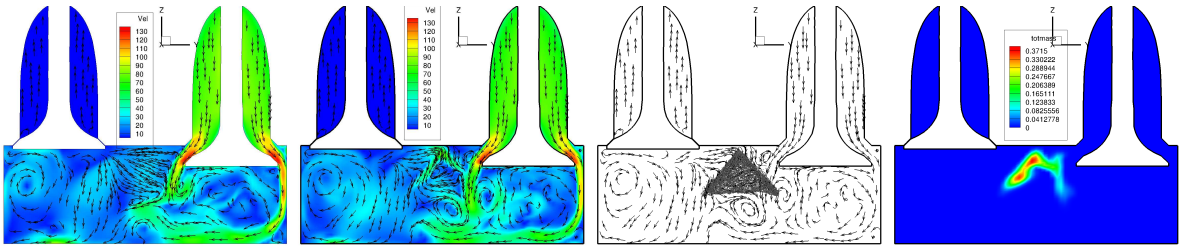
where $(\rho D)_g$ is the fuel vapor diffusivity in the air, and Sh_d the Sherwood number that accounts in the presently used convection model for boundary layer effects. It was determined by the following expression

$$Sh_d = \left(2.0 + 0.6 Re^{\frac{1}{2}} Sc^{\frac{1}{2}}\right) \frac{ln\left(1 + B_m\right)}{B_m} \tag{6}$$

where the Schmidt number $Sc = \mu_g/(\rho D)_g$, the Spalding mass transfer number $B_m = (Y_s - Y_\infty)/(1 - Y_s)$, Y_∞ and Y_s representing the mass fraction of fuel near the droplets and in the ambient gas, respectively. More details about the evaporation model used are provided in [34]. The evaporated mass fraction is transported with an appropriate transport equation in which the SGS scalar flux vector is modeled by a simple gradient assumption [18].

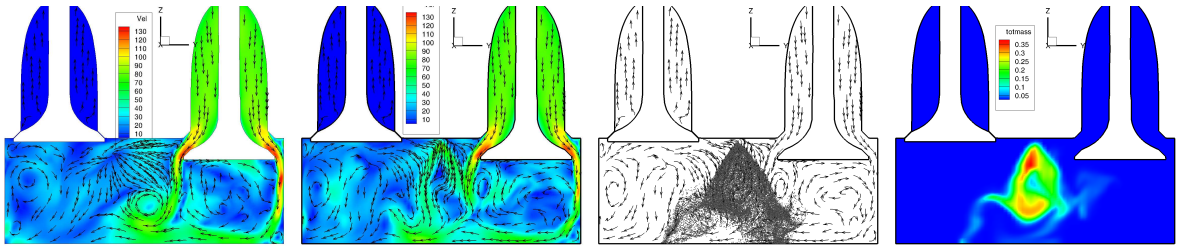
Wall film formation

Spray-wall interaction is also considered as an important phenomenon in IC-engines. In the case of GDI the fuel is injected directly in the combustion chamber. The injected fuels must be vaporized and mixed properly with the air charge in order to have desirable combustion and engine power. In most of IC-engine designs, the fuel spray may impinge on engine surfaces (e.g. piston crown, cylinder liner, valves) before vaporization and mixing are complete. Spray impingement has been shown to influence engine performance and emissions in both compression ignited (CI) and spark ignited engines (SI) [35]. The impingement mostly results in formation of wall film on engine surface, that influence the engine performance especially in transient control. It is a major factor affecting air -fuel ratio due to time lag resulting from a film of liquid fuel deposited on the piston surface. The time lag results in decreased engine response, increased fuel consumption and increased emissions. In order to improve the engine performances, it is essential to avoid the formation of liquid film on/inside the engine cylinder



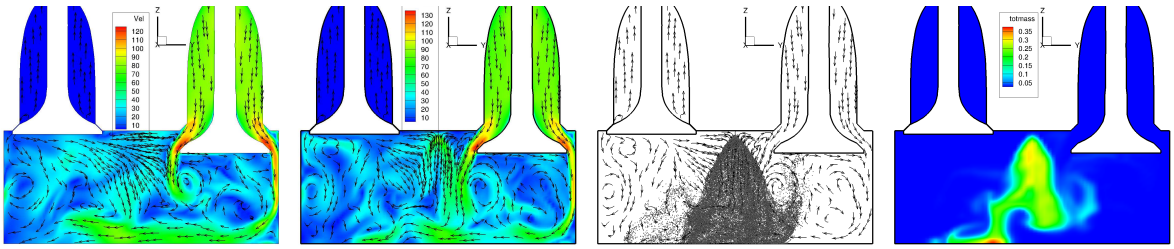
(a) (b) (c) (d)

Figure 7. The sectional view (x-plane) at CA plot 55° ATDC for (a) Velocity profile without spray (b) Velocity profile with GDI spray(c) spray profile (c) Evaporated fuel mass fraction



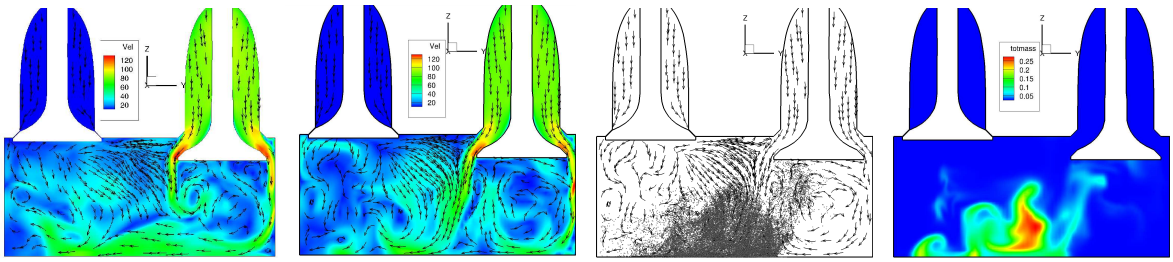
(a) (b) (c) (d)

Figure 8. The sectional view (x-plane) at CA plot 59° ATDC for (a) Velocity profile without spray (b) Velocity profile with GDI spray(c) spray profile (c) Evaporated fuel mass fraction



(a) (b) (c) (d)

Figure 9. The sectional view (x-plane) at CA plot 63° ATDC for (a) Velocity profile without spray (b) Velocity profile with GDI spray(c) spray profile (c) Evaporated fuel mass fraction



(a) (b) (c) (d)

Figure 10. The sectional view (x-plane) at CA plot 66° ATDC for (a) Velocity profile without spray (b) Velocity profile with GDI spray(c) spray profile (c) Evaporated fuel mass fraction

by design and parametric optimization. In the present study the wall film model suggested by O'Rouke et al. [36] is used, that include droplet splash, film spreading due to impingement forces, and motion due to film inertia. In the present study, the complete model is not described considering the model detail of the wall-film model. The interested reader may refer to [36].

Numerical Configurations

An optical gasoline engine [37] designed to support the development and validation activities for the CFD software is used for the simulation of evaporating spray here. The engine geometry is shown in Figure 1. It features two-valve with simple intake and exhaust port/runner geometry and a pancake-shape combustion chamber [37]. The total of ca. 0.9 million control volumes are used to represent the cylinder squish, valves and ports geometry (see Figure 2). The engine has bore and stroke dimension of 92 mm and 86 mm respectively, while the speed is 1200 rpm. The valve lift diagram is provided in Figure 3. For the numerical investigation of the fuel spray dynamics carried out in the present paper, a continental piezoinjector with outwardly opening nozzle, which represents one of the available GDI piezoinjector is used [6, 38]. The complete engine details and injection parameters are listed in Table 1.

Results and Discussion

Because comprehensive experimental data are not available on the evolving spray in this engine configuration, a numerical analysis is reported here. For the stationary cylinder case (no piston movements), a comprehensive validation of the spray atomization models (primary and secondary atomization), injection boundary condition, spray profile and spray dynamics has been carried out and reported in previous works [15, 16, 17]. Based on the successful assessment of these models and due to the lack of complete experimental data for the real engine configuration under study, focus is on the numerical analysis of the interaction of high speed intake air with evolving fuel spray and mixture formation. Figure 4 compares the cylinder pressure curve as a function of crank angle obtained by simulation and experiments [37]. This shows good agreement. To evaluate the turbulence model on IC-engine application, simulation is performed both with RANS $(k-\epsilon)$ and LES turbulence model. Figures 5- 6 display the velocity profile at 90° ATDC, when intake valve is opened for two different engine cycles. In contrast to RANS, LES model is able to resolve flow structures nicely. It is also clearly visible that, only the LES model is able to predict the the cycle-to-cycle variation of flow profile (see Figures 5b- 6b).
LES simulation is then performed only for one engine cycle with GDI spray, where the spray evolution properties are evaluated at various stage of engine crank angles. The results are presented in Figures 7-9 at various stage of engine crank angles for velocity vector/contour (with/without spray), superimposed spray profile, and evaporated fuel mass fraction. In Figure 7, it is clearly visible that the high speed intake air at CA 55° strikes the GDI spray and deforms it considerably. In this process the overall profile of the gas velocity changes completely, as it can be seen in the cases with and without spray. The high velocity region can also be seen along the GDI spray and the formation of the inward and outwards vortex is clearly visible below the hollow cone spray and in the vicinity of the intake air-fuel spray interaction. This also influences the mass fraction profile (see Figure 7d). The process of the air-fuel mixture preparation, that is vital for the IC-engine operation, is then tracked and its evolution is displayed in further Figures at crank angle of 59°, 63° and 66°, respectively (see Figures 8d-10d). In case of GDI, there is always chances of the high speed non-evaporated fuel getting deposited on the piston surface and subsequent forms liquid film on the wall. The deposited fuel then picks up heat from the piston surface and subsequently gets evaporated as visible in Figure 9d. This behavior is more pronounced in later stage of fuel injection as shown in Figure 10 for CA 66° ATDC, where the slightly large amount of fuel is deposited on the piston surface leading to a large amount of evaporated fuel mass fraction on Figure 10d. In ideal case, the injected fuel should evaporate completely and form proper air-fuel mixture to have desirable engine performance. However, the formation of the liquid film directly affects the engine performance especially in transient control. It is a major factor affecting air -fuel ratio due to time lag resulting from a liquid film deposited on the piston surface. This time lag results in decreased engine response, increased fuel consumption and increased emissions.

Summary and Outlook

A comparative study is carried out with RANS and LES turbulence model. LES results shows the improvement in resolving the flow structure and predicting the cycle-to-cycle variations. A preliminary validation with experimental data on engine pressure curve is performed. A qualitative study is then carried out using LES, thereby a comprehensive fuel injection model is applied to simulate a real engine configuration with moving piston and valves. The CFD model is able to capture the transient behavior of evolving spray. It shows how the intake charge motion considerably influences spray dynamics and vice versa, thereby air-fuel mixture formation. The simulation

results also show the evidence of the formation of liquid film on the piston wall which is undesirable for the optimum engine performance.
The presented result is being used as a basis for further analysis of unsteady effects along with cycle-to-cycle variations in real engine configurations for sufficient large number of engine cycles. To take into account the ignition and subsequent combustion. A detail tabulated chemistry model is being incorporated to carry out complete engine analysis.

Acknowledgements

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