Modelling the spray and combustion processes in diesel engine using coupled Euler-Eulerian and Euler-Lagrangian approach

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ABSTRACT

The focus of this paper is to show that the existing and developed models are capable for describing spray formation, combustion and pollutant formation processes. The Euler-Eulerian approach was used for the spray modelling where the mathematical models of fuel jet disintegration and droplet evaporation are used. Spray combustion is modelled using the common Euler-Lagrangian approach. The coupling of two approaches have been performed by running simultaneous computations on separate computational domains with constantly exchanging mass, enthalpy and momentum sources. This research outlines the capability employing the coupled approach. The calculated results were compared with the available experimental data. It is concluded that the pressure and temperature evolution, combustion process and the emissions trends are well described using this approach. The coupled simulations could be used in further engine development retaining the high CPU efficiency taken from the Euler-Lagrangian simulations with an increased solution accuracy in the near-nozzle region employing the Euler-Eulerian approach.

KEYWORDS

CFD modelling, Eulerian, Lagrangian, coupling, combustion.

INTRODUCTION

Powering diesel engines and burning a vast amount of fossil fuel increases the concentration of pollutants dangerous for human health and for the environment. The most significant contributors are nitric oxides, carbonaceous particles, carbon monoxide and unburnt hydrocarbons. The regulation of these pollutants has been a hot topic for several decades and rigorous regulations are planned for the future. Huge scientific effort and time are dedicated for determining how various factors and fuel energy conversion influence the emissions of internal combustion engines. Detailed understanding of such processes is limited in experimental investigations and therefore, the Computational Fluid Dynamics tools can be employed in addition to experiments.

Numerous studies about spray processes have helped engineers establish the criteria needed to design and develop more efficient combustion and related fuel devices while minimizing the pollutant emissions 1, 2 and 3. The understanding of the complex nature of the fuel spray formed by high pressure injectors in the experimental investigations is limited and this understanding can be significantly improved by numerical simulations. The numerical

modelling of spray processes is a very challenging task as compared to a single phase flow. The challenges are due to the fluid interfaces between phases, and the property variations across the interfaces between phases. Thus, the spray models demand complicated techniques to couple the dynamics of the liquid droplets and the carrier gas. A variety of strategies have been formulated during the last years in order to address this problem. In general, most of these strategies fall into two basic formulation methods that are commonly used to couple the dynamics of the liquid phase and the gas phase: the Eulerian-Lagrangian method and the Eulerian-Eulerian method.

The Eulerian-Lagrangian method has been firstly used in the engineering applications 4, 5, 6, 7 and many others in recent years. In this approach, the spray is represented by finite numbers of parcels assuming that all the droplets within one parcel have similar size and the same physical properties. The motion and transport through the flow field are solved using the Lagrangian formulation, whilst the continuous gas phase is described solving the common conservation equations. The coupling between the phases is performed introducing the source terms for interfacial mass, momentum and energy exchange [9]. This approach have severe limitations. It is very sensitive to the numerical grid resolution in the near nozzle region [8] which results in inadequate description of dense sprays. However, Lagrangian approach is suitable for calculating the diluted region where lower volume fraction of the liquid phase is encountered. Furthermore, this approach suffers from the statistical convergence problems, as discussed in [10]. The Euler–Lagrangian formulation is most often used to reliably describe sprays produced by low pressure atomisation [11].

To overcome the mentioned approach disadvantages the Euler Eulerian multiphase approach can be employed. Here, both phases are treated as continuum and are conservation equations are solved for each phase separately with similar numerical techniques. This approach was first addressed by [12] and has been adopted and applied for numerical simulation, e.g., [13], [14], [15], [16], [17], [18], [19], [20] and others.

Compared to the Lagrangian scheme, the Eulerian scheme calculation is fairly efficient for flows of high droplet concentration, whilst the Lagrangian scheme show better solution for the diluted flows. Knowing this, the two mentioned approaches can be used together to overcome their disadvantages and improve the spray modelling. In this work, the coupling concept has been presented where the validated Eulerian multiphase spray approach was used together with the Lagrangian DDM spray approach to take advantage of the capabilities inherent in both methods. This concept was then applied for coupled simulation of real internal combustion engine, which is particularly challenging for such modelling. Spray was calculated by the Eulerian multiphase spray method in a fine, non-moving mesh that covers only a small part of the engine downstream of the nozzle exit. The Eulerian multiphase spray simulation was coupled with single phase engine simulation performed in the coarser moving mesh that overlaps the spray mesh. The basic idea was to couple two different simulations, the Eulerian multiphase spray calculation in the dense spray region with the single-phase engine calculation applying DDM in the whole computational domain. This means that two different CFD codes, Eulerian multiphase spray code, referred here as spray code, and single-phase engine code, referred here as engine code, were performed simultaneously simulations.

A concept for simulation of different flow regimes, both dense and dilute spray, by using the Eulerian multiphase approach coupled by Lagrangian approach is proposed in **Error! Reference source not found.**21], [22]. In this paper, a coupling of the Eulerian multiphase spray simulation with Lagrangian DDM engine simulation was done by AVL FIRE® Code Coupling Interface (ACCI) [23]. Coupling of two simulations means that current field values of both simulations were used as either boundary condition values or source terms for other simulations. In this work, the flow field of the engine code calculations were used as boundary condition values for the Eulerian multiphase spray code calculation. In another direction, the

source terms (mass, momentum and energy) between the liquid phases and the gaseous phase of the Eulerian multiphase spray code calculation were transferred to the gas phase calculation of the engine code in order to synchronise the flow field.

MATHEMATICAL MODELLING

The basis of the Eulerian spray method is the multiphase approach obtained through the ensemble averaging process of the conservation equations. The gas and the liquid phase are considered as continuum represented by the volume fractions. The gas phase is modelled as the primary phase, whilst the droplets are treated as secondary phase. The droplets are divided into a finite number of classes represented by a droplet diameter range. Table 1 shows the phase and class specification in the Eulerian multiphase size of classes approach. The vapour is transported by a separate scalar transport equation within the gaseous phase. The phases from 2 to n-1 are the liquid droplet phases. The last phase, phase n, is modelled as the bulk liquid phase flowing out from the nozzle.

Table 1. The phase specification of the Eulerian spray model

Phase	1	2, …, n-1	n
Content	Gas mixture	Droplets	Bulk liquid

A set of conservation equations is being solved both for the gas and liquid phase. This leads to a great number of conservation equations to be solved especially when defining a higher number of droplet classes. Details on the conservation equation and the modelled source terms can be found in [24]. Equations (1), (2) and (3) represent the mass, momentum, and enthalpy conservation equations for phase k [23] and [24]. The terms e Γ_{kl}, $\mathbf{M}_{kl}$ and H_{kl}, stand for the mass, momentum and enthalpy exchange terms between phase k and phase l. They contain the complete physics of the spray model, whilst the left hand side determines the rate of change and the convective transport. Equation (4) represents the volume fraction compatibility condition that must be fulfilled as a prerequisite of the conservative approach.

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \mathbf{v}_k \right) = \sum_{l=1,l \neq k}^{n} \Gamma_{kl} \tag{1}$$

$$\frac{\partial \alpha_k \rho_k \mathbf{v}_k}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \mathbf{v}_k \mathbf{v}_k \right) = -\alpha_k \nabla p + \nabla \cdot \alpha_k \left(\boldsymbol{\tau}_k + \boldsymbol{\tau}_k^t \right) + \alpha_k \rho_k \mathbf{f} +$$
$$+ \sum_{l=1,l \neq k}^{n} \mathbf{M}_{kl} + \mathbf{v}_k \sum_{l=1,l \neq k}^{n} \Gamma_{kl} \tag{2}$$

$$\frac{\partial \alpha_k \rho_k h_k}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \mathbf{v}_k h_k \right) = \nabla \cdot \alpha_k \left(\mathbf{q}_k + \mathbf{q}_k^t \right) + \alpha_k \rho_k \mathbf{f} \cdot \mathbf{v}_k$$
$$+ \alpha_k \rho_k \theta_k + \alpha_k \boldsymbol{\tau}_k : \nabla \mathbf{v}_k + \alpha_k \frac{dp}{dt} + \sum_{l=1,l \neq k}^{n} H_{kl} + h_k \sum_{l=1,l \neq k}^{n} \Gamma_{kl} \tag{3}$$

$$\sum_{k=1}^{n} \alpha_k = 1 \tag{4}$$

For reliable use of the Euler-Eulerian multiphase model a detailed verification has been performed [25]. The validation has been performed comparing the liquid and vapour penetration in comparison to the experimental data. The validation of the Euler-Lagrangian approach was performed in [24] where the mean pressure, temperature and pollutant emissions were compared to the experimental data. The confidence in the accuracy of the presented approach is based on the two above mentioned model validations. It can be concluded that the topic in [24] is calculating the pollutant emissions employing the Euler Lagrangian formulation which is different to topic in this manuscript, whilst the topic in the [25] is parameterisation of the breakup models employing the Euler Eulerian formulation which is different to topic in this manuscript.

As it was previously mentioned the Euler-Lagrangian approach was used for the purpose of this paper. Lagrangian formulation was used for tracking droplets motion through the flow field, whilst the Euler formulation was used for solving the gaseous phase [26].

The AVL Code Coupling Interface (ACCI) was used in this work as a separate software module to enable coupling between two different CFD simulations, the Eulerian spray multiphase calculation and the Lagrangian DDM spray single-phase engine calculation. This module provides the required data exchange between two simulations, i.e., two codes. Moreover, the ACCI module provides spatial mapping of data between different meshes, which was performed in a conservative manner based on a volume or area weighted interpolation. The coupling was implemented as a server-client system, where Eulerian multiphase spray simulation was calculated with the spray client and Lagrangian DDM single-phase engine simulation was calculated with the engine client. As mentioned previously, the goal of coupled simulation is to use the benefits of both simulations, Eulerian multiphase spray simulation and single-phase engine simulation, when calculating the fuel injection, mixture preparation and combustion in real engine configuration. The fuel injection process was calculated at the spray client with a fine mesh only near the nozzle hole. Mixture preparation, combustion and nitrogen emission formation were calculated at the engine client in whole engine configuration with coarser moving mesh.

The 3D non-moving computational domain, used for Eulerian multiphase spray simulation, is only a small part of the 3D moving engine domain.

As addressed, the ACCI was used to couple two separate domains: spray domain calculated with spray client applying the Eulerian multiphase spray method, and engine domain calculated with engine client applying the Lagrangian DDM method. ACCI performs the spatial mapping between different meshes and transfers the attribute values between them. The main task of the ACCI is to exchange either the boundary condition values or source terms between two clients. The data exchange was done at each coupling time step. Initialization of coupled simulation must be performed as the first step where the engine client sends the initial conditions such as pressure, temperature, turbulence kinetic energy, etc., to the coupling server. The spray client gets the initialization information from the coupling server.

The spray client transfers the source terms from the whole spray 3D volume mesh to the overlapping domain in the engine mesh. Since the spray client and engine client use different meshes, the source terms mapping was performed in a conservative manner using a weighting factor. This factor was calculated from the intersection volumes between spray and engine mesh according to the equation (5):

$$wf_{se} = \frac{CV_{se}}{CV_s} \tag{5}$$

for extensive attributes such as mass or momentum sources. For example, mass source term S_e in the control volume of the engine mesh was calculated from all values in the control volumes in spray mesh as:

$$S_e = \sum_s wf_{se} S_s .$$

(6)

Figure 1 illustrates the intersection of control volume of the source-interface spray mesh CV_s with control volume of the target-interface engine mesh CV_e. Source terms should be mapped from the spray mesh to the engine mesh.
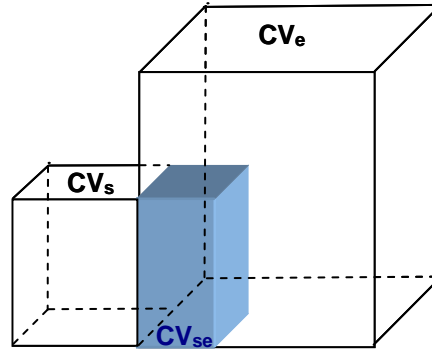

Figure 1. Intersection of control volumes between spray and engine mesh

In the case of non-extensive attributes such as mass fraction, velocity, pressure or temperature where these attributes do not depend on the size of control volumes the weighting factor is defined as:

$$wf_{se} = \frac{CV_{se}}{CV_e} .$$

(7)

The boundary condition values (pressure, velocity, turbulence and temperature) in the 3D volume mesh of the engine client at the end of engine time-step were mapped to the 2D surface boundaries of the spray client. These values were used as boundary conditions in the spray calculation. For this purpose two different boundary conditions were defined for the spray mesh, static pressure and velocity at a face selection surface.

Liquid phases that cross the boundary of the spray mesh were treated in the engine code by classical DDM model, producing new parcels in the engine domain. The details regarding the bidirectional coupling between the engine and spray domain is in detailed explained in [23], [27], and [30].

NUMERICAL SIMULATION

Since the combustion chamber geometry and the 6 hole injector configuration are symmetrical, the calculated engine domain is only 1/6 of the total chamber with one nozzle in order to save computational time. The Eulerian multiphase spray calculation was performed only close to the nozzle (full conical spray domain), while the Lagrangian spray calculation, combustion and formation of nitrogen emission were performed in the remaining combustion chamber (60 degree sector of cylinder), as illustrated in Figure 2.
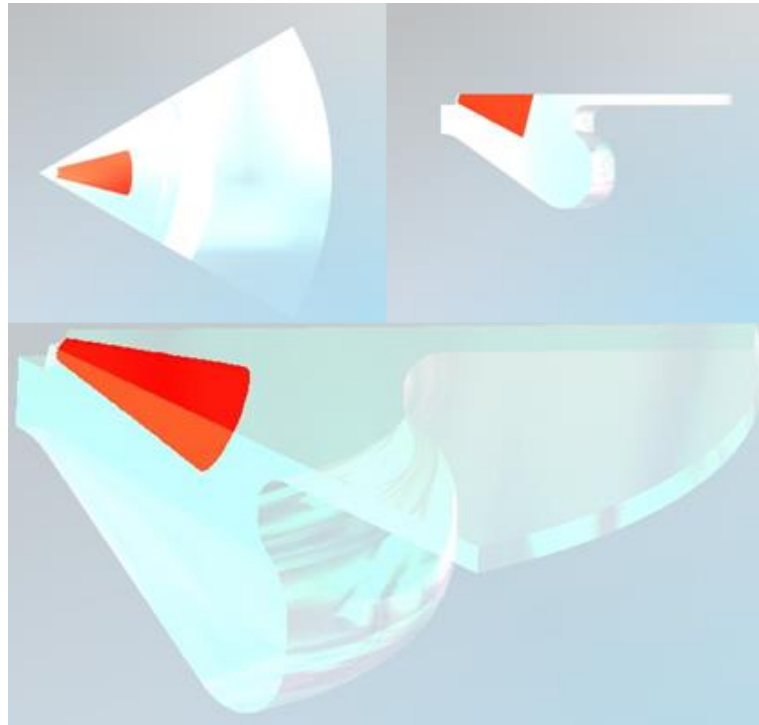
Figure 2. Engine and spray domain used for the simulation

The examined engine stroke is 89.4 mm, bore 81.5 mm, compression ratio 17.5 and revolving speed 4200 rpm. The boundary conditions used for engine simulation are presented in Figure 3. The cylinder geometry was assumed to be symmetric around the cylinder axis and cyclic boundary conditions were applied to the sides. A moving wall boundary condition was applied to the piston bowl. The in-cylinder thermodynamic state and flow distribution prior to injection of diesel fuel were obtained through simulation of the compression stroke. The engine simulation was run from 630.0 to deg CA until 738.2, but in the first part of the simulation the engine client was run alone in the period of 630 to 703.4 deg CA since there is no liquid fuel in the domain up to this point. Injection of diesel fuel starts at 703.4 deg CA. At this point the coupling of engine and spray simulations were initiated. This means coupled simulations were run from the beginning of the injection of diesel fuel (703.4 deg CA) through the end of the injection (738.2 deg CA). The in-cylinder region of the computational mesh consisted of 23664 control volumes at top dead centre (TDC) whilst the rezone procedure during the expansion stroke created computational domain consisting of around 80000 control volumes in the low dead canter (LDC).
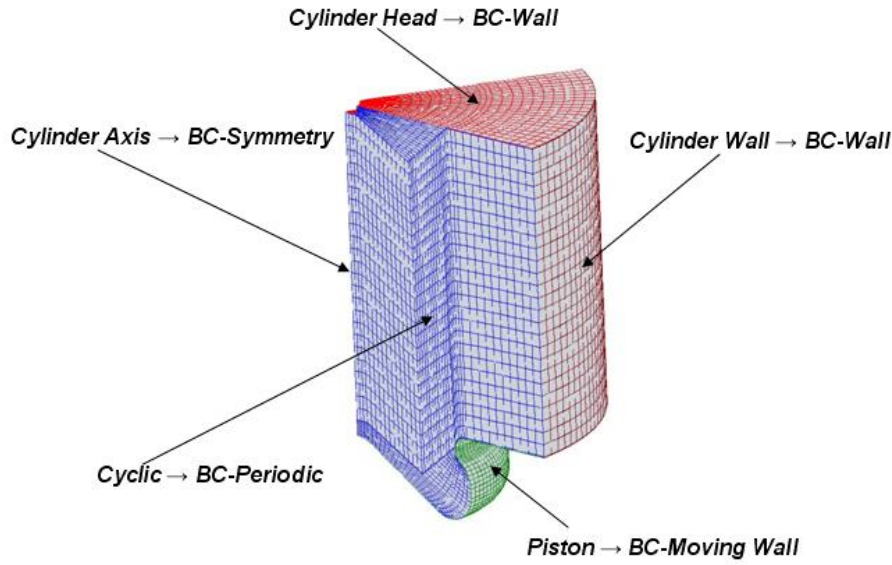
Figure 3. Engine boundary conditions

Turbulence was modelled by the standard k-epsilon model. The standard high Reynolds k-eps model could be used for the considered flow conditions. This model is the most widely used in CFD simulations of practical engineering applications and it yields realistic predictions of major mean-flow features. The diesel combustion was represented by the Eddy Break-up Model [28]. This model assumes that reaction rates are controlled by turbulence while chemical kinetics are neglected. The fuel consumption rate (reaction rate) is assumed to be inversely proportional to the turbulent mixing time scale (k/epsilon) and can be expressed in accordance with [29] as

$$w_F = A \frac{\varepsilon}{k} \min \left(Y_F, \frac{Y_{Ox}}{S}, B \frac{Y_{Pr}}{1+S} \right), \tag{8}$$

where Y denotes the local mean mass fraction of fuel, oxygen and product, while S is the relationship in the stoichiometric fuel/air reaction in equation (8), and A and B are empirical coefficients that are not generalized, but rather established for each reactive flow application. The first rate is calculated according to the Arrhenius reaction rate, the second calculated reaction rate represents the rate of dissipation of turbulent reactant eddies, while the third reaction rate is the rate of dissipation of turbulent eddies with products according to equation (8).

The central difference discretization scheme was used for the convective term in the continuity equation, while a hybrid between the central differences and the upwind scheme with a blending factor of 0.5 was used for the convective terms in the momentum equations. The upwind discretization scheme was used for the convective terms in the scalar equations. The convergence of the solution was achieved with proper set of the under-relaxation factors and sufficiently small time steps to fully account the dynamic spray behaviour. The diesel fuel with temperature of 353 K, density 769 kg/m3, specific heat 2296 J/kgK and molar viscosity equal to 6.4012e-04 kg/ms was used as fuel in this research. The effects of turbulent diffusion, evaporation and break-up of droplets were taken into account in engine simulations. The evaporation of droplets was modelled by the Abramzon/Sirignano model while for break-up the standard WAVE model was used [23].

An outline of the spray region of the computational mesh is given in Figure 4. The conical mesh consisted of 11760 control volumes. It was refined toward the spray inlet and the symmetry

axis. The diesel fuel was injected by the nozzle with an orifice diameter of 137 µ m into the cylinder. Injection starts near the end of the compression stroke at 703.4 deg CA and finishes at 738.2 deg CA.
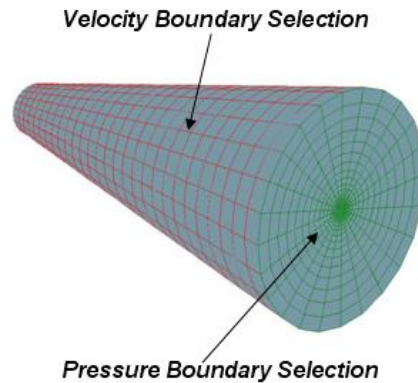

Figure 4. Spray boundary conditions

The Eulerian multiphase results were generated using six phases total, one gaseous phase, four droplet phases, and one bulk liquid phase. All phases were treated as interpenetrating multi-fluids represented by their volume fractions. The gas phase was treated as the primary phase, while the spray droplets were treated as the secondary phases. The droplets were classified into different size classes by volume fractions and diameters. The size class diameters are 5, 10, 20 and 40 µ m for the droplet phases and the nozzle diameter of 137 µ m was assigned to the bulk liquid phase. The mesh dependency of the Euler Eulerian and Euler Lagrangian simulation is mentioned in [24], [25].

The initial conditions used for engine calculations are taken from [30]. The pressure at the start of simulation (630 deg CA) was set to 0.45 MPa, temperature to 430 K. The cylinder was filled with air initialised with turbulent kinetic energy of 50 m^2/s^2 and turbulent length scale of 0.001 m. The wall boundary selections were initialized with the same temperature as the in-cylinder air. The fuel was injected into the domain according to the experimental velocity curve, as seen in Figure 5.
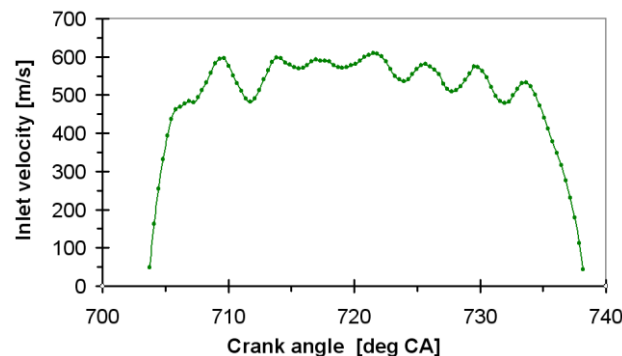

Figure 5. Injection velocity used for spray simulation

RESULTS

The main goal of coupled simulations has been to investigate the capabilities of the coupling concept between validated 3D Eulerian multi-phase simulation and validated NOx chemical reaction mechanisms for engine simulation. This means that the validated 3D Eulerian multi-phase model was used as a physical improvement of the spray process, while the combustion process was modelled on a single phase solver and furthermore was coupled with improved

NOx reaction mechanisms [25], [23] and [30]. Two types of coupled simulations were conducted in this work: swirl and non-swirl engine simulations. Two different cutting-planes are used to present the simulation results as shown in Figure 5.
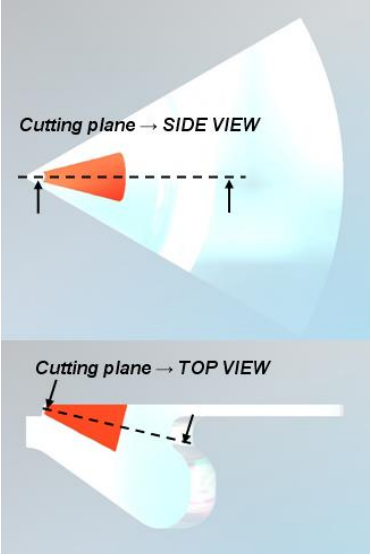

Figure 5. Cutting planes used for visualisation of simulation results

The gas phase velocity field is shown for 720 deg CA in Figure 6. As can be seen, the maximum velocity is higher at the Eulerian spray domain than at the engine domain due to better mesh resolution. In the spray simulation a significant volume fraction of the liquid phases occupies the control volumes in a region near the nozzle, whilst in the engine simulations there is only the gas phase. The plots also show good agreement of the gas flow field between two codes, indicating that the gas flow field of the engine simulation was well mapped to the surface boundaries of the spray client. In another direction, source terms resulting from spray simulation were mapped to the engine client. Adequate source mapping can be seen in Figure 6. Overall, it can be said that velocity was resolved more accurately in the spray simulation due to much finer mesh resolution, and the momentum exchange between the liquid and gaseous phases calculated by spray code were well mapped to the engine simulation, providing a more accurate flow field.
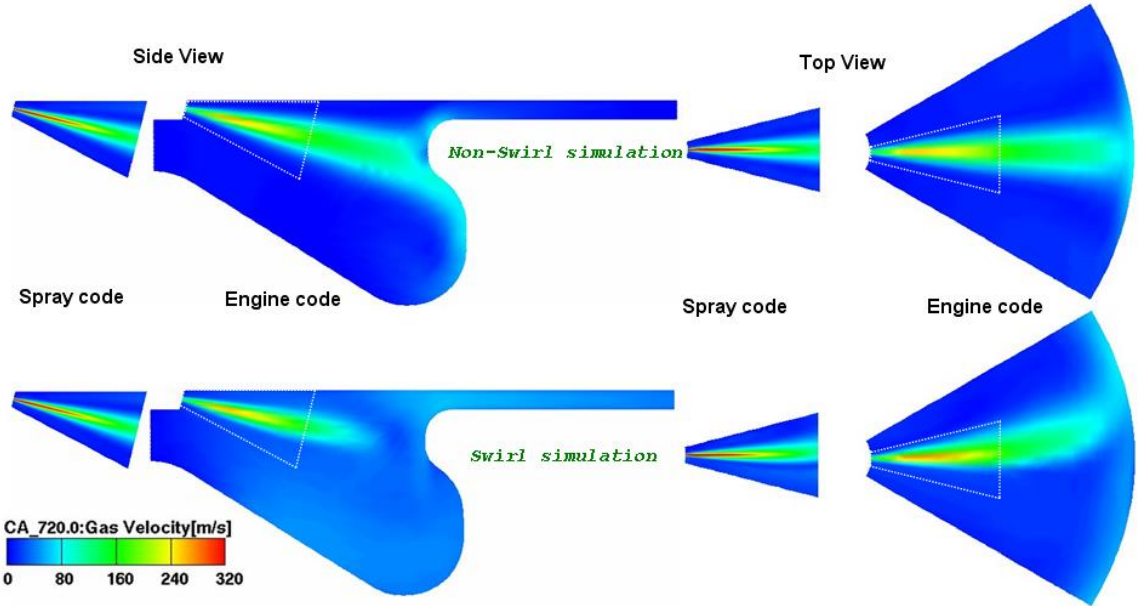
Figure 6. Gas velocity of the spray and engine code at 720 deg CA

Throughout the simulation the spray droplets disappear due to the evaporation process. The heat arrives at the droplets from the ambient gas by conduction and convection, producing the fuel vapor that leaves into the gas by convection and diffusion. Figure 7 shows a comparison of the fuel vapor mass fraction between spray and engine code. As can be seen, the spray and the engine fuel vapor results exhibit very similar trends and good agreement in the overlapping region. One can observe a difference between the swirl and non-swirl simulation. The swirl motion in the cylinder calculated by engine code impacts the spray simulation, and as can be seen, the fuel vapor is deviated. This confirms that the gas flow field is well calculated and the transfer of boundary condition values and source terms between the two simulations is good.
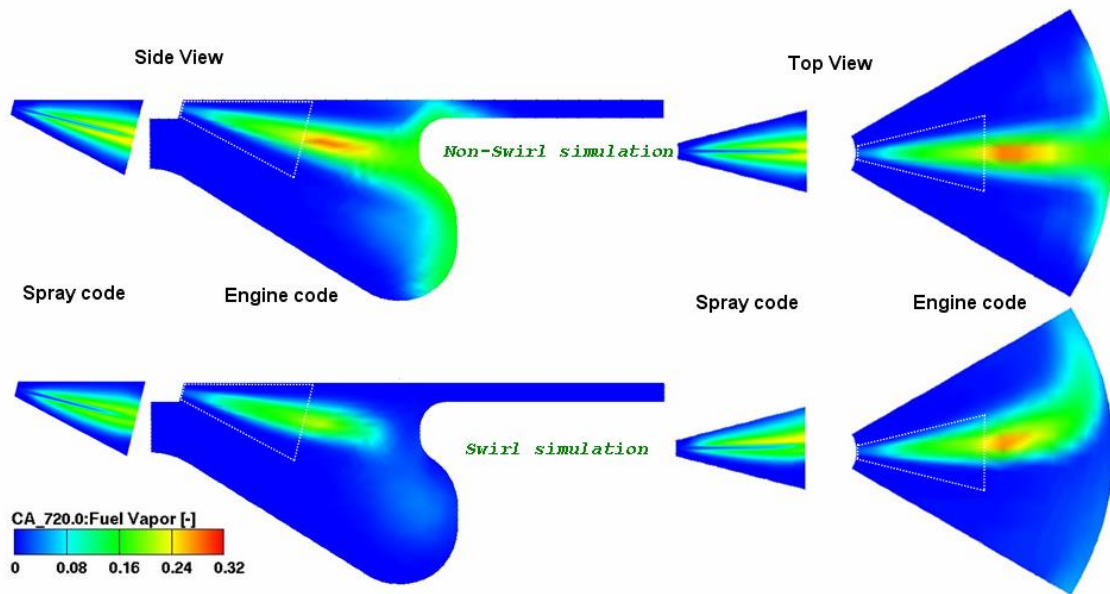

Figure 7. Fuel vapor of the spray and engine code at 720 deg CA

Figure 8 show the gas temperature distribution and nitrogen oxide (NO) mass fraction distribution of the swirl and non-swirl engine simulations. The regions of NO can be examined by looking at contours of NO and temperature. The formation of NO in the combustion processes in engine simulations was predicted using reduced chemical reaction mechanisms described in [23] and [30]. The used nitrogen scheme was based only on thermal NO formed by oxidation of atmospheric nitrogen in a fuel-lean environment. Prompt NO was neglected since this mechanism contributes only a minor part of the total NO in diesel engine.

The thermal NO mechanism arises from the thermal dissociation and subsequent reaction of nitrogen and oxygen molecules in combustion air at relatively high temperatures. It is extremely sensitive to the temperature and it is produced only in very hot products regions. Figure 8 shows a comparison of NO mass fraction distribution with the temperature distribution, indicating that NO occurs wherever there is high temperature.
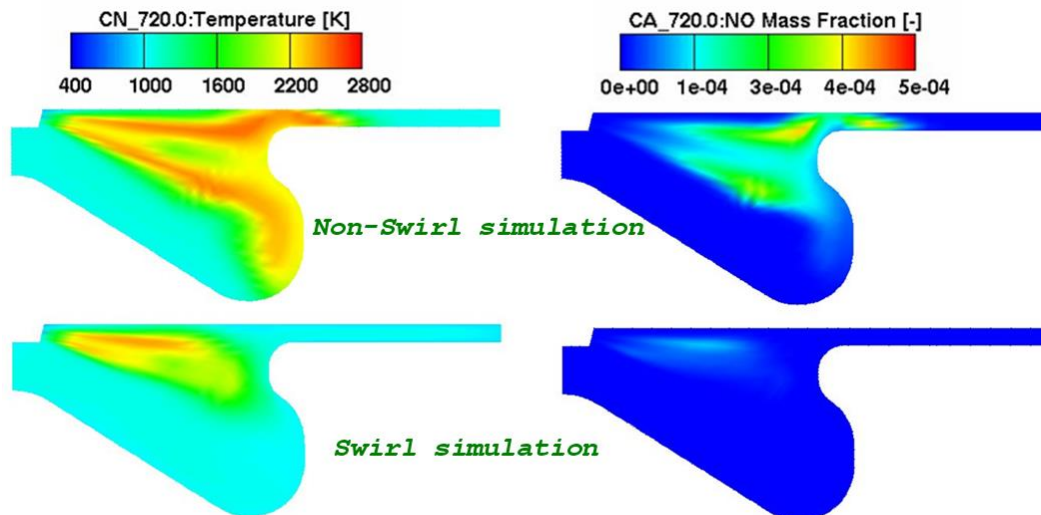
Figure 8. Temperature and NO distribution at 720 deg. CA - side view

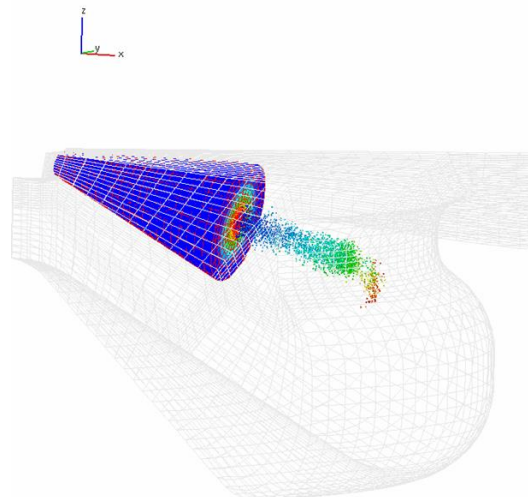The transition from the Eulerian to the Lagrangian approach is presented on the Figure 9.

Figure 9. DDM parcels produced in the engine domain

As it is visible on the upper figure, after the liquid phase reaches the end of the Eulerian spray domain the Lagrangian parcels are introduced. The mass, momentum and enthalpy source terms are transferred to the Lagrangian engine simulation.

CONCLUSION

To demonstrate the capability of the coupling concept, an integrated simulation approach was applied for calculation of the real internal combustion engine. An integrated simulation approach was based on the idea of coupling two different simulations, the Euler-Eulerian multiphase spray calculation performed only close to the nozzle in the dense spray region with the single-phase engine calculation applying DDM and the NOx chemical reaction mechanisms in the whole computational domain. The Eulerian multiphase spray simulation was performed on a separate, fine mesh, while the single-phase engine simulation was performed on coarser mesh, presenting the whole domain and arbitrarily overlapping the spray mesh. These simulations were coupled and performed simultaneously to take advantage of the capabilities inherent in both simulations. The flow field of the engine code calculations were used as boundary condition values for the Eulerian multiphase spray code calculation, and the source terms of the Eulerian multiphase spray code calculation were transferred to the gas phase

calculation of the engine code. The simulation results indicate that the coupling concept works well, allowing an efficient data transfer between the Eulerian multiphase spray and single-phase engine simulation. However, the time costs of the coupled simulation can be up to several time higher than simulations employing the Eulerian-Lagrangian approach only. It is important to note that further improvements can be made by implementation of the combustion process in the Eulerian multiphase domain, including the transfer of energy and vapour sources from the single-phase engine code to the Eulerian multiphase code. An integrated simulation method presented in this work can be improved by coupling with nozzle flow simulation, taking into account the influences from nozzle flow turbulence and cavitation dynamics on the primary break-up of the liquid fuel jet. It can be stated that the presented simulation methods can serve as an advanced tool to analyse and improve understanding of turbulent reacting multiphase flow in real combustion configurations. This approach can be used to describe the high pressure dense and dispersed liquid fuel spray behaviour and NOx formation, resulting in a better description of the fuel-air mixing process and the pollutant formation process, which are crucial issues to ensure better combustion efficiency and to reduce emission pollutants in modern combustion systems.

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