

Numerical Investigation of Non-Reacting and Reacting Diesel Sprays in Constant-Volume Vessels

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ABSTRACT

A numerical investigation on a series of Diesel spray experiments in constant-volume vessels is proposed. Non reacting conditions were used to assess the spray models and to determine the grid size required to correctly predict the fuel-air mixture formation process. To this end, not only computed liquid and vapor penetrations were compared with experimental data, but also a detailed comparison between computed and experimental mixture fraction distributions was performed at different distances from the injector. Grid dependency was reduced by introducing an Adaptive Local Mesh Refinement technique (ALMR) with an arbitrary level of refinement.

Once the capabilities of the current implemented spray models have been assessed, reacting conditions at different ambient densities and temperatures were considered. A Perfectly Stirred Reactor (PSR) combustion model, based on a direct integration of complex chemistry mechanisms over a homogenous cell, was adopted. A detailed comparison in terms of auto-ignition time and flame lift-off length is provided. Furthermore, the assumptions of the PSR model were verified by visualizing the mixture fraction variance ($\widetilde{Z''^2}$) distribution in the regions where combustion takes place, such that the role of possible interactions between chemistry and turbulence can be estimated.

INTRODUCTION

A deep understanding of the dominant physical and chemical phenomena characterizing the combustion process remains the fundamental prerequisite to improve the existing Diesel technology towards cleaner and more efficient engines. Accurate studies to investigate the in-cylinder spray evolution, the fuel-air mixing process,

the occurring auto-ignition and flame development are still very needed. Numerous experiments in constant-volume and constant-pressure vessels [1, 2] have clarified different aspects related to the structure of free spray jet flames at different operating conditions (ambient temperature and density, amount of EGR), while optical measurements in single cylinder test engines have helped to understand the complex interactions between the fuel spray and the in-cylinder flow-fields during the combustion process [3]. However these detailed investigation are typically performed in simplified configurations and therefore they cannot extensively be used from a design perspective to optimize a real engine geometry together with the possible injection strategies.

On the other hand, Computational Fluid Dynamics (CFD) represents a very useful tool to integrate the experimental activity to investigate the combustion process in Diesel engines and also be part of the industrial design and analysis. Despite the fact that any of the governing physical and chemical phenomena has been matter of investigation for decades, simulation results are still very dependent on the accuracy and set-up of the employed sub-models, on the numerical discretization and on the assumptions made to account for the turbulence-chemistry interactions [4, 5, 6, 7, 8, 9]. Among these sources of uncertainties, grid dependency plays a major role and it is directly linked with the adoption of the Eulerian-Lagrangian approach to model the spray evolution. The reasons for such dependency are mainly due to the difficulty in having a spatial resolution which guarantees a cell volume bigger than the volume of the droplets they contain, but which is also able to accurately resolve the gas phase development near the nozzle [10]. Furthermore the lack of statistical convergence in the Lagrangian treatment of the liquid phase [11], the relevance of the adopted interpolation process, whereby the gas quantities known at Eulerian

nodes are estimated at the parcel location [12] and the grid dependency caused by the physical sub-models introduce other possible sources of error. As a consequence, the capability of predicting the correct fuel and air mixedness prior to ignition has a very critical numerical dependency. Several improvements have been proposed to overcome this known limitation either based on new collision algorithms [13, 14] or proposing the implementation of a combined hybrid Eulerian-Eulerian and Eulerian-Lagrangian methodology [15] or making use of an adaptive locally refined mesh in the spray region [10, 16].

Within this context, the authors intend to simulate the Diesel spray combustion process with an adaptive local mesh refinement technique (ALMR) in combination with the Perfectly Stirred Reactor (PSR) combustion model. In this way, it is possible to start the simulation with a relatively coarse mesh which will be progressively refined only in the regions where the fuel is injected and mixes with air. An arbitrary level of refinement is allowed to reach the desired mesh size and achieve satisfactory results. The adaptive mesh refinement approach preserves the quality of the results and reduces the required computational time and as well as the pre-processing time, which is needed to generate a spray-optimized grid. The Perfectly Stirred Reactor (PSR) approach is used to model the combustion process [8, 7, 17], involving complex chemistry to describe the fuel oxidation process and neglecting any sub-grid interaction between turbulence and chemistry.

The capabilities of the proposed methodology were verified by simulating series of constant-volume diesel combustion experiments, taken from the SANDIA Engine combustion database, which considers a wide range of ambient environments among those typically experienced in a diesel engine [18].

COMPUTATIONAL MODELS

The authors have implemented the proposed approaches to model the Diesel spray combustion process into the OpenFOAM® code, release 1.5. The code is open-source and written in object oriented C++ language [19, 20, 21]. OpenFOAM handles polyhedral meshes of arbitrary shapes, contains almost the state of the art of physical and numerical models and for this reason it is the ideal tool to perform advanced research in a collaborative environment. In previous studies, OpenFOAM had already been successfully applied to simulate different Diesel spray combustion experiments [4, 17, 22, 23, 24].

SPRAY MODEL

The discrete droplet method (DDM) was adopted to simulate the evolution of Diesel sprays [25], in which the liquid is described by a Lagrangian approach and the vapor by Eulerian coordinates. The spray droplets

are described by stochastic particles which are usually referred as *parcels* [26]. Each parcel represents a class of identical, non-interacting droplets, and they are tracked through the physical space in a Lagrangian manner according to the mass, momentum and energy exchange with the gas (Eulerian) phase. Additional phenomenological models are required to describe the various physical processes taking place in the sub-grid length scales. The interaction between the Lagrangian and the Eulerian phases determines the fuel/air mixture formation process and modifies the flow-field in the computational domain. The phase coupling can be distinguished into 'gas-to-liquid' and 'liquid-to-gas'. The first one comprises the interpolation process, whereby gas quantities known at the Eulerian nodes are estimated at the parcel locations. The 'liquid-to-gas' refers to the summation of particle source terms in the Eulerian conservation laws.

GAS TO LIQUID COUPLING

Two different interpolation techniques were chosen to compute the gas quantities at the parcel positions. The *cell-point-face* approach is used to estimate the gas velocities at the parcel locations [4]. Firstly, the velocity field, which is stored at the mesh cell centers, is interpolated both at the mesh faces and mesh points locations. Then, a tetrahedron is built with the closest points around each parcel (cell centers, face centers, mesh points), as it is illustrated in Figure 1.

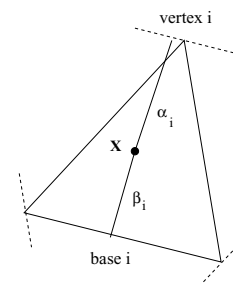


Figure 1: Interpolation of the velocity field at the parcel locations.

The distance between the parcel and one of the tetrahedron faces is α_i , while $\alpha_i + \beta_i$ represents the distance between the same face and its opposite vertex. The interpolated velocity at the parcel position x is:

$$\mathbf{u}(x) = \sum_{i=1}^4 \frac{\alpha_i}{\alpha_1 + \beta_i} \mathbf{u}_i \quad (1)$$

When this interpolation technique is used, each parcel experiences a continuous velocity field within the computational domain, such that the grid dependency of the spray simulations is reduced. For stability reasons, the same technique cannot be employed to estimate the gas phase temperature, pressure and density at the parcel positions: these quantities are assumed to have the same values of the cell center where the parcel is found [4].

LIQUID TO GAS COUPLING

Each parcel is tracked along its path by using the *face-to-face* algorithm. This makes possible to identify all the cells crossed by each parcel during one time step and to split the Lagrangian source terms of the Eulerian equations accordingly [4]. In this way, both the accuracy and the stability of the spray simulation are increased.

SPRAY SUB-MODELS

The DDM approach requires the adoption of sub-models to describe the spray breakup and evaporation that the parcels are subjected to before they become part of the gas phase. To model the spray breakup [27], both the Kelvin-Helmoltz and Rayleigh-Taylor mechanisms are accounted for. The Ranz-Marshall correlation [28] is used to model the droplet evaporation. Droplet to droplet interactions and turbulence dispersion effects are neglected.

REDUCTION OF GRID DEPENDENCIES

It is generally accepted [11, 29, 30, 31] that the grid dependency of the Eulerian-Lagrangian spray simulations is related to the various sub-models involved and to the inadequate spatial resolution hindering the coupling between the gas and liquid phase. This second aspect is the most important since it often requires an unphysical adjustment of the spray sub-models coefficients. This leads to the lack of convergency and consistency of the computed solution when the grid size is reduced.

In this work, the authors have followed more justifiable measures to reduce the grid dependency [30]:

1. Spray-adapted grids are adopted, such that the spray penetrates almost perpendicular into the cells.
2. Droplet to droplet interaction models are avoided since they often introduce a source of strong grid dependency.
3. The turbulence length scale is limited in the liquid jet region, since the liquid jet governs the relevant length scales.
4. An adaptive local mesh refinement technique is introduced to keep an acceptable grid size and, at the same time, to model the relevant length scales typical of the fuel-air mixture formation process.

TURBULENT LENGTH SCALE LIMITER

Investigations carried out by Abrahm and Otto [32, 30] revealed that the liquid jet is the driving force for mixture formation and the orifice diameter is the relevant length scale that needs to be discretized to achieve a satisfactory agreement with experimental data. However, the grid size used in the spray simulations is generally much higher

than the nozzle diameter ($2\div 5$ times) and this aspect is responsible for a strong dependency of the computed results on the ambient diffusivity. To overcome these limitations and to keep an acceptable grid size, Karrholm and Nordin [22] proposed to limit the turbulence length scale to the orifice diameter in the cells where the spray parcels are present. The same approach was followed by the authors in this work, adopting the standard $k - \varepsilon$ model. The turbulence integral length is defined as:

$$l_t = C_\mu \frac{k^{3/2}}{\varepsilon} \leq L_{sgs} \quad (2)$$

where k is the turbulent kinetic energy and ε represents its dissipation rate. L_{sgs} is the limiter length which is set to the nozzle diameter. Since k governs the scale of the fluctuating turbulent velocity and ε controls the size of the turbulent eddies, the limit was imposed as constraint on ε , after solving the equations for k and ε :

$$\varepsilon \geq C_\mu \frac{k^{3/2}}{L_{sgs}} \quad (3)$$

When the turbulence integral length is limited to the nozzle diameter, the computed vapor and liquid penetrations become less sensitive to both the grid size and the ambient diffusivity [33, 22].

ADAPTIVE LOCAL MESH REFINEMENT (ALMR)

Diesel spray combustion calculations are performed in constant-volume vessels or in internal combustion engines. Hence the grid size should correctly reproduce the geometrical domain to be simulated and it has to be fine enough in the regions where the fuel/air mixture formation and the combustion process occur. If the common cell shapes (tet, hex, prisms) are used and the mesh topology is not allowed to change during the simulation, the grid generation process becomes time consuming, needs experience and care and the resulting mesh is always a compromise between the two aforementioned requirements.

Within this context, adaptive local mesh refinement (ALMR) becomes very interesting since it enables a high mesh resolution of the spray liquid-gas interaction while the overall grid size is weakly increased. Different implementations of this technique were successfully applied for spray simulations [10, 29, 34]. In this work the authors apply such a technique to Diesel spray modeling in OpenFOAM. The code supports polyhedral meshes of arbitrary shapes and includes different algorithms which easily allow to modify the topology of the grid during the simulation by adding or removing grid points, faces and cells according to specified criteria [35]. This makes possible to easily perform adaptive local mesh refinement as it was illustrated in [20, 21, 36] for other fields of applications.