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Effect of mesh refinement and model parameters on LES simulation of diesel sprays

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ABSTRACT

Review of the recent literature on fuel spray modeling suggests that the use of Large Eddy Simulation (LES) approach is of fundamental importance in order to adequately represent the complex phenomena related to spray–turbulence interactions, which affect all physical processes of the mixture formation and combustion. However, some deficiencies have been identified related to the accuracy of non-reacting spray simulations, mainly related to the adequate set-up of different models and numerical parameters and, in particular, to mesh size, to adequately capture the spray turbulence interactions. This work presents the application of advanced turbulence modeling to the spray injection process in a static chamber, based on the implementation of a LES turbulence model in a Lagrangian spray based solver in OpenFOAM (open source code). Results obtained hitherto for non-reacting sprays proved that highly accurate results can be obtained for liquid and vapor length penetrations by correct modeling of spray phenomena and adequate mesh refinement to correctly capture turbulence–spray interactions. In addition, a new criterion for adaptive mesh refinement based on the droplet Stokes number, is proposed and tested. This criterion can be also used to evaluate to what extent the spray turbulent dispersion, is adequately captured with a given mesh refinement, using LES approach.

1. Introduction

Diesel engines are known for their higher fuel conversion efficiency, as a consequence of better thermal efficiency and reduced pumping work. Environmental and health related concerns and worries on fuel economy and greenhouse gas emissions have led to the introduction of ever more stringent emission standards. Lately concerns about NOx emissions have increased tremendously more so with the recent facts involving Diesel engines, where it has been found that on-road emissions to be higher than in the test cycle. The introduction of more demanding European emission cycle, starting gradually in September 2017 and reaching full implementation by September 2019, that reproduces more adequately the real driving conditions (RDE Real-World Driving Emissions) will enforce that the combustion system be designed with more care and with attention to various interrelated phenomena. Computational fluid dynamics simulation of engine in-cylinder processes is of fundamental importance in the combustion design process, but care has to be taken as there are still several unresolved issues in spray combustion modeling. In particular, the correct modeling of the spray–turbulence interactions will have important influence on the prediction of liquid and vapor penetration, mixture formation and, at the end, on the whole combustion process.

From a fuel spray simulation stand point, two major facts impact the liquid length penetration accuracy (Nordin, 2001; Baumgarten, 2006); (1) the gas phase velocity calculation at the parcel location, that can be done assuming the velocity of the closest node in the volume or interpolate to the other nodes (Fig. 1), and (2) the momentum transfer between liquid droplets and gas phase (Fig. 2). In the last, on a coarse grid the momentum transferred, from the parcel to the cell gas volume, will be diffused in a bigger volume and the gas acceleration will be smaller, maintaining a high relative velocity between parcel and gas and thus maintaining a high drag that will lead to reduced liquid length penetration. On the other hand, on a finer grid with the momentum transfer the gas velocity will increase faster, reducing the relative velocity between droplets and gas, leading to lower drag and as a consequence higher liquid length penetration.

Regarding the droplet size distribution, most spray simulation studies used the Kelvin–Helmholtz/Raileigh–Taylor (KH–RT) combined breakup models (Bharadwaj and Rutland, 2010; Wehrfritz et al., 2013; Elmtoft et al., 2015; Jangi et al., 2015), but the model parameters varied among them and, in some cases, using these tuning parameters to improve the correlation of simulation results to experimental results.

Another aspect observed in previous works is the lack of consistence to compare liquid length penetration (distance from the nozzle exit

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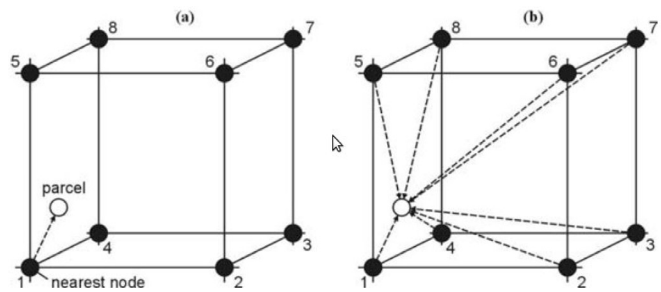

Fig. 1. Gas-droplet velocity calculation: (a) nearest vertex and (b) interpolation. Source: Baumgarten (2006).

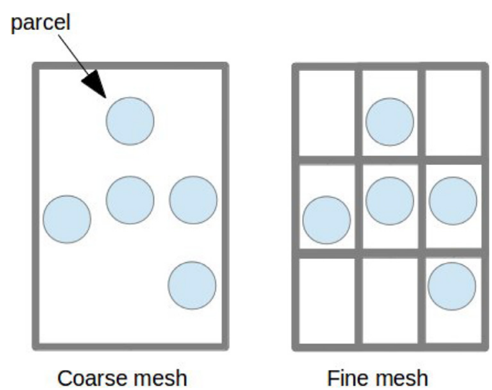

Fig. 2. Liquid–Gas phase momentum exchange.

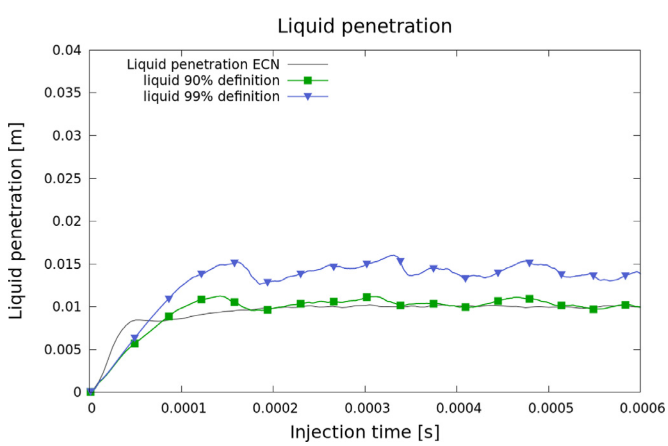

Fig. 3. Influence of liquid penetration definition on results comparison with experiments.

along the spray axis to the point where a predefined percentage of liquid fuel is still encountered) against experiments, sometimes even against the same experiment. The percentage definition varied from 90% to 99% among the various cited works. The definition used by the Engine Combustion Network (ECN), which should be used as reference, is 99% to compare simulation results against their experimental data. Therefore, even claiming that experimental value of liquid penetration are adequately reproduced by models, the penetration definition certainly influence this validation. Fig. 3 shows the liquid penetration obtained in this work with a coarse mesh (the same simulation), considering two different definitions for the liquid penetration. It can be observed that, changing this definition could lead to a wrong conclusion regarding the results comparison with experiments.

An investigation on the interaction between mesh size and number of injected parcels was done in Senecal et al. (2013), where the authors stated that with fine grids, if the liquid mass contained in the parcel was similar to the gas phase in the cell, a minimum of momentum transfer was required to get the gas phase to reach the same velocity of the parcel, thus the drag would be reduced to a minimum and as a consequence the liquid length penetration would be over predicted. They concluded that as the mesh was refined the number of injected parcels has to be increased, in order to have the amount of liquid mass in each parcel reduced, and thus minimizing this effect. These authors also considered that the injection of the spray in a single point would have the same effect of reduction in drag, so they proposed the injection to be performed along a circle with the same diameter of the injector nozzle. They also concluded that, for spray modeling with LES approach, the mesh independence condition should be replaced by what these authors called “mesh convergence”, i.e., if the mesh would be refined beyond a certain size results would get worse. Regarding the liquid length penetration definition they used the value of 95% and the minimum cell size of 31.25 μm with adaptive mesh refinement. They also used dynamic droplet distortion model, droplet collision model and stochastic turbulence dispersion model.

Spray simulation using LES modeling was also investigated in Xue et al. (2013). The showed good correlation with experimental results but considered the value of 90% for the definition of liquid length penetration. The minimum cell size used in their work was 31.25μm with adaptive mesh refinement and included dynamic droplet distortion (TAB), droplet collision and stochastic turbulence dispersion models.

An attempt to improve the precision of the simulations of spray by reducing the size of the droplets injected by the blob method, maintaining the point injection was done in Elmtoft et al. (2015). Instead of injecting blobs with the same size of the nozzle diameter, the initial Blobs’ size range from a fraction of 0.10 to 0.25 of the nozzle diameter. They used 97% for the definition for liquid length penetration. The minimum cell size used in their work was 62.5 μ m with adaptive mesh refinement and also included dynamic droplet distortion, droplet collision and stochastic turbulence dispersion models.

Other studies was performed in Banerjee and Rutland (2015), in this case with constant mesh size along the simulations (i.e. not used AMR), with minimum cells sizes at the spray region of 125 μ m. They reported good correlation of liquid penetration with experimental data but only after a certain time after injection, in the region which they defined as steady state liquid jet, then, their model was no able of capturing adequately the initial part of penetration. In addition, considered 97% the definition for liquid length penetration. They reported also results for vapor penetration, and even using 0.05(5%) fraction as definition, different from 0.1 recommended by the ECN, did not show good correlations.

Concerning spray and flow turbulence interaction, some models presented in literature (some of these previously cited) for Diesel engine spray included these interactions considering spray induced turbulence (*SIT*) and stochastic turbulence dispersion (*STD*) (Lee et al., 2002; Bharadwaj and Rutland, 2010; Tsang et al., 2014; Gong et al., 2014b; 2014a; Zhou et al., 2015). In the LES context, the *SIT* phenomenon in usually included in the models through a source term in the sub-grid TKE equation, which takes into account the sub-grid TKE generation due to droplet velocity fluctuations, which, on its turn, is calculated through an stochastic model (see Eqs. (23)–(26)). The *STD* phenomenon is the counterpart of *SIT* on liquid phase and considers the droplet dispersion due to the sub-grid turbulence (once in the LES context, the dispersion due to resolved scales is directly accounted through interfacial momentum exchange). A detailed analysis of the inclusion of *SIT* and *STD* in the context of LES model was presented in Jangi et al. (2015). In that work, which used experimental data from the ECN for comparison, it was identified that vapor penetration was not greatly affected by either *SIT* or *STD*, while liquid penetration length was over predicted if *STD* was not included in the model. They found that the liquid length penetration was not impacted by *SIT*. The authors stated that the reason why previous works using LES approach