Numerical Simulations of a Simultaneous Direct Injection of Liquid And Gaseous Fuels Into a Constant Volume Chamber

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Abstract
Numerical simulations of the dual fuelling process by simultaneous direct injection of liquid and gaseous fuels into a combustion chamber were performed. Diesel fuel and CH₄ were injected into a constant volume vessel through separate nozzles. Injection started for both fuels at the same time. The presented simulations were done using the AVL Fire code – the CFD software dedicated to engine simulations. This work was the first step in a process of modeling the full engine cycle, including combustion. The aim of the study was to validate the spray model before applying it to more complex simulations. One major simplification was made to speed up the calculation process: instead of full chamber geometry only a 60 deg sector of the cylindrical chamber containing only two nozzles, one for gaseous fuel and one for liquid was investigated. The simulation results were compared with literature data [12]. The images from the numerical solution presenting spray droplets and CH₄ concentration were compared with images made by the shadowgraph technique [12].

Keywords: Spray, direct injection, simultaneous injection, dual fuel injection

1. Introduction
Although the simultaneous direct injection of two or more fuels is not a new idea, it has not been widely implemented. It is far less popular than simultaneous injection combining port fuel injection (PFI) and direct-injection (DI). Systems combining direct injection and port injection have been investigated, developed and implemented especially in the area of gas engines [2, 10]. There have also been studies involving gasoline engines simultaneously fuelled with alternative fuels [14]. But the technology for the simultaneous direct injection of two or more different fuels has only been implemented by two companies: Westport for heavy duty vehicles and Wärtsilä for stationary engines. This solution has made it possible to use even associated gases of almost any quality as fuels [7]. This is because this kind of fuel system is not as sensitive to fuel quality and variations in fuel composition and properties as other engine fuel systems.

The stationary and marine engine industry will certainly look for possibilities of applying environmental friendly fuels and by-products as fuels. This will inevitably lend impetus to the development of fuel systems able to handle these fuels. In
this situation engine manufacturers will look for tools to improve the design process, such as CFD codes. Thus, efficient models for engine simulations need to be developed and validated. With respect to previous numerical work relating to the dual fuelling process, the main focus was on modeling the combustion of premixed gas-air mixtures ignited by diesel pilot injection. Miao and Milton developed a 3-D numerical model dedicated to dual fuel engine simulations [8]. They focused on the combustion issue and modeled the pilot fuel injection in a simplified way. In that case it was fully justified, especially as the amount of liquid spray was very small compared to the amount of gaseous fuel. But in the case of systems with simultaneous direct injection of both fuels, the liquid spray is of major importance. These kinds of fuel system are usually intended for both: gas operation (where the amount of liquid is minimal) and for fuel sharing mode (where the share of liquid fuel in total fuel consumption can be very high). The injection issue in systems that combine direct injection of both liquid and gaseous fuels was researched by White [12] and by White and others [13]. They created a numerical model using Fluent software and validated the spray model available in this software.

Although liquid spray models in internal combustion engines have been widely validated, the focus in this work was on liquid injection. There were two reasons for this. The first was the interaction between the liquid spray and the gas jet – a simultaneous gas jet provides an area of high velocity and turbulence kinetic energy gradients which could be crucial for the liquid spray model. The second reason was the fact that the gas outflow simulation was done by modeling the full flow through the nozzle. This means that no gas jet model was applied and the gas jet was mainly dependent on the turbulence model.

2. Numerical model

The presented simulations were done using the AVL Fire code – the CFD software based on the Finite Volume approach dedicated to engine simulations. This tool has a broad variety of applications. For turbulent conditions fluctuating parameters are averaged using the RANS method (Reynolds Averaged Navier-Stokes). There are several turbulence models available. For this case the k-zeta-f model was chosen. This model was developed by Hanjalic, Popovac and Hadziabdij [6]. This model is based on Durbin’s elliptic relaxation concept, which solves a transport equation for the velocity scales ratio \( \zeta = \frac{\overline{v^2}}{k} \) instead of the equation for \( \overline{v^2} \) [6]. The \( \overline{v^2} \) is the velocity scale and k is the turbulence kinetic energy. Durbin’s model is described in [3]. The authors claim that due to a more convenient formulation of the equation for elliptic function f and especially of the wall boundary condition for this function, it is more robust and less sensitive to non-uniformities and clustering of the computational grid than Durbin’s model [6]. The advantages of this model were important in the gas nozzle region, where the wall effects were very strong. Therefore, for this case this model was regarded as the best of those available in AVL Fire code.

Another crucial element of the numerical model, besides the turbulence model, was the spray model. For liquid injection the Discrete Droplet Model (DDM) was used in the conducted simulations. The DDM model has advantages over the Continuous Droplet Model (CDM) in terms of dispersed sprays, because it has much lower computational requirements.

In the DDM approach, the spray is represented by finite numbers of droplet groups, called droplet parcels. It is assumed that all the droplets within one parcel are similar in size and that they have the same physical properties [11]. Each parcel is considered as a particle and is tracked individually in the Lagrangian particle tracking framework [5].

In the CDM approach the spray is represented by the volume fractions of one bulk liquid and several droplet size class phases [4]. For the dilute spray region, the DDM approach has a significant benefit, as the computational effort for additional spray parcels increasing the number of nodes in the droplet size PDF is significantly smaller than that for additional droplet size classes in the Eulerian-Eulerian framework [4].
When using a DDM multiphase model, the character of the simulated spray depends on the break-up submodel applied. The spray breakup model governs droplet breakup. There is a broad variety of break-up submodels available in AVL Fire. Each spray break-up model application field depends mainly on the Webber number, and the Webber Number in turn depends on the nature of the injection. For high pressure direct injection, where the Webber number is much higher than in gasoline ported injection, the most suitable break-up model is the Wave model. Thus the Wave model was chosen for secondary break-up modeling in the investigated case. This model is based on the Kelvin-Helmholtz instability of a liquid jet, where the viscous forces produce waves on the liquid surface and new droplets are formed from the surface waves. Waves grow on the droplet surface with a growth rate $\Omega$ and a wave-length $\Lambda$, and the sizes of the newly-formed droplets are determined from the wavelength and growth rate of this instability [11]. The growth rate $\Omega$ and its corresponding wavelength $\Lambda$ are calculated from the relevant properties of the liquid and gas.

Due to the break-up and production of new droplets, the size of the parent droplets is reduced and the rate of change of this parent droplets is given by [11].

$$\frac{dr}{dt} = \frac{r - r_{\text{stable}}}{\tau_a}, \quad r_{\text{stable}} \leq r$$  \hspace{1cm} (1)

The break-up droplet radius is given by:

$$r_{\text{stable}} = B_0\Lambda$$  \hspace{1cm} (2)

and the break-up time is given by:

$$\tau_a = 3.726 \cdot B_1 \frac{r}{\Lambda \Omega}$$  \hspace{1cm} (3)

The rate of break-up in this model can be adjusted by two constants: $B_0$ – droplet radius constant and $B_1$ – droplet break-up time constant. In the presented simulation $B_0$ was set at 0.61 and $B_1$ was set at 20. These values are recommended by the authors of the model [9] and are default values in AVL Fire software [1]. The flow rate of the diesel fuel was $5 \frac{g}{s}$ and was constant during the injection time, which was 0.4 ms. After this time the diesel fuel flow was stopped abruptly.

As for gas injection, the flow rate was set according to [12]. White [12] adjusted the gas mass flow for simulations using Fluent CFD software. Since Fire is a very similar tool, it was decided to use the gas mass flow optimized by White [12]. The gas mass flow rate is presented in Table 1. The gas mass flow developed over 4 ms and after that remained constant. Nevertheless, the focus in the conducted simulation was on the early stage of the injection.

The computational domain (Fig. 2) was divided into 673,000 elements. The generated grid was a hybrid type grid consisting of a few regions with structural mesh and

<table>
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<tr>
<th>time, ms</th>
<th>Gas mass flow rate, $\frac{g}{s}$</th>
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<tr>
<td>0</td>
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<tr>
<td>0.1</td>
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<td>0.2</td>
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<td>1</td>
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<td>1.3</td>
<td>1.5</td>
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<td>1.8</td>
<td>2</td>
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<td>2.5</td>
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<td>3.5</td>
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Figure 1: Section of the mesh
one small region with nonstructural mesh. Most of the elements were hexagonal. Nevertheless, 35,000 tetragonal elements were used to connect the mesh in the nozzle with the main chamber mesh (Fig. 1). The boundary conditions for this model were specified as follows:

On the side walls there were symmetry conditions. On the other walls there were adiabatic wall conditions. The inlet boundary condition is presented in Figure 2.

3. Results

The simulation results were compared with experimental ones taken from the literature [12]. Images from the numerical solution presenting spray droplets and contours of CH\textsubscript{4} concentration were compared with images presented in [12] made by the shadowgraph technique. This technique provides a visualized representation of the droplets and the density gradients as well.

Initially only diesel fuel injection was under investigation. The reason for this was to find out if the Wave model B\textsubscript{0} and B\textsubscript{1} constants, recommended in [9], are suitable for conditions in the experiment conducted in [12]. Figure 3 compares the diesel fuel injection simulation results with the experimental results from [12]. It can be seen in Figure 3 that in this case the gas jet did not influence the liquid jet to a great extent. The liquid jet evolved in a similar fashion to single liquid fuel injection. The only difference was at the beginning, where the numerical spray was observed to grow faster.

In terms of the comparison with the experimental results obtained by the shadowgraph technique, only the spray cloud formed by droplets was important.

Figure 3 appears to show that the evolution of the modeled spray was essentially the same as in the experiment conducted by White [12]. The only difference was at the beginning, where the numerical spray developed faster. The shape of the tip of the calculated spray was much less diffuse than the spray observed by White [12] using the shadowgraph technique. This may be regarded as an imperfection in the numerical spray model, which assumes that the spray evolves in space in the shape of a spherical cone of a certain angle. However, the penetration evolution seemed to be essentially the same. Thus, for further investigation of the dual injection the same values of Wave model constants: B\textsubscript{0} and B\textsubscript{1} were used.

The comparison of the simultaneous injection of diesel and gaseous fuel simulation results with the experimental ones from [12] is shown in Figure 4. It can be seen in Figure 4 that in this case the gas jet did not influence the liquid jet to a great extent. The liquid jet evolved in a similar fashion to single liquid fuel injection. Although the focus was on evolution of the liquid spray in the early stage of injection, the phenomena observed after 2 ms in Figures 3 and 4 merit some comment. After 2 ms some artifacts on the bottom part of the numerical domain can be noticed. These are reflected droplets from the bottom of the computational domain. The reflection of the droplets results from the fact that there was no liquid-wall interaction model applied. As mentioned before, the focus was on the early stage of the injection and the development of the spray...
Figure 3: Comparison of the diesel fuel injection simulation results presented as spray accumulated view (right) with experimental results obtained by the shadowgraph technique (left) from [12]
Figure 4: Comparison of the dual fuel injection simulation results presented as spray accumulated view (right) with experimental results obtained by the shadowgraph technique (left) from [12]. The upper nozzle is for the gaseous fuel and the lower one is for the liquid fuel.
was of primary importance, not the spray-wall interaction.

4. Conclusions

The Wave model is generally found to be the best break-up model for high pressure sprays in engine simulations. Even though there was no quantitative comparison of simulated results with the experimental data and the presented comparison was only qualitative, it can be concluded that the DDM approach with the Wave break-up model produces reasonable results. To draw more detailed conclusions, more detailed data from the experiments is needed. The figures obtained by the shadowgraph technique only allow one to compare the shape of the accumulated spray. Thus, only general conclusions could be drawn in this case.

As for pure diesel injection, the diesel spray penetration appeared to be slightly higher for the numerical solution, especially at the beginning of the injection.

In the experimental cases there is always a time lag between the command signal and the reaction time of the injection system. In numerical simulations there is no such delay. The delay in the experimental case was estimated by White [12] and was taken into account in this comparison with the numerical solution. Nevertheless, this delay could be included in the simulations of the diesel spray by defining the flow rate evolution in a way that is closer to reality. This move is planned for future research. Moreover, the simulation results showed that the gas jet in the case of simultaneous direct injection of a liquid and gaseous fuel has little influence on the liquid spray.

Acknowledgement

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References

[14] X. Wu, R. Daniel, G. Tian, H. Xu, Z. Huang, and

Nomenclature

Λ wave length
Ω wave growth rate
B₀ model constant
B₁ model constant
r radius of the droplet
r_{stable} break-up droplet radius
tₜ break-up time