Evaluation of breakup models for marine diesel spray simulations

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Abstract

The open-source CFD software OpenFOAM was used to simulate evaporating, high pressure marine diesel sprays. The most frequently used models, based on Kelvin-Helmholtz and Rayleigh-Taylor instabilities, are adopted to describe the breakup of liquid fuel. The proposed approach was first validated using experimental data from the Engine Combustion Network for heavy-duty diesel engine sprays. A satisfactory agreement with SANDIA's experimental data demonstrated that the simulations can correctly capture the spray processes.
2D simulations were then performed using the same approach and compared with the optical spray measurements obtained from the GUCCI (Ghent University Combustion Chamber I) setup. Significantly higher penetration predicted by simulation implied that the current approach cannot reproduce the marine diesel spray processes and thus needs to be improved. A quantitative analysis of the different cases is made to seek possibilities for improvement.

Keywords
Marine diesel spray, CFD, Breakup models

Introduction

Pollutant emission standards in the shipping sector have been lagging behind those in for instance the automotive sector, as a result of which international shipping is now responsible for an emission of harmful NOx that is similar to the NOx emission of the whole of Europe [1]. In diesel engines the spray characteristics have a direct influence on the fuel conversion and formation of harmful substances. The fuel injection and atomization processes are extremely complex involving transient two-phase, turbulent flows at high pressures, with a wide range of temporal and spatial scales [2]. Pollutant formation is strongly affected by the state of mixing during the combustion process. The spray characteristics have a direct influence on the mixture formation and fuel conversion since they determine droplet size and positions. Studying diesel spray characteristics is therefore essential to optimize combustion in diesel engines.
Many experimental investigations of fuel spray characteristics are carried out in optically accessible constant volume combustion chambers, like the Sandia Combustion Vessel (SCV) [3], the Spray Combustion Chamber (SCC) of Wärtsilä Switzerland [4] and the Ghent University Combustion Chamber I (GUCCI) [5, 6]. Using Computational Fluid Dynamics (CFD) is today becoming increasingly necessary in the optimization of the in-cylinder processes of internal combustion engines. The detailed modelling of the spray is a prerequisite for the accurate calculation of ignition, combustion and pollutant formation.
In the present work, 2D simulations are performed using the OpenFOAM® code together with Lib-Engine, which is a set of libraries and solvers developed by the Internal Combustion Engine group of the Politecnico di Milano [7]. In the simulations, the blob method [8] is used as the injection model, and the Kelvin-Helmholtz and Rayleigh-Taylor (KH/RT) [9] model is adopted for the breakup of liquid fuel. The capabilities of the proposed method are first validated by simulating experimental studies in the Sandia Combustion Vessel [10, 11]. Then, the same method is employed to simulate the conditions typically for medium speed marine diesel engines. Experimental measurements obtained on the GUCCI setup are used to evaluate the computational results.

Computational Models

The Eulerian-Lagrangian approach is employed to model the fuel spray. In this approach, the conservation equations for the continuous gas phase are solved in a Eulerian way, and for the description of the disperse phase (droplets) the Lagrangian methodology is used. Additional phenomenological sub-models are then needed to describe the processes occurring with the droplets. The computational sub-model for droplet break-up in this work is the blob-KH/RT model. The blob method was developed by Reitz and Diwakar [8], and assumes that the injected liquid jet is represented by large spherical blobs. The diameter of these blobs equals the nozzle hole diameter and

their number is determined from the mass flow rate. The Kelvin-Helmholtz instability model is used to predict the primary break-up of the intact liquid core of the diesel jet, while the secondary break-up of individual drops is modelled with the KH model in conjunction with the Rayleigh-Taylor accelerative instability model [4].
According to the stability analysis of the Kelvin-Helmholtz model, the injected liquid jet breaks up due to its interaction with the gas as it penetrates, yielding a core which contains relatively large drops. The drop radius of the newly formed droplet, r_{new} , is assumed to be proportional to the wavelength Λ_{KH} of unstable waves. The radius of the new droplets and the wavelength can be obtained from:

$$r_{new} = B_0 \cdot \Lambda_{KH} \tag{1}$$

$$\frac{\Lambda_{KH}}{r_0} = \frac{9.02(1+0.45\sqrt{Z})(1+0.4\,T^{0.7})}{(1+0.865We_g^{1.67})^{0.6}} \tag{2}$$

where

$$Z=\frac{(We_l)^{0.5}}{Re_l},\ T=Z\,(We_g)^{0.5},\ We_g=\frac{\rho_g r_0 u_{rel}^2}{\sigma},\ We_l=\frac{\rho_l r_0 u_{rel}^2}{\sigma},\ Re_l=\frac{\rho_l r_0 u_{rel}}{\mu_l} \tag{3}$$

$B_0 = 0.61$ is a constant. Z ,We, Re, T , σ , u_{rel} , ρ, μ_l and r_0 are respectively the Ohnesorge number, the Weber number, the Reynolds number, the Taylor number, the surface tension, the relative velocity magnitude between the two-phases, the density, the liquid viscosity and the radius of the undisturbed liquid jet. More details about the KH/RT model can be found in the work by Beale et al. [9] and Patterson et al. [12]. It can be seen from equations (1)-(3) that the breakup process is strongly influenced by the Reynolds and Weber numbers of the injected liquid jet.
The reduction rate of the liquid jet radius and the breakup time (τ_{bu}) are expressed as

$$\frac{dr}{dt} = -\frac{r_0 - r_{new}}{\tau_{bu}} \tag{4}$$

$$\tau_{bu} = 3.788 \cdot B_1 \frac{r}{\Lambda \cdot \Omega} \tag{5}$$

$$\Omega = \frac{0.34+0.38We_g^{1.5}}{(1+Z)(1+1.4\cdot T^{0.6})}\left(\frac{\sigma}{\rho_l r_0^3}\right)^{0.5} \tag{6}$$

Where Ω is the growth rate of the most unstable surface wave and B_1 is an adjustable model constant including the influence of the nozzle hole flow on spray break-up. The value of B_1 =10 is chosen for the present study.
For the gas phase, the mass, momentum and energy equations are solved for a compressible, multi-component gas flow using a RANS (Reynolds Average Navier-Stokes) approach. For this work, the standard k – ϵ model was chosen for the modelling of turbulence in the spray simulation.

Test cases

Validation of the computational models is performed using three sets of measurement data. Case 1 and Case 2, measured in the Sandia Combustion Vessel (SCV) within the ECN (Engine Combustion Network), correspond to heavy-duty engines. Case 3 is representative of medium-speed marine engines and was measured [13] in the GUCCI setup. Due to its physical properties and similar reaction chemistry to diesel fuel, n-dodecane was chosen as reference fuel. In order to provide more accurate boundary conditions, a computer model [14] of the pump-line-nozzle (PLN) injection system was developed using Simcenter Amesim and validated using the GUCCI setup. Figure 1 shows the injection velocity profile of Case 2 and Case 3. A summary of the conditions used in this work is listed in Table 1.
Lucchini et al.[7] investigated the spray-mesh-turbulence interactions for evaporating sprays at engine conditions and concluded that the best results are provided by a mesh size which is five times greater than the nozzle diameter. A grid independence test has been conducted for the 2D simulations in this work according to the conclusion above. Accounting for the size of the combustion chamber and the nozzle diameter, a mesh with 11664 cells was chosen for Case 1 and Case 2, and a mesh with 2592 cells was used for Case 3.

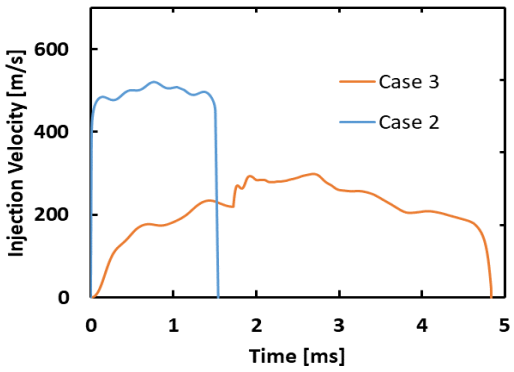

Figure 1. Injection velocity profile of Case2 and Case 3

Table 1. Conditions for test cases

	Case 1	Case 2	Case 3
Facility	SCV	SCV	GUCCI
Injection system	Common rail	Common rail	Pump-Line-Nozzle
Application	Automotive	Automotive	Marine
Fuel	n-dodecane	n-dodecane	n-dodecane
Nozzle diameter [mm]	0.0837	0.0894	0.4400
Injection duration [ms]	1.5	1.5	4.8
Injected fuel mass [mg]	3.33	3.83	111.90
Ambient Temperature (K)	900	700	700
Ambient density (kg/m^3)	23.01	22.80	22.50

Results and discussion

Figure 2 presents the comparison of numerical results against experimental data in terms of vapor and liquid penetration for Case 1. The employed spray model is able to describe the spray penetration history, though the numerical result of liquid length is about 10% higher than the measurement.

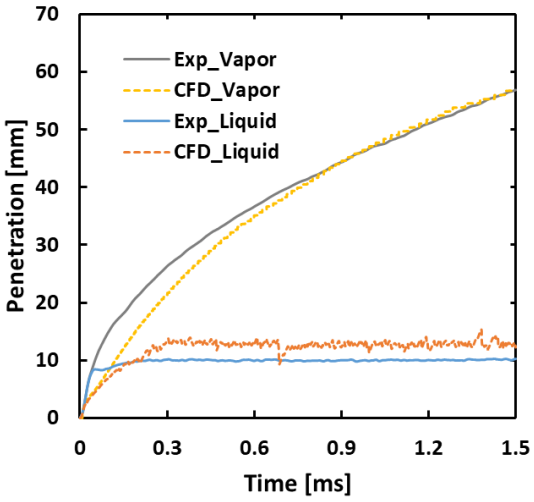

Figure 2. Numerical and measured penetrations for Case 1.

Since the vapor penetration measurement for Case 2 is not available in the ECN database, Figure 3 only compares the liquid penetration. There is generally good agreement between simulations and measurements, except for an underestimation in the early stage (0 – 0.2 ms).
As seen in Figure 4, the simulation for Case 3 overestimates both the vapor and liquid penetration significantly. This also means that the simulation underestimates the spray disintegration process.

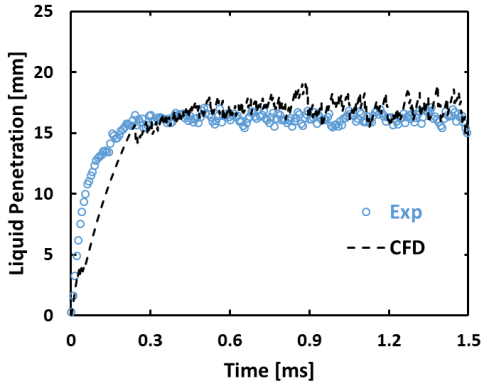

Figure 3. Numerical and measured liquid penetrations for Case 2.

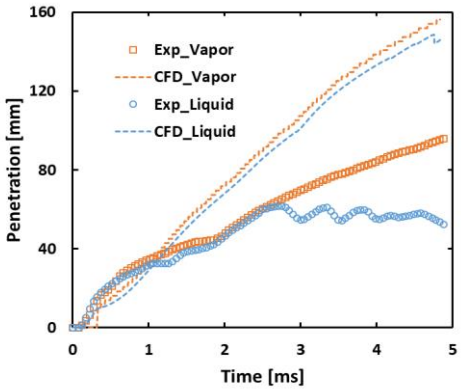

Figure 4. Numerical and measured penetrations for Case 3.

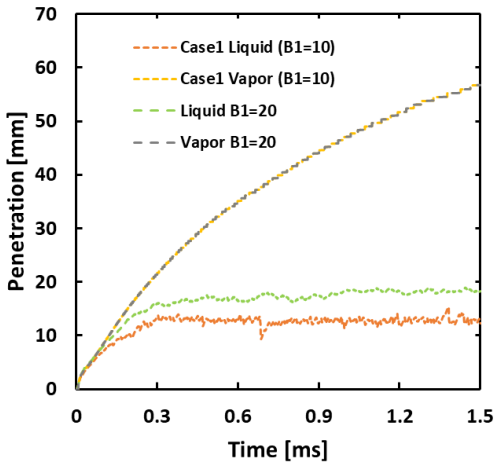

Figure 5. Effect of B_1 on penetrations for Case 1.

The effect of model constant B_1 in equation (5) is investigated. Figure 5 illustrates the effect of the break-up constant B_1 for Case 1. The liquid phase shows a significant sensitivity to the break-up constant, while the vapor penetration is slightly different. A higher value of B_1 results in reduced break-up and increased penetration, while a smaller value leads to increased spray disintegration and reduced penetration. The result here is consistent with the work by Patterson et al.[12]. However, the comparison for Case 3 from Figure 6 shows that the penetration length is less sensitive to this constant than in Case 1.

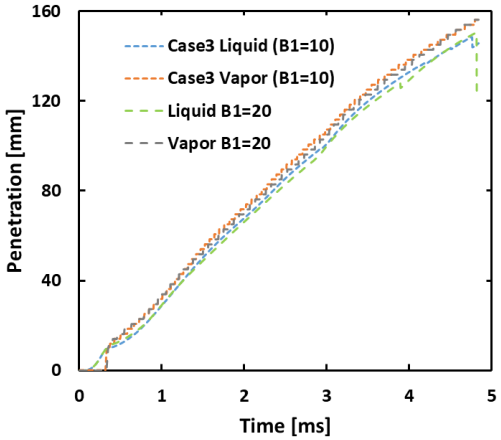

Figure 6. Effect of B_1 on penetrations for Case 3.

In the following part of this section, the applicability of the blob-KH/RT model to marine diesel spray simulation is discussed. As seen in Table 1, the ambient temperatures of Case 2 and Case 3 are the same, and the ambient gas densities for the two cases are similar. The main differences between Case 2 and Case 3 are the initial injection conditions, which represent automotive engines and medium speed marine engines, respectively. Therefore, the discussion below focuses on Case 2 and Case 3.

In order to make quantitative comparisons of the two cases above, some reasonable assumptions are made:

- Fluid properties (density, viscosity) of n-dodecane at the nozzle exit are constant values (713 kg/m^3 for density and 0.001 kg·m^{-1}·s^{-1} for viscosity) during the injection process.
- Surface tension at the liquid-gas interface at the nozzle is 0.02 kg/s^2 according to Liu and Reitz [15].
- The velocity of the ambient gas is much smaller than the fuel injection velocity , so $U_{inj} \approx u_{rel}$.

Based on these assumptions, the liquid Weber number (We_l), Reynolds number (Re_l) and Ohnesorge number Z at the nozzle hole exit can be calculated. Using the injection velocity profile of Case 2 and Case 3, the liquid Weber number and Reynolds number are obtained and shown in Figure 7 and Figure 8, respectively. Compared to Case 2, the Reynolds number of Case 3 is much higher, while the Weber number is lower at the onset of the injection.

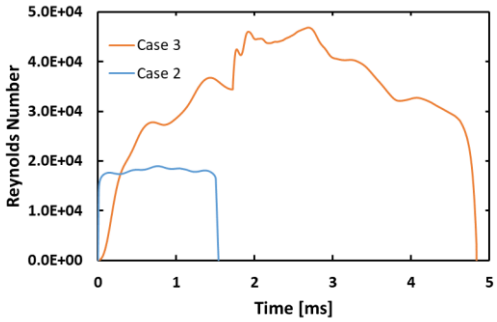

Figure 7. Reynolds number for Case 2 and Case 3.

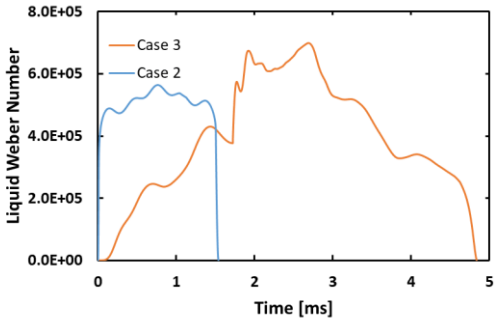

Figure 8. Liquid Weber number for Case 2 and Case 3.

The Ohnesorge numbers, which are not related to the injection velocity, are 0.0396 (Case 2) and 0.0178 (Case 3). In marine diesel engines, the nozzle diameter of injectors is normally of the order of 0.1 mm and larger, which is

about an order of magnitude larger than in automotive applications. From equation (3), a lower value of the Ohnesorge number leads to a smaller value of the RHS (right-hand side) term of equation (2), which results in reduced breakup. Meanwhile, the initial droplets (undisturbed liquid jet) diameter of Case 3 is rather large, so the newly formed droplets evaporate very slowly. Moreover, a lower injection velocity leads to a smaller value of gas Weber number (equation 3), which results in a slow growth rate Ω of the most unstable surface wave according to the theoretical analysis given by Reitz et al. [16, 17]. The discussion above reveals that at relatively low speeds the liquid fuel does not break up easily.

Figure 4 also shows that the simulation predicts a faster penetration than the measurement, which is mainly caused by the primary breakup being too slow in the simulation. Baumgarten [18] summarized four possible mechanisms of primary break-up: aerodynamics induced (KH model) break-up, turbulence induced break-up, cavitation induced break-up and velocity relaxation induced break-up. Usually, more than one mechanism occurs simultaneously and cannot be clearly separated from each other. The simulation and measurement for Case 3 demonstrate that the aerodynamics induced break-up is not the dominating mechanism in medium speed marine engines. The model should be improved to include other possible breakup mechanisms.

Conclusions

In this work simulations based on the blob-KH/RT model, representative of heavy-duty engines and medium-speed marine engines, have been performed. A satisfactory agreement with SANDIA's experimental data demonstrated that this approach can correctly capture the spray processes in automotive diesel engines. However, the over-prediction of penetration by the simulation implies that the blob-KH/RT is incapable of modelling marine diesel sprays with a relatively low Ohnesorge number. It is concluded that a modification of the current model is needed, accounting for the high Reynolds and low Weber numbers for accurate prediction of diesel sprays in marine engines.

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Nomenclature

r_{new}	newly formed droplet radius [m]
r_0	droplet radius of undisturbed liquid jet [m]
Λ_{KH}	wavelength [m]
Z	non-dimensional Ohnesorge number [/]
T	non-dimensional Taylor number [/]
Re_l	non-dimensional Reynolds number of liquid jet [/]
We_l	non-dimensional Weber number of liquid jet [/]
We_g	non-dimensional Weber number of gas [/]
ρ_g	density of gas [kg/m^3]
ρ_l	density of liquid jet [kg/m^3]
σ	surface tension [kg/s^2]
μ_l	dynamic viscosity [N•s/m^2]
u_{rel}	relative velocity [m/s]
U_{inj}	injection velocity [m/s]
D	injector nozzle diameter [m]
Ω	growth rate of most unstable wave [s^{-1}]
τ	characteristic time scale [s]

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