

Modelling of Fuel Injector In-Nozzle Cavitation and Early Spray Breakup Using a Multiphase Volume of Fluid Method

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Abstract

Fuel injector in-nozzle flow and early spray breakup is modelled using a compressible, multiphase Volume of Fluid Large Eddy Simulation implemented in the OpenFOAM environment. The volume fraction transport equations for liquid, vapour and gas phases are reformulated to include phase change source terms. These terms are modelled using the cavitation formulation by Schnerr, which is extended to eliminate non-physical mass transfer rates. The numerical method is validated by comparing the simulated mass flow rates, pressure and liquid volume fraction distributions at different cavitation conditions against published experimental data. Favourable comparison between simulations and experiments is achieved with minor discrepancies attributable to uncertainties in fuel properties and assumptions made in numerical models. Applications of the code to simulation of in-nozzle phenomena and primary breakup of the injected spray from a sharp edged nozzle reveals that in-nozzle flow separation, wall shear and cavitation contribute significantly to the fragmentation of the jet.

Introduction

Modern diesel engines comprise multiple systems that govern complex combustion processes. The characteristics of combustion in the engine chamber has direct effects on the overall efficiency and emission of diesel engines. One of the main factors contributing to an efficient combustion process is the degree to which the diesel spray is atomised. The atomisation of a diesel spray can be attributed to interaction with ambient gas and in-nozzle flow characteristics such as flow separation and cavitation. In this study, characteristics of in-nozzle flow particularly the onset of flow separation and cavitation which are often considered to be the main reasons for primary breakup [11] are numerically investigated.

In many experimental studies [1, 3], the onset of cavitation in diesel injectors has been reported to enhance atomisation of the emerging diesel spray and increase the dispersion angle. For a nozzle with a sharp inlet, the high pressure gradient and fluid inertia cause the flow to separate and form a region of contracted flow. This reduces the effective area and creates a recirculation zone in which pressure can reduce to, or below vapour pressure. Cavities generated after the sharp entrance can accumulate along the nozzle wall and may extend to the nozzle exit. Depending on the relative length of the cavities and nozzle, vapour bubbles may collapse outside of the nozzle exit enhancing jet breakup. However, there are situations where flow separation and cavitation can result in complete detachment of fluid flow from the nozzle wall. In those cases, air can be drawn into low pressure regions of the nozzle, resulting in hydraulic flip. Upon the occurrence of hydraulic flip, the in-nozzle flow does not experience wall shear. Consequently, the effect of wall shear minimises and spray atomisation may be suppressed, which leads to a narrower spray [12].

Recently, implementation of the Volume of Fluid (VOF) method for prediction of primary spray breakup with the effects of in-nozzle flow has been reported by Ghiji *et al.* [4]. As compared to homogenous [10], Eulerian-Lagrangian Coupling [5] and two fluid models [6], the VOF method is advantageous because it is able to capture a sharp liquid-gas interface in a volume conservative manner. The incompressible two-phase VOF method has also been integrated with cavitation models to study internal nozzle cavitation and its effects on the emerging spray by Marcer *et al.* [7]. However, in diesel engines, liquid fuel, fuel vapour and air can often co-exist in the chamber and phase change due to either cavitation or evaporation occurs exclusively between fuel and vapour. Also, the injection of fuel may exceed the speed of sound in the gas phase within the chamber due to high injection pressure. Modelling the diesel spray atomisation therefore falls into the framework of compressible multiphase flow with phase change. Thus, the main objective of the present study is to develop a compressible multiphase VOF method with cavitation modelling capability for improved diesel spray simulations.

Description of the VOF Approach

For a multiphase flow with phase change, transport equations for all phases can be given as:

$$\frac{\partial(\rho_l \alpha_l)}{\partial t} + \nabla \cdot (\rho_l \alpha_l U_l) = \dot{m} \quad (1)$$

$$\frac{\partial(\rho_v \alpha_v)}{\partial t} + \nabla \cdot (\rho_v \alpha_v U_v) = -\dot{m} \quad (2)$$

$$\frac{\partial(\rho_i \alpha_i)}{\partial t} + \nabla \cdot (\rho_i \alpha_i U_i) = 0 \quad (3)$$

where \dot{m} is the phase change mass transfer rate, subscripts l and v represents the liquid and vapour phases respectively, while i represents the phases that do not take part in the phase change process. The rate of mass exchange can be expressed as:

$$\dot{m} = \dot{m}^+ - \dot{m}^- \quad (4)$$

The rate of condensation \dot{m}^+ and vaporisation \dot{m}^- of the liquid phase on the phase interface is modelled by Schnerr and Sauer model [8]:

$$\begin{cases} \nabla \cdot (\alpha_l U_l) + \nabla \cdot (\alpha_v U_v) + \nabla \cdot (\alpha_i U_i) = \nabla \cdot U(a) \\ \nabla \cdot U = - \left(\frac{\alpha_l}{\rho_l} \left[\frac{D\rho_l}{Dt} \right] + \frac{\alpha_v}{\rho_v} \left[\frac{D\rho_v}{Dt} \right] + \frac{\alpha_i}{\rho_i} \left[\frac{D\rho_i}{Dt} \right] \right) + \dot{m} \left(\frac{1}{\rho_l} - \frac{1}{\rho_v} \right) \end{cases} (b) \quad (5)$$

Detailed implementation of this model is discussed in the next section. By adding and subtracting $\nabla \cdot (\alpha_l U)$ on the LHS of equation (1-3), expanding the convection terms and utilising equation (5), the final form of the multiphase transport equations comprising phase change source terms can be obtained. For simplicity, only the transport equation for the liquid phase is shown:

$$\begin{aligned}
& \frac{\partial \alpha_i}{\partial t} + \nabla \cdot (\alpha_i U) + \nabla \cdot (\alpha_i \alpha_v (U_i - U_v) + \alpha_i \alpha_l (U_l - U_i)) \\
&= -\frac{\alpha_l}{\rho_l} \left[\frac{D\rho_l}{Dt} \right] (1 - \alpha_i) + \alpha_i (\nabla \cdot U) + \alpha_i \left[\frac{\alpha_v}{\rho_v} \frac{D\rho_v}{Dt} + \frac{\alpha_l}{\rho_l} \frac{D\rho_l}{Dt} \right] \\
&+ \dot{m} \left(\frac{1}{\rho_l} - \alpha_i \left(\frac{1}{\rho_l} - \frac{1}{\rho_v} \right) \right)
\end{aligned} \tag{6}$$

The present study employs VOF with Large Eddy Simulation (LES) turbulence modelling. The VOF-LES is based on a mathematical model composed of governing equations for the conservation of mass and momentum of a multiphase system, accredited to De Villiers *et al.* [2]. This system comprises three immiscible, compressible fluids and accounts for the surface tension between them. Details of the VOF-LES formulation can be found in previous work [4].

Schnerr and Sauer Model

The Schnerr and Sauer model is based on bubble dynamics derived from the generalised Rayleigh-Plesset equation. In the present study, a phase change limiter $\max(1 - \alpha_l - \alpha_i, 0)$ is added to eliminate unbounded volume fractions caused by physically unrealistic condensation and vaporisation rates. The modified Schnerr and Sauer model is defined as:

$$\begin{cases}
\dot{m}^- = \frac{3\rho_l \rho_v}{\rho} \alpha_i \max(1 - \alpha_l - \alpha_i, 0) (rR_b) \\
\quad * \sqrt{\frac{2}{3\rho_l (|p - p_v| + 0.001p_v)}} \min(p - p_v, 0) \\
\dot{m}^+ = \frac{3\rho_l \rho_v}{\rho} \alpha_i \max(1 - \alpha_l - \alpha_i, 0) (rR_b) \\
\quad * \sqrt{\frac{2}{3\rho_l (|p - p_v| + 0.001p_v)}} \max(p - p_v, 0)
\end{cases} \tag{7}$$

The inverse of the cavitation nuclei radius R_b^{-1} is related to α_l , α_i and bubble density n by:

$$R_b^{-1} = \left(\frac{4\pi n \alpha_l}{3(\max(1 - \alpha_l - \alpha_i, 0) + \alpha_{nuc})} \right)^{\frac{1}{3}} \tag{8}$$

where the nucleation site volume fraction:

$$\alpha_{nuc} = \frac{n\pi (d_{Nuc})^3}{6 + n\pi (d_{Nuc})^3} \tag{9}$$

is used to avoid division by zero. In the present study, bubble diameter d_{Nuc} is set as $0.1 \mu\text{m}$ (20% of the smallest mesh size $0.47 \mu\text{m}$) and bubble density n is set to $2.0 \times 10^9 \text{ cm}^{-3}$ based on the suggestion of Schnerr *et al.* [8].

Validation of the Numerical Model

The experimental data from Winklhofer *et al.* [13] is used for a comprehensive model validation. In the work of Winklhofer *et al.*, measurements are taken for diesel fuel passing through a $300 \mu\text{m}$ thick square channel where the injection pressure is fixed at 100 bar and the back pressure is varied to change the extent of cavitation from inception through to choked flow. The channel has an inlet width of $301 \mu\text{m}$ and is slightly converging through a length of $1000 \mu\text{m}$ to give an outlet width of $284 \mu\text{m}$. Detailed geometry for the square channel used in the present study can be found in [13]. Fuel inlet is set at the left end of the geometry, while a simplified non-reflective pressure outlet is applied to the right

end. The remaining face patches of the computational domain are configured to be no-slip and adiabatic walls with a zero-gradient boundary condition for all hydrodynamic variables. Cavitation is normally characterised by a global cavitation number (CN) commonly defined as:

$$CN = \frac{p_{inj} - p_{out}}{p_{out} - p_v} \tag{10}$$

Detailed properties of the fuel and operating conditions are given in Table 1.

Parameter	Value
Injection pressure p_{inj}	100 bar
Fuel	n-dodecane
Fuel density ρ_l	832 kg/m ³
Fuel dynamic viscosity	0.0065 N s/m ²
Surface tension	0.03 N/m
Vapour density ρ_v	0.1361 kg/m ³
Vapour pressure p_v	2000 Pa
Vapour dynamic viscosity	5.953×10^{-6} N s/m ²
Temperature	304 K
Ambient pressure p_{out}	30-80 bar
Cavitation number	0.25-2.33
Max velocity	150 m/s
Fuel Reynolds number Re	1817-5452

Table 1: Fuel properties and boundary conditions based on experimental setup [13].

Kolmogorov scale representing the smallest turbulence scale of the flow can then be estimated using the following formulation:

$$\eta = \frac{W}{(Re)^{\frac{1}{4}}} \tag{11}$$

where W is the channel outlet length and μ the dynamic viscosity of the liquid phase and Re is the liquid phase Reynolds number. However, a single Kolmogorov scale cannot be determined due to density variation in a compressible flow. Thus, only the liquid phase Kolmogorov scale is evaluated to be $0.47 \mu\text{m}$ because liquid fuel is relatively incompressible compared to air and vapour. The mesh is constructed by layering elements from the nozzle wall with a minimum size of $0.5 \mu\text{m}$ and a growth rate of 1.05 as shown in Figure 1. In total 6×10^6 hexahedral elements are used.

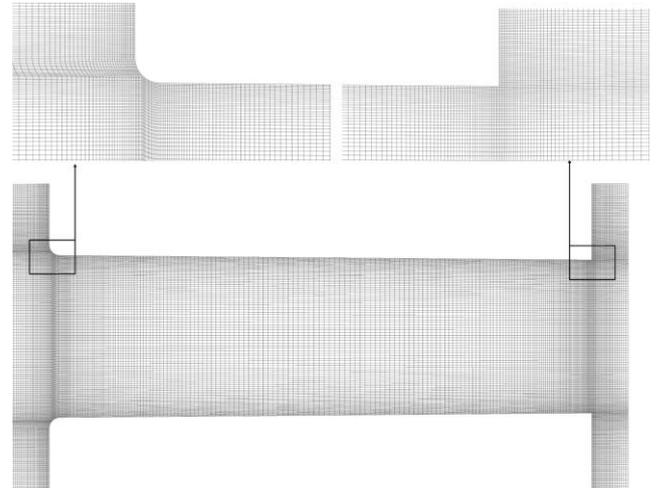


Figure 1: Computational domain for the square channel showing grid refinement at the inlet and outlet corners.

Comparison of simulated and measured mass flow rates at different flow conditions are presented in Figure 2. The developed

numerical model captures the effect of pressure on mass flow rates with favourable accuracy. The trend that mass flow rate increases almost linearly with increasing difference between injection and back pressures is also well captured. When the difference between injection and back pressures has exceeded 70 bar, both experiment and simulation show that further reducing the back pressure has only a minor effect on the rate of injection. This is because, at $\Delta p = 70$ bar, the flow has become choked (e.g. mass flow rate does not increase with decrease in back pressure).

Both the simulation and experiment demonstrate reduction in pressure downstream of the channel entrance before cavitation inception, as shown in Figure 3. The extent of the low pressure region simulated is consistent with experimental measurements. Cavitation inception occurs when the back pressure is set to 40 bar (Figure 3(b)). As the back pressure decreases, vapour cavities start to form in the recirculation zone and accumulate along the channel wall. At 30 bar back pressure the flow is fully choked and complete flow separation from the channel entrance occurs (Figure 3(c)). Deviation between simulations and experiments, in terms of extent and morphology of the cavitation, can be attributed to uncertainties in fluid properties and omission of surface imperfections on the round entrance and channel wall in the numerical model. These uncertainties, however, are difficult to eliminate in numerical simulations due to limited computing power.

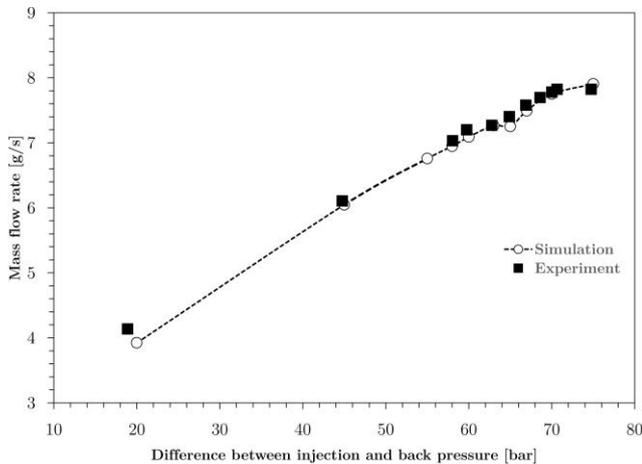


Figure 2: Comparison of simulated and measured mass flow rates at different back pressure conditions.

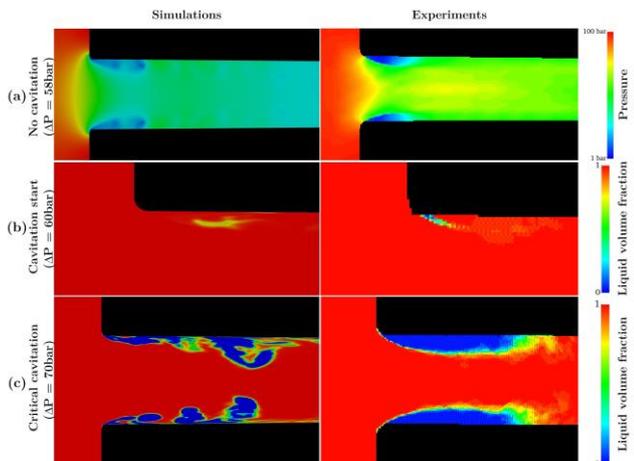


Figure 3: Comparison of contour plots of simulated (time averaged) and measured (averaged over 20 images) pressure and liquid volume fraction distributions in the channel at $\Delta p = 58, 60$ and 70 bar.

Characterisation of nozzle flow and primary breakup

Experimental conditions summarised in Ghiji *et al.*[4], relevant to a non-evaporating spray injected into a constant volume chamber

from a sharp edged nozzle are simulated. The properties of the diesel fuel and vapour, except for the temperature and Reynolds number, are given in Table 1. The ambient region (chamber) is non-reactive and initially filled with compressed air at 30 bar. The computational domain representing a diesel injector including the sac, nozzle and a portion of the chamber is shown in Figure 4. Boundary conditions are similar to the experimental setup of Ghiji *et al.* [4]. However, due to the lack of detailed knowledge of the time varying pressure profile in the injector sac, the pressure at the sac inlet is assumed to increase linearly from 30 bar to 600 bar in 100 μ s.

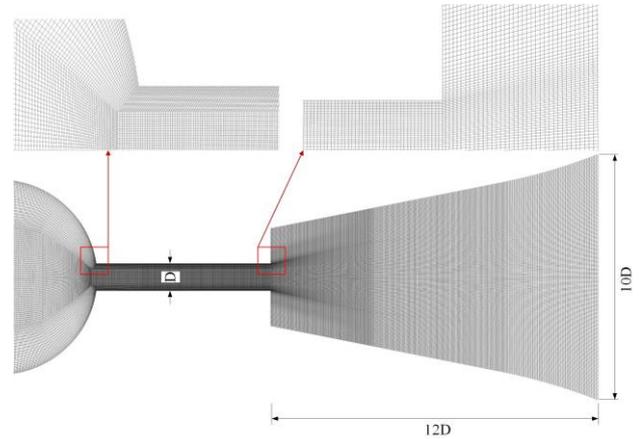


Figure 4: Dimensions and mesh topology for the computational domain. Refined hexahedral elements of $0.7 \mu\text{m}$ (based on Kolmogorov scale for the developed spray) are distributed in the nozzle at the wall. The mesh size increases gradually from the nozzle with a grow rate of 1.02. In total, 12×10^6 hexahedral elements.

The penetrating spray and the nozzle flow are represented in Figure 5 by a liquid volume fraction isosurface ($\alpha = 0.9$) coloured by velocity magnitude. At $19 \mu\text{s}$ After Start of Injection (ASOI), the emerging spray predicted by the two models is of similar shape. The mushroom like structure at the leading edge is the result of interaction of the compressed air ahead of the penetrating tip and the liquid jet. Surface instabilities start to develop at the edge of the mushroom structure and only minor disturbances are observed on the liquid surface. At $20 \mu\text{s}$ ASOI, a ring of cavitation bubbles is predicted by the cavitation model in the separation region near the nozzle entrance. By $37 \mu\text{s}$ ASOI aerodynamic forces start to strip small scale structures such as liquid ligaments and droplets from the liquid surface in the wake and at the edge of the 'mushroom'. At this stage, cavities that formed earlier at the nozzle entrance and developed in-nozzle turbulence begin to emerge from the nozzle exit. The collapse of the cavitation bubbles and the in-nozzle turbulence enhance surface instabilities on the jet. The non-cavitating code predicts a much less disturbed exiting jet. However, the opposite trend is observed after the occurrence of complete flow detachment when wall shear disappears in the cavitation simulation at $56 \mu\text{s}$ ASOI. After transition to hydraulic flip, the cavitation model predicts that the spray dispersion is narrowed and there is an intact liquid core leaving the nozzle exit. The near wall region is completely filled with mixtures composed of liquid, vapour and ambient gas which are connected to the chamber. At this stage the non-cavitating code captures a more turbulent exiting jet than the cavitation models. This is attributed to the persistent presence of wall shear which introduces turbulent disturbances on the surface of the jet.

Sectional contour plots of diesel volume fraction, total pressure and rate of condensation at $37 \mu\text{s}$ ASOI showing details of the collapse region of the jet are shown in Figure 6. Once cavities extend outside the nozzle exit, they collapse within the liquid jet with pressure recovery. However, low pressure regions appear

where cavities collapse. This may be attributable to liquid inertia and cavity oscillations. Localised low pressure regions and convex surface protrusions are observed to correlate spatially with regions of high vapour condensation rate. The presence and collapse of cavities within the liquid jet creates pressure gradients, as observed by Schnerr *et al.*[9]. The presence of collapsing cavitation bubbles within the emerging jet suggests they play a role in the greater development of surface instabilities and breakup in the cavitating cases compared with the non-cavitating despite the presence of turbulence.

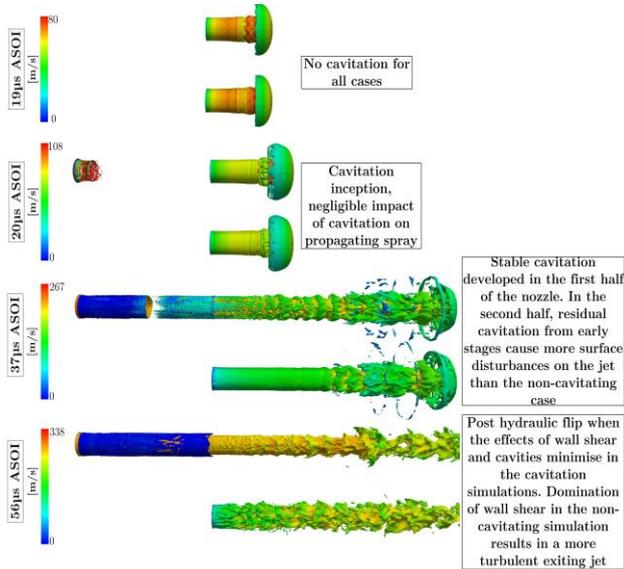


Figure 5: Penetrating spray represented by a liquid volume isosurface ($\alpha = 0.9$) coloured by velocity magnitude. Top: Schnerr, Bottom: Non-cavitating.

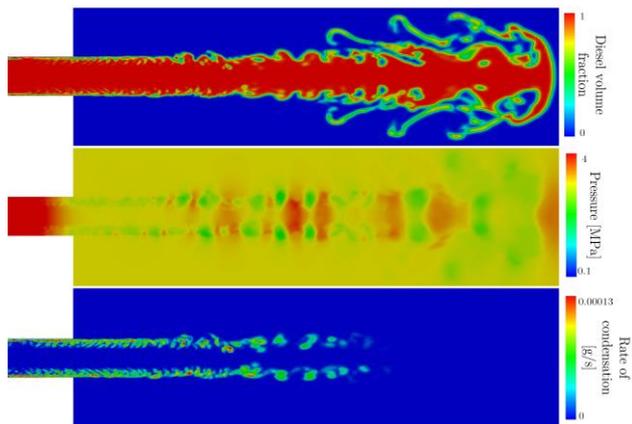


Figure 6: Sectional contour plots of diesel volume fraction, total pressure and rate of condensation at 37 μ s ASOI. Localised low pressure regions and convex surface protrusions are observed to correlate spatially with regions of high vapour condensation rate.

Conclusions

The onset of in-nozzle cavitation and its effects on the morphology and breakup of the early spray are successfully modelled using a compressible multiphase VOF cavitation LES code. The numerical simulations reveal that:

- The pressure in the contraction region can reduce to vapour pressure, leading to vaporisation of fuel and formation of vapour cavities.

- Vapour cavities forming at the nozzle inlet can grow to an extent that detaching bubbles collapse within the liquid jet after exiting the nozzle, enhancing jet breakup.
- Apart from in-nozzle flow separation and cavitation, another important factor contributing to the primary breakup of the spray is the wall shear experienced by the jet in the nozzle.

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