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Simulating the effect of in-nozzle cavitation on liquid atomisation using a three-phase model

M.G. Mithun*[,1], P. Koukouvnis[1], I. K. Karathanassis[1], M. Gavaises[1]

[1]*City, University of London, UK*

Abstract

The aim of this article is to present a fully compressible three-phase (liquid, vapour, air and mixture) cavitation model and its application to the simulation of in-nozzle cavitation effects on liquid atomization. The model employs a combination of barotropic cavitation model with an implicit sharp interface capturing Volume of Fluid (VoF) approximation. The results from the simulation is compared against the experimental results obtained by (1) for injection of water into air from a step nozzle. Large Eddy Simulation (LES) model is utilized for resolving turbulence. Simulations are performed for a condition where developing cavitation is observed. Model validation is achieved by qualitative comparison against the available images for the cavitation, spray pattern. The model predictions suggest that the experimentally observed void inside the nozzle is not purely vapour but a mixture of both vapour and back-flowing air. The simulation also identified a periodic air entrainment that occurs at developing cavitation condition which further improves primary atomization.

Keywords: three-phase flow; cavitation; Volume of Fluid; Large Eddy Simulation; atomization

Introduction

Many researchers in the past have reported that the in-nozzle flow has a major influence on the spray formation. Among geometric and other in-nozzle flow features, cavitation has the major effect on the spray. Despite knowing this fact, there are only very few numerical studies available in literature where the interaction between cavitation and spray is considered (2,3). Most of the studies either consider only the in-nozzle flow with/without cavitation or the primary/secondary atomization without cavitation.

In past, models based on approaches such as the Eulerian-Lagrangian (4,5) and Eulerian-Eulerian (6,7) or their combination (8,9) were widely utilized for modelling spray atomization. Their choice purely depends on the physics sought, Lagrangian based models are best suited at lean spray modelling and the fully Eulerian models are proved to be better for dense spray predictions. Another popular approach is the interface tracking methods such as the VoF (10,11) which is useful when many topological changes such as interface pinching and merging occurs and the interface motion are to be tracked accurately.

For modelling cavitation, heterogeneous models which consider the non-equilibrium between the phases and the homogeneous mixture models (12) where the slip between the phases is neglected are widely utilized. Models that solve transport equation for the secondary phase with appropriate mass transfer terms (13) and the single-fluid approach which uses an equation of state (EoS), to relates density with pressure and temperature or pressure alone (barotropic) are the most popular of homogeneous models. The barotropic models, based on the assumption of pressure equilibrium and infinite mass transfer between the phases are best suited for complex simulations owing to their simplicity and numerical stability (14).

In order to numerically study the effect of in-nozzle flow on primary atomization, a model that can handle the transport and interaction between the three phases present, namely liquid, vapour and air, is required. There are only very few studies available in the literature which deal with such problem and they are typically an extension of an existing cavitation model (15,16). An alternative approach for modelling the co-existence of three-phases is by employing the Volume of Fluid (VoF). To the author's knowledge, there are five studies available in literature, that attempted to link a two-phase VoF model with a cavitation model for studying the in-nozzle effects on atomization (2,3,17–19). These models differ in the way cavitation and compressibility is treated. A linear barotropic model with VoF was used for modelling atomization in a gasoline injector by (2). A comparative study of two transport-based cavitation models with application of VoF can be found in (19) for atomization occurring from a single solid cone injector. Further studies that assume the phases to be incompressible can be found in (3,17).

In this study, we present a compressible three-phase model which considers compressibility of both the mixture and pure phases, using non-linear isentropic relations. Such a consideration in compressibility is essential to capture the

*Corresponding Author, Mithun MG: mithun.murali-girija@city.ac.uk

nonlinear effects of the flow even when phase change is not dominant. All the three-phase models available in literature and presented above, consider the phases to be incompressible or assume linear compressibility. To the best of author's knowledge, this is the first work to consider a non-linear compressible model in conjunction with VoF and LES for studying primary atomization.

1. Three-Phase Model

The cavitation model used in this study is a piecewise barotropic function employing three different equations corresponding to liquid, liquid-vapour mixture and vapour phases. The Tait equation of state is used for modelling liquid ($\rho \geq \rho_l$); the pure vapour phase ($\rho < \rho_v$) is modelled using the isentropic gas equation and the equation for the mixture phase ($\rho_v \leq \rho \leq \rho_l$) is derived by integrating Eq- 1.1 with respect to mixture density for an isentropic process, using the Wallis speed of sound; the reader can refer to (14) for the detailed derivation:

$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s \qquad \text{Eq- 1.1}$$

where c is the speed of sound, and α is the volume fraction.
Combination of the individual equations of state with the assumption of the homogeneous equilibrium, results in Eq- 1.2 for a two-phase mixture:

$$p = \begin{cases} B\left[\left(\frac{\rho}{\rho_l(T_l)}\right)^N - 1\right] + p_{sat,l} & \rho \geq \rho_l \\ \frac{c_v^2 c_l^2 \rho_l \rho_v (\rho_v - \rho_l)}{c_v^2 \rho_v^2 - c_l^2 \rho_l^2} \ln\left(\frac{\rho}{c_l^2 \rho_l (\rho_l - \rho) + c_v^2 \rho_v (\rho - \rho_v)}\right) + p_{ref} & \rho_v \leq \rho \leq \rho_l \\ C_{vap} \rho^\kappa & \rho < \rho_v \end{cases} \qquad \text{Eq- 1.2}$$

In Eq- 1.2, B is the bulk modulus, $\rho_{sat,l}$, $p_{sat,l}$ and N are the saturation density, saturation pressure and the stiffness of the liquid, respectively. The parameter p_{ref} in the mixture equation is tuned to ensure continuous variation of density between the liquid and mixture phases. C_{vap} is the constant of the isentropic process and κ is the heat capacity ratio for the vapour phase. The subscript m, v and l corresponds to mixture vapour and liquid phases, respectively.
The third phase, i.e. the non-condensable gas (air) is modelled using isentropic gas equation Eq- 1.3, and it is assumed to be immiscible with the barotropic fluid.

$$p = C_{gas} \rho^\gamma \qquad \text{Eq- 1.3}$$

where, C_{gas} is the constant of the isentropic process for air and γ is the heat capacity ratio for air. The thermodynamic properties of water, vapour and gas (air) along with the constants used in Eq- 1.2 and Eq- 1.3 are listed in Table 1.
The barotropic fluid and the non-condensable gas equations (Eq- 1.2 and Eq- 1.3) are then combined using an implicit VoF model to closure the interaction of the three-phase system. The discretization of the phase volume fraction is performed using the compressive scheme, similar to the CICSAM (Compressive interface capturing for arbitrary meshes) scheme of (20). The discretization of the governing equations used in this study is based on the finite volume approach as implemented in ANSYS Fluent v17.1. In the results that follows, the variables are made non-dimensional based on based on the mean velocity inside the nozzle ($V_n = 18.3\ m/s$) and the length of the bottom wall ($l_{ref} = 9mm$).

2. Test case and simulation setup

The experimental geometry and the computational domain used for the simulation are shown in Figure 1. Pressurized tap water at 293K is injected through the nozzle to ambient air at 1bar and then gravitated to a buffer tank. The computational domain is extended to model the ambient air as shown. A block structured mesh with appropriate refinement near the walls is used to ensure $y^+ < 1$. The initial estimate of the mesh resolution for LES is calculated based on the Kolmogorov and Taylor length scales (~0.84 µm and ~48 µm computed for the maximum injection pressure condition). At the inlet, the absolute pressure is set to 3bar which corresponds to a developing cavitation condition inside the nozzle. The outlet pressure is set to ambient (1bar).

3. Results and Discussion

The results are presented for an injection pressure ($p_{inj} = 3bar$) at which developing cavitation occurs inside the nozzle. The comparison of the in-nozzle cavitation and the near-exit spray formation between the experimental result

*Corresponding Author, Mithun MG: mithun.murali-girija@city.ac.uk

(1) and the present simulation is shown in Figure 2. The asymmetry in geometry initiates cavitation inside the nozzle with more cavitation occurring from the lower wall compared to the upper wall. The results presented in Figure 2 confirms that the liquid jet atomizes faster on the cavitating side of the step nozzle as more ligaments and droplets are formed on this side. Compared to the experiments, the numerical simulation shows the entrainment of ambient air moving backwards inside the orifice and the total void seen inside the nozzle is a mixture of vapour and gas as highlighted in the Figure 2. This could be the case in experiment as well, however differentiating between the gaseous and vaporous cavitation during experiments is still an open question. The comparison of the void fraction and spray pattern shows a good match between the experimental result and simulation.

The evolution of the spray at developing cavitation condition is shown Figure 3. The formation of mushroom head during the early stages of the spray development due to the aerodynamic instabilities and the initial droplet formation from the periphery of the mushroom can be seen from Figure 3(a, b). The relative velocity difference between the water and ambient air initiates the Kelvin-Helmholtz instabilities at the interface. However, their effects on jet disintegration is limited due to the high density ratio between the two fluids in the present study (ratio of liquid over air density ~ 1000) in line with the observations of (21). As the time progress, the flow inside the nozzle becomes turbulent, and the interaction the turbulent structures with the liquid-air interface initiates the disintegration of the jet core, Figure 3d. At the same time, the sheet cavity formed at the inlet edge of the bottom wall quickly transforms into small vortices that are transported downstream by the flow. The variation in vortex transport velocity causes these vortices to merge together to form vapour clouds. The presence of the low-pressure cloud at the exit produce a pressure gradient across the interface that pulls the ambient air into the nozzle. A strong primary atomization and a sharp increase in spray cone angle is observed during this event, Figure 3(e, f). The entrained gas pushes the liquid away from the wall causing a restriction to the flow, a reduction in spray width and an increase the jet velocity is associated with this. An effect of which can be seen in Figure 3i towards the end of the domain. Subsequently, the pressure build-up caused by the flow restriction pushes the entrained gas back, recovering the flow area. An increase in atomisation and spray width is again observed during this event. The entrainment of the air in this case is a cyclic process and its frequency depends on the dynamics of the cavitation.

4. Conclusions

This paper presents a fully compressible three-phase model developed by utilizing a barotropic cavitation model along with a sharp interface VoF approach with application of LES for resolving turbulence. The simulations result is compared against the experimental result from (1) and further utilized to enhance the understanding of the complex interaction between the in-nozzle flow and primary atomization. It is identified that the main in-nozzle effects that influences the primary atomization are the cavitation, air entrainment and the liquid turbulence. In addition to that, aerodynamic forces further assist the atomisation process to a smaller extent. The capability of the model to distinguish between the vapour and air has revealed that the voids reported in the experiment is not entirely vapour but a mixture of vapour and entrained air. A periodic phenomenon of air-entrainment is observed at developing cavitation condition which is found to enhance the atomisation process. From the results obtained, it can be stated that developing cavitation is a favourable condition for better primary atomization. However, a detailed study on the erosion occurring at this condition is required before making a conclusion, as high erosive potential vapour cloud generation due to vortex merging is observed at this condition.

Table 1: Thermodynamic properties for water, vapour and gas at 20^oC.

Liquid Properties			Vapour properties			Gas Properties		
B	3.07	GPa	C_{vap}	27234.7	Pa/(kg/m^3)	C_{gas}	75267.84	Pa/(kg/m^3)
N	7.15	--	κ	1.327	--	γ	1.4	--
$\rho_{sat,L}$	998.16	Kg/m^3	$\rho_{sat,V}$	0.0173	Kg/m^3			
$C_{sat,L}$	1483.26	m/s	$C_{sat,V}$	97.9	m/s			
$P_{sat,L}$	4664.4	Pa	$P_{sat,V}$	125	Pa			
μ_L	1.02e-03	Pa s	μ_V	9.75e-06	Pa s	μ_g	1.78e-5	Pa s
Surface tension	*0.0728*	*N/m*						

*Corresponding Author, Mithun MG: mithun.murali-girija@city.ac.uk

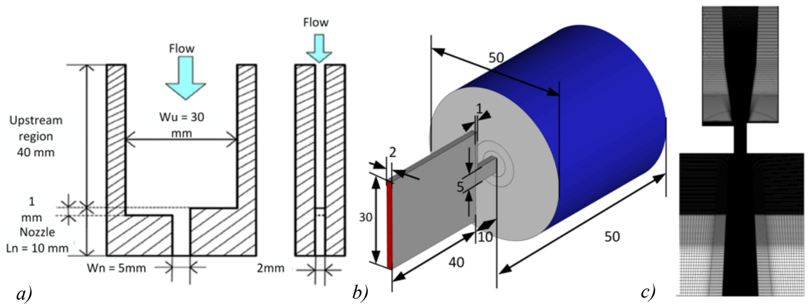

Figure 1: a) Step- Nozzle geometry as reported in (1) b) Computational domain c) the numerical grid used for LES.

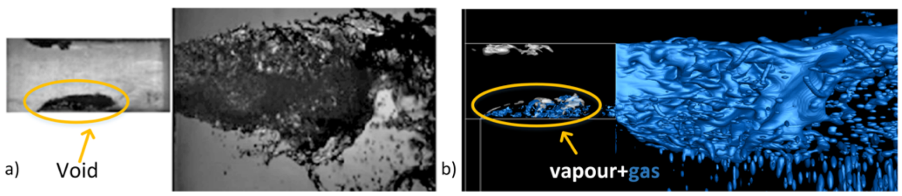

Figure 2: Comparison of in-nozzle cavitation and near-exit spray formation between experimental results from (1) and current numerical study at 3 bar inlet pressure. Iso-surfaces of 50% vapour (white) and 95% gas(blue) are shown.

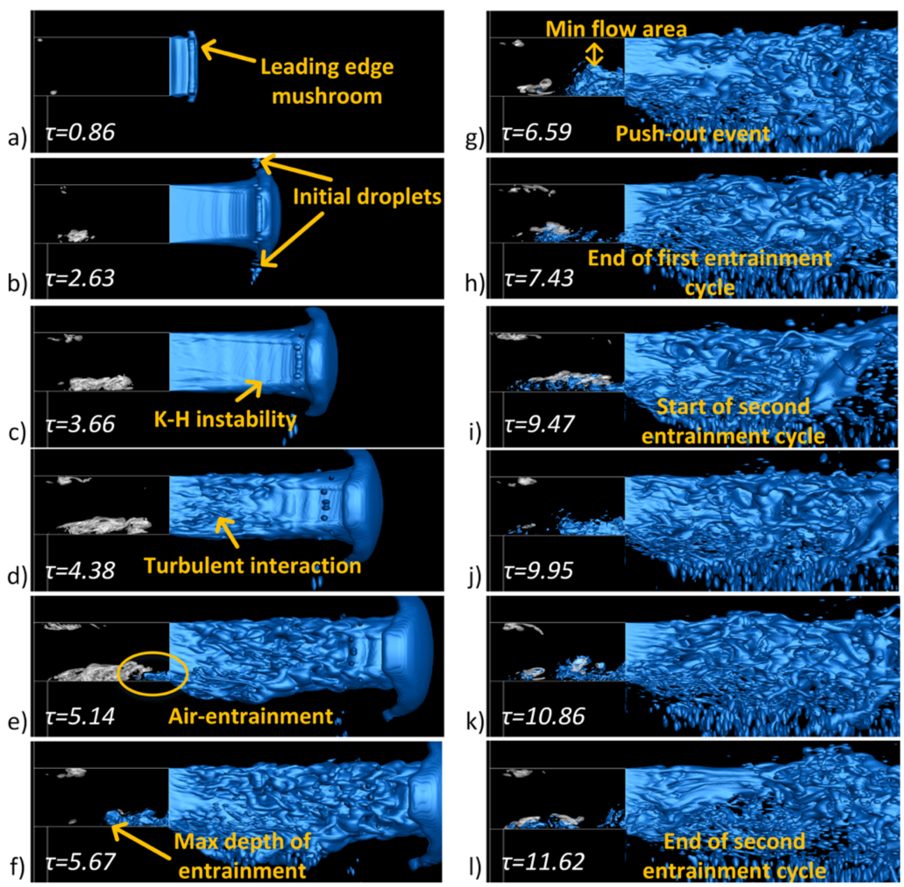

Figure 3: Evolution of in-nozzle cavitation and liquid jet at P_{inj}=3bar. Iso-surfaces of 50% vapour (white) and 95% gas (blue) volume fraction shown. The instances are chosen randomly over time to highlight the major events.

*Corresponding Author, Mithun MG: mithun.murali-girija@city.ac.uk

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*Corresponding Author, Mithun MG: mithun.murali-girija@city.ac.uk