

Large Eddy Simulation of GDI Single-Hole Flow and Near-Field Spray

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ABSTRACT

The improvement of spray atomization and penetration characteristics of GDI multi-hole injector sprays is a major component of the engine combustion developments, in order to achieve the fuel economy and emissions standards. Significant R&D efforts are directed towards optimization of the nozzle designs, in order to achieve optimum multi-objective spray characteristics.

The Volume-of-Fluid Large-Eddy-Simulation (VOF-LES) of the injector internal flow and spray break-up processes offers a computational capability to aid development of a fundamental knowledge of the liquid jet breakup process. It is a unique simulation method capable of simultaneous analysis of the injector nozzle internal flow and the near-field jet breakup process. Hence it provides a powerful tool to investigate the influence of nozzle design parameters on the spray geometric and atomization features and, consequently, reduces reliance on hardware trial-and-tests for multi-objective spray optimizations.

This publication reports investigations of a single, axisymmetric nozzle-hole, pertinent to GDI multi-hole injector nozzle geometry, with the aid of the current state-of-the-art VOF-LES method. The focus of the study is the influence of nozzle design and geometric features on the plume structure and its primary break-up process. Specifically, the influence of nozzle length-to-diameter ratio (l/d), counter-bore, and nozzle tapered geometry on the jet primary breakup are studied. Analysis of alternative nozzle geometries reveal the influence of marked influence of nozzle shape and l/d ratio on the nozzle flow structure, hydraulic efficiency and the jet breakup characteristics. There is marked influence of flow separation and hydraulic flip in the nozzle hole for amplification of the Kelvin-Helmholtz instabilities and the jet breakup length.

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INTRODUCTION

The optimization of the multi-hole GDI injector spray characteristics (atomization, spray plume cone angle, spray plume penetration, etc.), within the constraints imposed by engine geometry (e.g. avoidance of spray impingement on all solid surfaces) is a crucial component of the combustion system optimization to meet the fuel consumption and emission objectives [1].

The GDI multi-hole injector must fulfill several requirements: (1) precise fuel metering (with a uniform or defined hole-to-hole flow rate distribution), (2) precise spray plume geometric features (spray targeting geometry, etc.), and (3) required atomization characteristics (plume cone angle, spray droplet-size distribution, etc.). The simultaneous fulfillment of these requirements renders design optimization

of the GDI injector valve group for a specific combustion chamber geometry a non-trivial and often iterative process. This complexity owes to the coupling of the injector fuel metering, spray targeting and atomization characteristics, as a result of the influence of the nozzle geometry on all features of the spray. Currently, the GDI injector seat / nozzle design draws on significant empirical knowledge, developed through experimental valve-group Design-of-Experiment programs. The major drawback of this method, apart from the cost and time requirement, is the difficulty to investigate one aspect of the spray characteristics in isolation (without affecting other spray features) in order to establish a direct and conclusive correlation. One approach to address this complexity and establish an understanding of the relationship between the seat / nozzle geometry and the spray geometry / characteristics

is through application of advanced computational fluid dynamic (CFD) methods.

Over the recent two decades, there has been significant recognition of the influence of the injector valve group design on the flow structure within the injector nozzle and the subsequent liquid jet primary breakup and atomization characteristics. The nozzles representative of the diesel fuel injectors have received the most intensive R&D attention, leading to identification of multiple fluid dynamic phenomena as influential factors that affect the spray primary breakup, including the cavitation [2, 3, 4, 5], turbulence [6, 7, 8] and vortices [9, 10, 11] that form upstream or within the nozzle hole. It is notable that often these phenomena are concurrent and coupled, for instance the cavitation or coherent vortices can markedly influence the nozzle velocity distribution as well as promoting turbulence levels.

The GDI multi-hole injector valve-group and spray atomization is receiving more attention [12, 13, 14], in line with the broad adoption of direct injection for gasoline engines as well as advances of the GDI combustion system (e.g. the adoption of injector center-mount layout for the homogenous combustion systems) and the more stringent requirements on fuel economy and emissions, especially the particulate number emission target under consideration. The experimental data shows dependence of the spray plume structure and atomization on the geometry of the GDI multi-hole nozzles, in addition to expected influence of the of pintle-sac geometry (owing to its influence on the flow upstream of the nozzle hole). In this respect, despite the conceptual similarity with the diesel injectors, it is expected that the differences in the GDI nozzle geometry (in particular the small nozzle length-to-diameter (l/d) ratio) and operation pressure (hence the rate of acceleration and nozzle-exit liquid jet velocity) are significant to render the key nozzle fluid dynamic and breakup features different than the diesel injector nozzles. For example, it is expected that the short nozzle l/d renders the jet breakup characteristics sensitive to the nozzle entrance flow conditions and occurrence of the hydraulic flip phenomenon [13]. The implication is that an accurate computational analysis of the flow within the injector valve-group is an integral component of the analysis of the spray near-field breakup and atomization characteristics.

The VOF-LES method for analysis of the jet breakup process has been under development and verification over the past decade. The capability of the method has been broadly demonstrated [15, 16, 17, 18], although in all cases, the injector internal flow domain was excluded and the liquid jet VOF-LES simulations were performed with assumed nozzle-exit flow conditions (with imposed disturbances, to represent turbulent fluctuations). The importance of the nozzle-exit flow condition on the jet breakup was investigated in the DNS 'numerical experiments' of Sander and Weigand [19] that demonstrated significant influence of the issuing jet velocity profile and turbulence disturbances on the jet primary breakup. The recent combined VOF-LES and spray

imaging studies of the GDI conical and planar-sheet liquid jet atomization [20,21] incorporated the valve-group/nozzle into the computational domain, in order to couple the injector internal flow with the jet primary breakup process, and to alleviate the uncertainty / complexity associated with prescribing the nozzle-exit stationary (varying in time and space) velocity conditions. These simulations provided good quantitative prediction of the jet breakup process (e.g. the Kelvin-Helmholtz instability wave length) and demonstrated (1) the strong dependence of the spray geometry and atomization characteristics on the details of the nozzle geometry, and (2) the capability of the VOF-LES method to capture the effect of nozzle design on the jet primary breakup structure. Therefore, the VOF-LES of the injector valve-group internal flow and near-field primary breakup offers a useful tool for investigation of the GDI multi-hole specific seat-nozzle design / geometric features and the associated effect on the liquid plume structure and its primary break-up.

This paper describes studies of the valve-group (seat and nozzle) flow and the near-field breakup of full-cone liquid jets from a single hole (axisymmetric) injector, using thru-hole with counterbore type nozzles, carried out with the aid of the multi-fluid VOF-LES method. The valve-group geometry, in terms of the seat geometric features (sac geometry, pintle stroke, etc.) and the nozzle geometry (nozzle size, l/d, counter-bore, etc.) are representative of the GDI multi-hole injector. The paper presents VOF-LES simulation of the seat-nozzle flow and near-field jet breakup for alternative nozzle geometries, that are the subject of current interest including varying nozzle hole l/d, counter-bore and the tapered nozzle hole geometry, in order to investigate their specific influence on the jet primary breakup characteristics. A comparison of the simulation results with the round jet breakup/atomization theories [6, 8] is provided.

THE COMPUTATIONAL METHOD

CONSERVATION EQUATIONS OF MULTI-PHASE SYSTEM

The mathematical modeling practice is similar to De Villiers et al [22]. It comprises of the transport equations for the conservation of mass and momentum of a two-phase flow system, comprised of two immiscible, compressible or incompressible Newtonian fluids, including the surface tension. The single set of conservation equations that describe the flow of a two-phase mixture are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0 \quad (1)$$

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U \otimes U) = -\nabla P + \nabla \cdot \tau + \int_{S(t)} \sigma \kappa \delta(x - x') ds \quad (2)$$

Where, U is the velocity, ρ is the density, σ is the surface tension coefficient, τ is the stress tensor, κ is the curvature of the liquid surface, n represents a unit vector normal to the liquid surface, and $\nabla \cdot ()$ and $\nabla \cdot ()$ denote the gradient and the divergence operations, respectively.

The integral term in equation (2) represents the momentum source due to surface tension: it is effective at the interface of the liquid surface $S(t)$ over the entire liquid volume. This is an important source term in the numerical simulation of the liquid jet breakup process. The evaluation of this term is achieved through the Continuum Surface Force (CSF) model of Brackbill et. al. [23] as:

$$\int_{S(t)} \sigma \kappa \delta(x - x') ds \approx \sigma \kappa \nabla \alpha \quad (3)$$

Where α is the “volume -of-liquid” phase-fraction, which is obtained from solution of a transport equation, and κ is the “curvature of the interface”, estimated from the solution of the phase-fraction α as:

$$\kappa = \nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right) \quad (4)$$

Equation (4) is valid for cases with constant surface tension, as in the case of present study. In case of variable surface tension, e.g. in case of spatially non-uniform composition or temperature distribution, surface tension gradients are encountered that generate additional shear stress at the interface that must be taken into account.

LARGE-EDDY-SIMULATION METHOD

The VOF-LES equations are derived from equations (1), (2), (3), through a process of local volume averaging of the phase-weighted hydrodynamic variables. This entails decomposition of the dependent variables into resolvable and computational sub-grid scales of turbulent fluctuations, and application of a filter that removes the sub-grid scale fluctuations from the direct numerical simulation. The filtering process, in conjunction with the non-linear term in equation (2), produces additional terms, involving correlations of the hydrodynamic variable fluctuations at sub-grid scales that require closure with the aid of mathematical models. The most notable of these terms is the Sub-Grid-Scale (SGS) stress tensor that represents the effect of unresolved scales of turbulence on the momentum transport process and its viscose dissipation.

The Sub-Grid-Scale (SGS) stress is defined as:

$$\tau_{sgs} = \overline{U(t)U(t)} - \overline{U}(t)\overline{U}(t) \quad (5)$$

Where $U(t)$ is the instantaneous resolved velocity field. The closure of the SGS stress is effected through a sub-grid-scale “eddy-viscosity” model as:

$$\tau_{sgs} = \frac{2}{3} \kappa \mathbf{I} - \frac{\mu_{sgs}}{\rho} (\nabla \overline{U} + \nabla \overline{U}^T) \quad (6)$$

Where κ is the SGS turbulence kinetic energy and μ_{sgs} is the SGS turbulent viscosity. These SGS turbulence parameters are obtained through solution of a transport equation for the SGS turbulence kinetic energy, according to Yoshizawa [24].

$$\frac{\partial \kappa}{\partial t} + \nabla \cdot (\kappa \overline{U}) = -\nabla \cdot [(v + v_{sgs}) \nabla \kappa + \tau_{sgs} \overline{U}] - \frac{1}{2} \tau_{sgs} : (\nabla \overline{U} + \nabla \overline{U}^T) - \varepsilon \quad (7)$$

Where $\varepsilon = C_\varepsilon \kappa^{3/2} / \Delta$ is the SGS turbulence dissipation rate, $v_{sgs} = C_\kappa \kappa^{1/2} / \Delta$ and Δ is the SGS length scale (equivalent to the local computational cell size). The turbulence model constants have the values $C_\kappa = 0.07$ and $C_\varepsilon = 1.05$, in accordance with Yoshizawa [24].

The additional SGS terms associated with the transport equations (2) which involve correlations of the sub-grid fluctuations of the phase-fraction, density, surface tension, etc., are all neglected in the absence of mathematical closure models, following the work of de Villiers et al [22].

VOF-BASED INTERFACE-TRACKING METHOD

The principle of the “Volume of Fluid” (VOF) approach is that a two- (or indeed multi-) phases system can be represented as a mixture of phases in which the phase-fraction distribution includes sharp, yet resolvable, transitions between the phases. Accordingly, the interface in a two-phase flow system is computed with the aid of the transport equation for the liquid volume fraction as the indicator function to locate the interface. The transport equation for the phase fraction α , for two incompressible fluids, is:

$$\frac{\partial \rho \alpha}{\partial t} + \nabla \cdot (\rho U \alpha) = 0 \quad (8)$$

According to the definition of α , the mixture thermo-physical properties are calculated as:

$$\rho = \alpha \rho_f + (1 - \alpha) \rho_g \quad (9)$$

$$\mu = \alpha \eta_f + (1 - \alpha) \mu_g \quad (10)$$

The VOF interface capturing/tracking method is a simple and flexible approach for simulation of multi-phase systems with free surfaces, especially for circumstances that the surface tension effects are not dominant. The main challenge of the VOF methodology relates to the accuracy of the numerical scheme, in order to assure that it simultaneously

provides the boundedness and conservation of the flow variables, and that the interface remains sharp, yet not affected by numerical dispersion and mesh alignment bias [25].

Of the several important numerical issues in simulation of free surface flows using the VOF method, the conservation of phase fraction, in conjunction with requirements for a non-diffusive interface capturing / tracking numerical method, are the most critical. In particular, this is important in case of flows with large density ratios, where small inaccuracies in volume fraction solution can lead to significant errors in calculation of physical and fluid-dynamic properties. In addition, especially in the case of free-surface flows, an accurate, non-diffusive phase-fraction solution is critical for proper evaluation of the surface curvature, which is required for determination of the surface tension force and the corresponding pressure gradient across the free surface.

In the present simulations, an advanced method formulated by Open-FOAM Ltd. [26] that adopts a two-fluid formulation of the conventional volume-of-fluid concept, within the frame-work of the finite-volume method, is used. The method employs a formulation of the phase transport equation that includes a "compression velocity" term [27] which acts to "compress" the VOF interface and maintain a sharp interface resolution. Appropriate numerical schemes are employed to ensure the bounded temporal/spatial discretization, and minimum mesh biasing, of the compression term and convection of the phase fraction transport equation, without numerical diffusion/dispersion of the liquid-gas interface.

A comparison of the VOF interface capturing /tracking and the numerical solution method in the Open-FOAM code with the alternative "Interface Reconstruction" scheme [28] for prediction of a Rayleigh jet breakup, provides closely similar predictions of the jet structure, breakup length and droplet size between the two computational methods, in close agreement with the measurements and theoretical analysis [28].

VORTEX EDUCTION METHOD

Identification of vortical coherent structures is an important component of computational flow visualization with the aid of Direct and Large-Eddy simulation methods. In the present study, the quantity Q is adopted for identification of vortex cores [29, 30]. The quantity Q is defined as:

$$Q = 1/2 * [\|W\|^2 - \|S\|^2] \quad (11)$$

Where W is defined as the anti-symmetric part of the velocity gradient tensor:

$$\begin{aligned} \|W\| &= [W : W]^{1/2} \\ W &= 1/2 * [\nabla \bar{U} - (\nabla \bar{U})^T] \end{aligned} \quad (12)$$

Where S is the local rate of strain tensor:

$$\begin{aligned} \|S\| &= 1/2 * [S : S]^{1/2} \\ S &= 1/2 * [\nabla \bar{U} + (\nabla \bar{U})^T] \end{aligned} \quad (13)$$

A large positive Q represents flow regions where the rate of strain is dominated by the rate of rotation. The use of Q (instead of the vorticity magnitude $\omega = |\nabla \times \bar{U}|$) is advocated, especially for identifying vortex cores in wall-bounded flows.

SEMI-EMPERICAL JET BREAKUP MODELS

The breakup of liquid jets has been the subject of fluid-dynamic enquiry and mathematical analysis for over a century. There exist various analytical-empirical relations, derived from the linear stability theory, to categorize the jet breakup regimes and to estimate the important parameters of jet breakup, such as the wave-length of the dominant jet-interface instability or the jet breakup length [6, 8, 37]. These relations solely rely on the aerodynamic parameters of the jet and do not take into account the nozzle geometry (e.g. l/d , nozzle entrance geometry, etc.) and the nozzle internal flow (e.g. jet velocity profile at nozzle exit). It is of interest to compare the VOF-LES simulation results with the available standard jet breakup analytical-empirical relations.

The relations for the jet-interface maximum growth-rate wave and its wave-length, derived from the round-jet linear stability analysis [6, 37] are given as:

$$\frac{\Lambda}{a} = 9.02 \frac{(1 + 0.45Z^{0.5})(1 + 0.4T^{0.7})}{(1 + 0.87We_{gas}^{1.67})^{0.6}} \quad (14)$$

$$\Omega \left[\frac{\rho_{liquid} a^3}{\sigma} \right]^{0.5} = \frac{(0.34 + 0.38We_{gas}^{1.5})}{(1 + Z)(1 + 1.4T^{0.6})} \quad (15)$$

With the dimensionless parameters defined as $Z = We_{liquid}^{0.5} / Re_{liquid}$, $T = ZWe_{air}^{0.5}$, $We_{liquid} = \rho_{liquid} a / \sigma$, $We_{air} = \rho_{air} a / \sigma$ and $Re_{liquid} = Ua / \nu_{liquid}$. U is the liquid jet relative velocity and $a (= 0.5d)$ is the jet radius.

The relations the round jet breakup length (in a quiescent ambient) L / a are derived from the Taylor's analysis of high-speed liquid jet breakup, as [8]:

$$L / a = B(\rho_{liquid} / \rho_{gas})^{0.5} / f(T) \quad (16)$$

With the parameter $B = 4.04$, recommended for typical diesel spray nozzles. The Taylor's parameter T and $f(T)$ defined as:

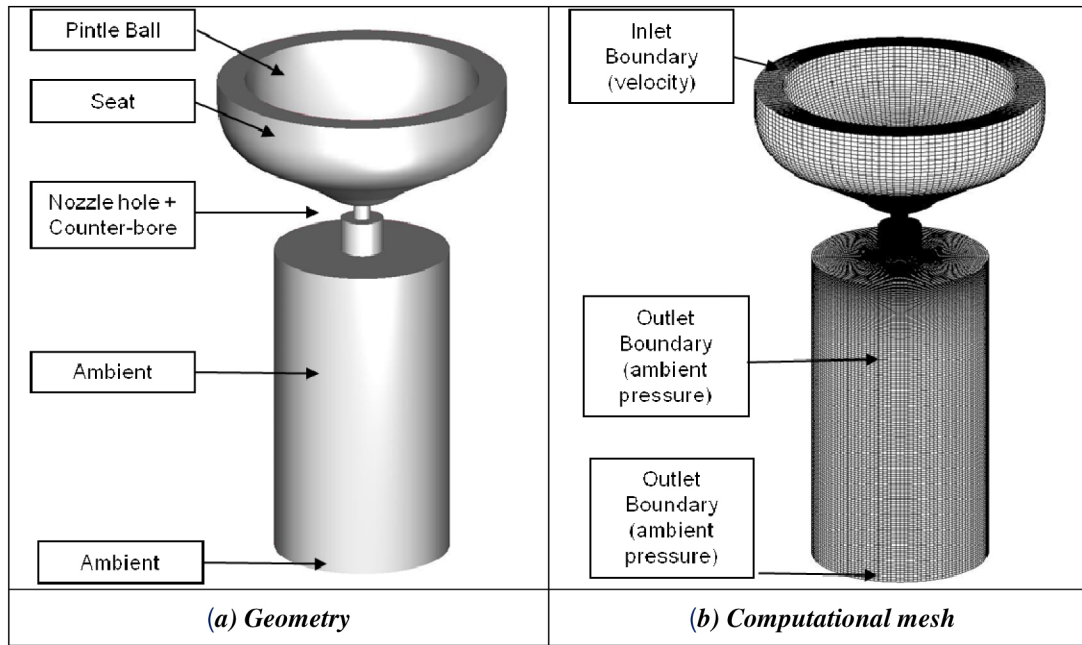


Figure 1. Computational domain, mesh and boundaries

$$T = (\rho_{liquid} / \rho_{gas})(Re_{liquid} / We_{liquid})^2 \quad (17)$$

$$f(T) = \sqrt{3} / 6 [1 - \exp(-10T)] \quad (18)$$

These relations are employed for calculation of the jet breakup parameters, for comparison with the VOF-LES simulation results.

THE NUMERICAL SOLUTION METHOD

All computations are performed using Open-FOAM [26] an open source finite-volume CFD tool-box. The solution method for the VOF-LES conservation equations in OpenFOAM incorporates a “compressive” formulation of the phase-fraction transport equation, employs special NVD/TVD and blend of central/upwind schemes for spatial discretization of the transport terms, and a blend of the Crank-Nicholson and Euler-implicit integration schemes for the phase-fraction and the governing conservation equations. The numerical method is intended to afford second-order spatial and temporal discretization / integration accuracy and to assure that the schemes are bounded and preserve the proper physical limits of the fluid dynamic variables.

The “pressure implicit with splitting of operators” (PISO) [31] algorithm, specifically suited to transient flows, is employed for coupled solution of the mass and momentum conservation equations, through coupling of the velocity and the pressure fields.

Computational Domain and Mesh

Figure 1 presents the three-dimensional computational domain that comprises the injector valve-group flow domain and its immediate near-field ambient. The computational mesh is of the order 2.5M cells (1.M cells within the injector domain and 1.5M cells within the ambient) and affords a spatial resolution in the range 2-5 μm (within the injector seat-nozzle) to 30 μm (within the far-field ambient). The topic of requisite mesh resolution in LES simulations is of notable importance: previous VOF-LES simulations of the injector valve-group geometries [20, 21] have demonstrated that this level of spatial discretization can provide quantitatively reliable numerical solutions. The numerical integration time-step is imposed by various stability criteria, and is of the order 1.E-9 second. The calculations pertain to the injector pintle at the full-open position: therefore, the LES results represent the transient development of the flow for the injector in full-open position.

The pintle motion is not included in the simulation, due to severe requirements of the VOF-LES method for mesh geometric quality (e.g. orthogonality, aspect ratio, etc.) that would not permit the extensive mesh deformation required to accommodate the pintle displacement (of order 60 μm). Hence, the transient simulation of the seat-nozzle flow development is performed on a fixed geometry mesh, without direct representation of the pintle motion. To this effect, the simulation initial condition is that the nozzle - from inlet to the pintle sealing band - is filled with liquid at rest (the rest of the computational domain is filled with stagnant air at ambient conditions). At start of the calculation ($t > 0$.) the liquid phase at the inlet boundary is accelerated to its final velocity (corresponding to the nozzle hole static flow for

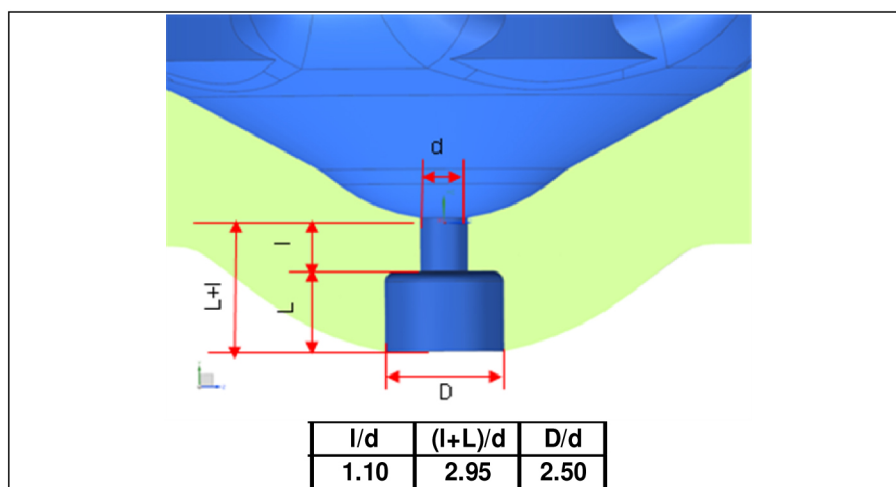


Figure 2. Nozzle geometry and dimensional parameters

20MPa fuel system pressure) over a short time interval (of order 5 μ s) and then is kept constant.

Boundary Conditions

In the present calculations, the liquid is n-Heptane at $T=293^\circ\text{K}$ temperature. The following boundary conditions are employed:

- Inlet: Uniform inlet velocity, as per the individual nozzle static flow for 20MPa fuel pressure (without imposition of artificial velocity disturbances),
- Outlets: Non-reflective, uniform static ambient pressure,
- Walls: zero-slip velocity condition, in conjunction with no treatments of the near-wall fluid-dynamic variables, except for imposing the zero-gradient condition, normal-to-wall, for the sub-grid-scale turbulent kinetic energy

The nozzles studied have different discharge coefficients; hence the imposed inlet velocity was adjusted to ensure a boundary static pressure of 20 MPa for all cases. Consequently, the relevant nozzle fluid-dynamic parameters (static flow, Re , We , etc.) are not identical. The choice of velocity boundary condition is for flexibility considerations (in anticipation of turbulent flow boundary conditions).

The outlet boundaries are at sufficient distance from the nozzle, to ensure minimum reflection of pressure disturbances that may influence the jet breakup process.

THE SIMULATION RESULTS

CASE 1: BASE NOZZLE GEOMETRY

The geometry and nozzle dimensions of the “Base” GDI nozzle are presented in Figure 2. The nozzle diameter ‘d’ is of order 0.2mm. This geometry is representative of the design features of the current production GDI nozzles that incorporate a “counter-bore” to achieve a small nozzle l/d ratio, irrespective of the seat thickness imposed by the structural integrity considerations.

Transient Jet Development

The transient development of the flow within the injector seat and nozzle is illustrated by the evolution of the iso-surface plots of $VOF=0.5$ (colored by the instantaneous velocity), at selected times after the start of simulation, in Figure 3. Figure 4 presents the corresponding VOF contour plots on a symmetry cut-plane through the geometry.

The transient nozzle flow is markedly affected by the entrapped air in the sac volume, beneath the pintle. The initial liquid jet is fully attached at entrance to the nozzle. The entrapment and discharge of the trapped air by the liquid causes formation of an attached liquid jet with an unsteady air core, as illustrated by the VOF iso-surface / contour plots for $t = 30\mu\text{s}$, $40\mu\text{s}$ and $50\mu\text{s}$. Also notable is the perfect axisymmetric structure of the flow within the nozzle, which is indicative of the high level of resolution and numerical accuracy of the solution. The VOF plots at $t=40\mu\text{s}$ already show the development of the liquid jet irregular instabilities within the immediate downstream of the nozzle exit.

With diminishing of the air entrapped in the sac volume and reduction of the jet core air volume flow rate, the liquid jet separates at the nozzle entrance edge and, owing to the short nozzle l/d , extends to the nozzle outlet. This causes ingestion of the ambient air into nozzle (which forms an air annulus that separates the liquid jet from the nozzle wall). The phenomenon is known as “hydraulic flip” and its occurrence is indicated in Figure 4, by the VOF plot at $t = 75\mu\text{s}$. The full establishment of the hydraulic flip takes between the $t=75\mu\text{s}$ and $t = 100\mu\text{s}$; thereafter the liquid jet is fully detached at the nozzle entrance and the ingested air penetrates the full nozzle length to form a complete hydraulic flip. This is the structure of the steady-state stationary turbulent jet that prevails for $t > 100\mu\text{s}$. This structure is very stable (no temporal or cyclic variation of the jet separation, velocity profile, occurrence of partial hydraulic flip, Kelvin-Helmholtz interface waves).