

Coupled LES Jet Primary Breakup - Lagrangian Spray Simulation of a GDi Multi-Hole Fuel Injector

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ABSTRACT

This paper presents results of a coupling of the Volume-of-Fluid Large-Eddy simulation (VOF-LES) of the jet primary breakup with a Lagrangian stochastic spray simulation of a GDi multi-hole injector. The objective is to assess the potential of replacing the phenomenological models of jet primary atomization with the stochastic parcel size - velocity data extracted from the VOF-LES analysis. The paper describes the methodology and assesses the predictive capability achieved, through comparison of the Lagrangian far-field spray simulation results with the complete experimental spray characterization data under the atmospheric ambient conditions.

The injector sac-nozzle flow and jet primary breakup simulation is performed with the Open-FOAM code. The simulation of the spray development processes - of propagation, evaporation and secondary atomization - is performed with the AVL-FIRE commercial CFD code adopting the standard Lagrangian discrete droplet method.

The comparison demonstrates good quantitative agreement for prediction of all significant far-field spray plume parameters, notably the trajectory, spread angle, tip penetration, foot-print pattern and the droplet-size probability distribution function.

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INTRODUCTION

The spray primary breakup is an important intermediate phase in the spray atomization process. It represents the disintegration of the continuum liquid jet issuing from the nozzle as a result of the specific velocity, turbulence and vorticity conditions imparted onto it by the seat-nozzle geometry and the aerodynamic interactions with the ambient air (the nozzle flow cavitation compounds this complexity). It also represents a major area of shortcoming in the current Lagrangian methods for the spray analysis: the process is represented by heuristic and semi-analytical mathematical models that cannot be directly verified with the aid of experimental data, owing to the difficulty of spray droplet-size distribution measurement in the optically-dense near-nozzle region [1].

The mathematical modelling of the processes that contribute to the primary atomization is challenging. There is increasing recognition of the substantial influence of the injector seat-nozzle geometry - and its fluid dynamic features - on the jet primary breakup structure and, thereof, the spray morphology and macroscale parameters [1,2,3,4,5,6]. These influences are evident in the substantial difference between the breakup characteristics of GDi multi-hole sprays and the diesel sprays, which in large part are due to the

seat-nozzle geometric features [2,3,4,5,6]. The available mathematical models of spray primary atomization are generally developed on the basis of the jet aerodynamic stability principles with additional phenomenological modelling account of the complex nozzle flow hydrodynamics (e.g. flow separation, turbulence, cavitation, etc.) [1, 7, 8].

In view of the experimental complexity to measure spray in the nozzle near-field region of primary atomization, it is impossible to ascertain the predictive capability of various primary atomization models available in the literature [1,7, 8]. Commonly, the primary and secondary atomization models are selected and their parameters are calibrated jointly based on the far-field spray macroscale data (e.g. the spray tip penetration). Therefore the predictive capability of the current primary atomization models cannot be established independently (excluding the plume cone angle, which is one verifiable output of some primary atomization models). In practice, absence of due attention to the nozzle flow complexities (e.g. flow separation within the nozzle hole) often results in an over-simplified description of the liquid jet condition (e.g. erroneous prescription of the velocity profile). This is a notable contributor to the inability of

the spray atomization models - verified under one set of test conditions - to correctly predict the effect of changes in the fuel pressure and/or ambient conditions.

One approach to improve the predictive accuracy of Lagrangian spray simulations is through the so-called Eulerian-Lagrangian method, in which Unsteady Reynolds-Averaged Navier-Stokes (URANS) multi-phase simulation of the injector seat-nozzle flow is performed to account for the real geometry influence on the liquid jet condition at the nozzle exit (velocity profile, turbulence, liquid / vapor phase fraction). This approach still requires use and parameter-set calibration of phenomenological models of jet primary atomization, in order to determine the spray initial conditions [8, 9]. Its advantage - over a geometry-drawn prescription of the jet velocity and turbulence profiles - is the proper account of the seat-nozzle geometry influence on the nozzle-entrance flow conditions and, thereby, the liquid jet velocity, turbulence and phase-fraction at the nozzle exit.

The motivation for the present work is the development and verification of a methodology - and its constituent components - for a fully 'predictive' spray simulation method for use in the conventional CFD simulations of the GDI in-cylinder spray pattern optimization. The ultimate objective is to enable complete simulation of the spray processes based on the seat-nozzle geometric data. This entails a CFD method for prediction of the seat-nozzle flow and jet primary atomization, with intrinsic capability to reproduce the influence of seat- nozzle geometry on the plume breakup and macro-scale characteristics. The subsequent droplet atomization (i.e. droplet breakup induced by the aerodynamic - mechanical instabilities) is viewed to be governed by simpler, more universal physics and likely amenable to accurate mathematical modelling.

The Large Eddy Simulation (LES) offers potential for a direct (i.e. without resort to mathematical models) simulation of the seat-nozzle flow and near-field jet primary break-up process. If its predictive accuracy is verified, it can fill a major missing block in the current Lagrangian stochastic discrete-droplet spray simulation methodology by providing an accurate description of the spray initial droplet size-velocity probability distribution. This would afford two key advantages: (1) a capability to properly account for the complex effects of nozzle geometry on the spray primary breakup, and, hence, the complete spray atomization process, and (2) a complete simulation tool-chain for analysis of all major elements of the spray atomization and transport processes.

The LES of liquid jet primary atomization has been the subject of significant development and verification over the past decade. The capability of the method, based on the VOF or the Level-Set methods, for prediction of the interface deformation and breakup due to the capillary and aerodynamic forces has been broadly verified [10,11,12,13,14]. In applications to high pressure jet breakup, VOF-LES studies of the GDI multi-hole spray have demonstrated the capability to capture the effect of nozzle geometry on the jet breakup structure and provide good quantitative prediction of the plume near-field macroscale parameters, verified through comparison with the near-field spray shadow-graphic and X-ray imaging data [4,5,6].

The quantitative analysis of the VOF-LES GDI plume primary atomization has provided physically realistic droplet size - velocity probability distribution functions [15].

This paper is a successor of the quantitative analysis of the VOF-LES GDI plume primary atomization [15]. It attempts to assess the predictive accuracy of VOF-LES jet primary atomization data as initial conditions for Lagrangian spray simulations. The predictive accuracy is assessed through comparison of the Lagrangian simulated far-field spray with the experimental spray characterization data. The study pertains to a purpose-build GDI seat design with three skew-angled nozzle holes. The time-integrated probability density functions of the nozzle near-field droplet size and velocity data, extracted from VOF-LES simulation [15] are used as stochastic initial conditions for a Lagrangian simulation of the spray processes with the AVL-FIRE CFD code [16], adopting the conventional discrete droplet model. A WAVE type model is used for the droplet breakup due to the droplet - air interactions. The simulated far-field spray droplet-size distribution, plume geometry, plume spread angle and the transient tip penetration under atmospheric ambient conditions are compared with the experimental data.

The objective of this study is to advance the previous work [15] by (1) development of a method for provision of the stochastic data from LES to the Lagrangian spray simulation method, (2) to verify that accurate definition of the near-field plume is sufficient for accurate prediction of the far-field spray geometry (i.e. the nozzle-exit droplet size-velocity pdf determines the plume propagation and dispersion), and (3) to indirectly evaluate the VOF-LES primary droplet-size distribution data, in the absence of experimental measurements, by examining the accuracy of the predicted temporal spray tip penetration and the far-field spray droplet-size distribution probability density function.

The good predictive accuracy of the method to simulate the complete far-field spray characteristics demonstrates that these objectives are fulfilled. The study shows that coupling of the VOF-LES with the Lagrangian method offers a feasible route towards a complete simulation tool-chain for a 'predictive' spray processes simulation method.

THE VOF-LES COMPUTATIONAL METHOD

A detailed description of the VOF-LES mathematical model and the numerical solution method employed here is available in the literature [4,5,6]. The methodology is formally identical to the VOF-based liquid interface tracking method in Open-FOAM [17, 18] used by various groups for the study of free-surface liquid breakup processes [12, 13]. However details of the numerical methods and the solution algorithms used may differ, with substantial implications for the numerical stability and accuracy of the solution.

In general, the challenges of the VOF-LES method application to liquid jet atomization problem are twofold: (1) those related to the LES method, notably the adequate spatial resolution, the suitable sub-grid-scale turbulence model and the solution numerical accuracy and (2) those associated with the interface capturing/tracking scheme and preserving a sharp interface in the presence of severe distortions.

deformation, stretching and tearing. The high computational resource requirement of the method is an additional constraint in its engineering application, requiring a judicial balance between the spatial resolution and the computational demand.

In the case of high pressure liquid jet breakup simulation, the spatial mesh resolution plays a critical role with respect to the length-scale of the smallest resolvable interface deformation. Consequently, the computational mesh size should satisfy resolution requirements with respect to both the flow Reynolds number (i.e. the turbulence scales) as well as the Weber number (i.e. the most unstable interface Kelvin- Helmholtz wavelength) conditions.

The topic of interface transport in two-phase flow systems has been the subject of numerous studies that have led to the development of multiple methods, all of which involve solution of a transport equation for a conserved variable which enables tracking and locating of the interface [19, 20, 21, 22, 23, 24 and the references cited therein]. One approach is the VOF method, originally devised by Hirt and Nicolas [20] and an alternative approach is the Level-Set method of Osher and Sethian [21]. In both cases, accurate solution of the interface transport equation requires sophisticated mathematical treatments and application of auxiliary schemes (such as the hybrid Particle-Level Set method [23]) in order to prevent loss of interface details [22,23,24]. A limitation of the Level-Set method for two-phase flow in complex geometries, such as the injector internal flow domain, is the constraint of the Cartesian computational mesh [11]. The advantage of the VOF method is the flexibility to handle complex flow domain geometry due to absence of restriction on the computational mesh topology (as long as mesh quality does not hinder accurate solution of the governing conservation/transport equations). The penalty it incurs -without use of interface reconstruction schemes such as the piece-wise linear interface construction ‘PLIC’ method [25] - is a more diffusive solution of the interface (i.e. loss of the interface sharpness [26]).

Conservation Equations of Multi-Phase System

The VOF-LES methodology used in the present analysis is limited to two-phase immiscible, incompressible flows and excludes a treatment of the flow cavitation. The mathematical model is composed of the governing equations for the conservation of mass and momentum of a two-phase flow system, comprised of two immiscible, incompressible Newtonian fluids, that includes the surface tension force. The set of conservation equations that describe the flow of the two-phase mixture are:

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

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

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, and n represents a unit vector normal to the liquid surface. The operators $\nabla(\cdot)$ and $\nabla \cdot (\cdot)$ 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 adopting the Continuum Surface Force (CSF) model of Brackbill et al [27] as:

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

Where α is the “volume-of-liquid” phase-fraction obtained from solution of a transport equation and κ is the “curvature of the interface” evaluated from the solution of the phase-fraction α .

Large Eddy Simulation Method

The VOF-LES equations are derived from equations (1) (2), (3), through a process of volume averaging of the phase-weighted hydrodynamic variables. This entails decomposition of the dependent variables into resolvable and irresolvable (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 viscous dissipation. The Sub-Grid-Scale (SGS) stress is defined as:

$$\tau_{sgs} = \overline{U(t) \cdot U(t)} - \overline{U}(t) \cdot \overline{U}(t) \quad (4)$$

Where $U(t)$ is the instantaneous resolved velocity field. The closure of the sub-grid-scale stresses is affected through a Smagorinski-Lilly eddy-viscosity model.

VOF Interface Tracking Method

The principle of the ‘Volume of Fluid’ (VOF) approach is that a two-phase 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:

$$\frac{\partial \rho \alpha}{\partial t} + \nabla \cdot (\rho U \alpha) = 0 \quad (5)$$

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

$$\rho = \alpha \rho_f + (1 - \alpha) \rho_g \quad (6)$$

$$\mu = \alpha \mu_f + (1 - \alpha) \mu_g \quad (7)$$

In the present simulations, an advanced method formulated in Open-FOAM [17] 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 [18] which acts to maintain a sharp interface resolution, without resort to interface capturing enchantment methods.

Numerical Solution Method

The numerical solution of the VOF-LES conservation equations is performed using Open-FOAM [17] an open-source finite-volume CFD tool-box. The solution method employs a blend of temporal and spatial discretization schemes to achieve second-order temporal and spatial numerical accuracy, and to ensure that the fluid dynamic variables remain bounded. The Numerical solution of the primitive-variable flow equations is obtained with a modified PISO algorithm [17]. It should be noted that details of the numerical solution method (discretization scheme, algebraic solver, residual error, etc.) exert significant influence on the stability, realizability and numerical accuracy of the VOF and the hydrodynamic field solutions.

Computational Domain and Mesh

Figure 1 presents a view of the purpose-built 3-hole GDi seat geometry, manufactured to have three identical flow holes and counter-bore nozzles, arranged with 120° circumferential spacing.



Figure 1. The purpose-built GDi seat design with 3 identical nozzles at uniform 120° circumferential spacing

Figure 2 provides a view of the nozzle-hole geometry and its dimensional parameters. The flow hole diameter ‘d’ is of the order O(0.2mm) and the nozzle geometric features (skew angle β , l/d, etc.) are representative of the current GDi multi-hole seat design.

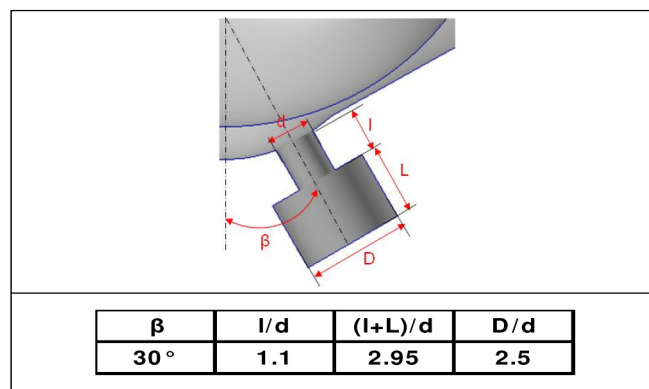


Figure 2. Nozzle geometry and dimensional parameters

Figure 3 presents the three-dimensional computational domain: it includes the injector valve-group flow domain and a segment of the contiguous near-field ambient space. The computational mesh is of the order 5 M cells (1M cells within the injector domain and 4M cells within the ambient) and affords a spatial resolution in the range 2-5 μm within the injector seat-nozzle flow domain. This mesh resolution is of the order of the turbulent liquid jet Taylor microscale (see Table3). Thus, it enables direct resolution of the velocity field of the energy containing and inertial range of the turbulence spectra in the LES calculation.

The pintle motion is not modelled in the simulation, due to severe constraints on mesh quality in the LES simulations that cannot be provided with a deforming mesh. Therefore, the VOF-LES transient seat-nozzle flow simulation is performed on a fixed-geometry mesh with the pintle at the nominal stroke position. Consequently, the initial temporal development of the seat-nozzle flow and jet primary breakup, though likely qualitatively representative, is not an authentic simulation of the injector pintle-opening phase. This is not critical since the focus of this study is on analysis of the ‘stationary’ spray characteristics pertinent to the fully-open pintle condition.

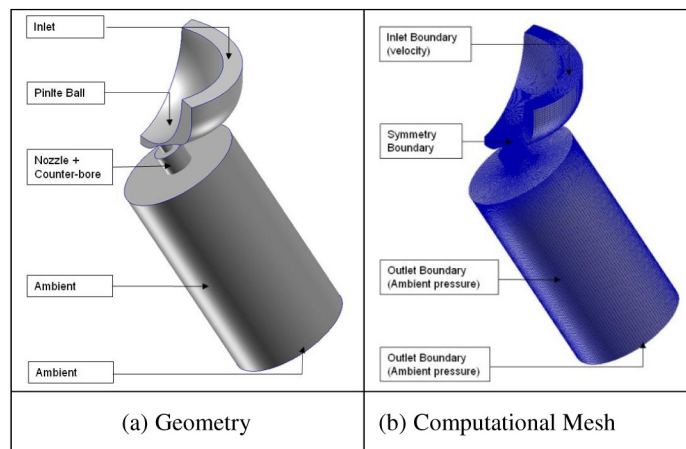


Figure 3. Geometry and computational mesh of the LES seat-nozzle and ambient domain, flow boundaries and boundary conditions