A Coupling between Internal Flow and Primary Breakup Simulations - Case of a Compound Nozzle

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Abstract
This paper is intended to demonstrate the capability of a numerical approach to retrieve the involved primary breakup process in the case of a single triple disk compound injector.
The present study is based on a coupling between internal flow modeling and primary breakup simulations. First internal flow simulations are achieved with a turbulence modeled by a RANS approach. This part of the study mainly focuses on the determination of the secondary flow and the turbulence level at the nozzle exit. The calculated issuing flow characteristics through the velocity profiles are then used as initial conditions for DNS simulations of the primary breakup.
Methodologies of each simulation part are described and numerical results of the primary breakup are compared to visualizations on a real size nozzle.

1. Introduction

In port-fuel spark-ignition engines, sprays are injected in the intake manifold and low-pressure injectors with compound nozzle are commonly used. The concept of compound nozzle is to enhance atomization by promoting the turbulence level of the issuing liquid flow. Compound nozzles consist of two or three superimposed disks with eccentric orifices that impose drastic deflections to the internal flow. Heyse et al. [1] pointed out that compound nozzles offer the best atomization efficiency and allow pollutant emissions to be reduced. The nozzles are intended to be optimized in order to increase the turbulence level at the periphery of the discharged liquid jets. Besides the turbulence level, the liquid flow at a compound nozzle exit section exhibits a double vortex secondary flow. This flow structure was returned by numerical calculations ([2-4]). Ren and Sayar [2] suggested that the contribution of this secondary flow to the atomization was more important than the one of liquid turbulence. Triballier et al. [4] confirmed the contribution of the secondary flow by showing that this flow structure induces a flattening of the liquid jet as soon as it leaves the nozzle discharge orifice as it can be observed in Figure 1.

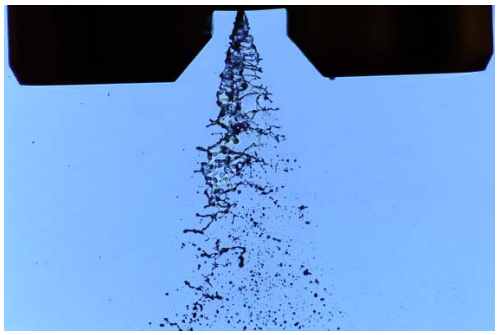

Figure 1: Example of a liquid jet discharged from a compound nozzle (from Triballier et al [4])

In port-fuel gasoline engines, the injection pressure is kept low and leads to the production of slow liquid jets at the nozzle exit. Chen et al. [5] showed that the aerodynamic forces are then absent from the primary breakup. Therefore, the breakup process is driven by turbulence and capillary forces only. Several studies reported that the turbulent intensity at the injector exit is a function of nozzle geometry and injection pressure [4-7]. This explains the strong influence of the nozzle geometry on the spray characteristics evidenced by experimental investigations. Therefore, the improvement of compound nozzles requires an accurate description of the internal flow as well as a better understanding of the primary breakup process that takes place in the present situation. Considering the small dimensions of the nozzle, the internal flow description is often derived from simulations. In the published studies, RANS models (either standard k-ε or RNG k-ε) were used. For instance, Glodowski et al. [7] found correlations between the turbulence kinetic energy of the issuing liquid flow and the Sauter mean diameter of the spray. Considering the turbulence of the issuing flow, Chen et al. [2] developed atomization models that reported calculated Sauter mean diameters of the same order of PDPA measurements.

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In recent years numerous studies have been devoted to two phase flow modeling and, in particular, the transport processes of droplets in turbulent flows have been more and more precisely described by numerical simulations. However, it clearly appears that one step beyond is to develop specific approaches to describe interface behaviors. Recent progress have been obtained by coupling three methods, the Level Set method for the interface tracking, the Ghost Fluid method for interface discontinuities and the VOF method for mass conservation (Ménard et al [8]). A numerical code has been developed for 3D geometries, and MPI parallelization is used.

The objective of the present study is to produce predictive simulation of the jet break-up by using internal flow results at the jet exit as input data for the DNS code. Simulations are carried out with or without predicted turbulent inlet conditions and qualitative comparisons with experimental visualization are presented.

2. Internal flow inside a triple disk nozzle

The investigated nozzles are composed of three superimposed disks (see figure 2). The liquid enters the nozzle through disk 1, passes through the cavity disk (disk 2) and issues from the nozzle through the discharge disk (disk 3). All the disks are circular. A previous investigation [6] concentrated on the effects of the height of the cavity disk and the eccentricity of the discharge orifice and showed that these two geometrical parameters strongly affect the secondary flow and the turbulence level at the outlet orifice.

In the studied simulations, we consider water atomization in air under atmospheric conditions. The Reynolds number at the exit of disk 3 is equal to 2400, and the gaseous Weber number is 1.6.

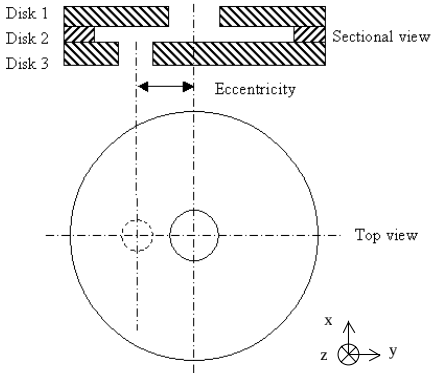


Figure 2: Design of the nozzle

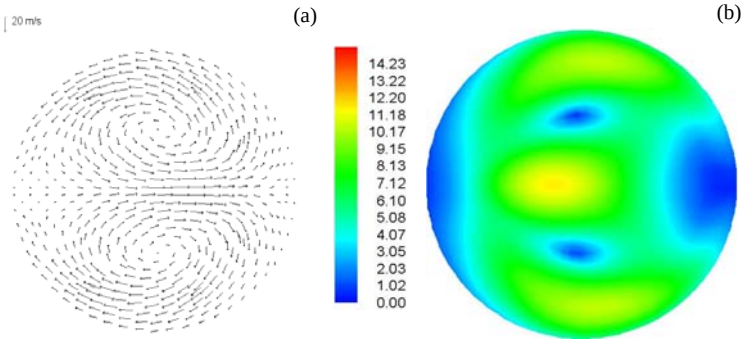


Figure 3: Nozzle exit (a): non axial velocity, (b): turbulent kinetic energy, ΔP_i = 3 bar, RNG k-ε simulation

Figure 3 presents an illustration of the flow at the exit section. Figure 3a shows the mean non-axial velocity field and Figure 3b shows the turbulent kinetic energy. Note that the turbulent kinetic energy is not axi-symmetric and that the turbulence is mainly concentrated along the walls. This important result highlights that the liquid turbulence can affect the liquid-gas interface at the nozzle outlet. Based on the liquid flow morphology, three kinetic energies per unit liquid volume at the nozzle exit are defined. These energies are the axial kinetic energy, E_a, the non-axial kinetic energy, E_k and the turbulent kinetic energy, $\rho_L T_{ke}$. These energies are deduced from simulations and calculated at the nozzle exit.

Dumouchel et al. [6] found also that the spray surface energy per unit liquid volume, deduced from drop-size distribution measurements, increased linearly with the sum of the non-axial and the turbulent kinetic energies, i.e., $E_k + \rho_L T_{ke}$. This sum was defined as the energy available for atomization. Among all the tested compound nozzles in [6], the one that reported the greatest energy available for atomization and that therefore produced the finest spray had the dimensions given in Table 1.

Disk	Thickness (µm)	Diameter (µm)	Eccentricity (µm)
1	177	300	0
2	75	2254	0
3	75	180	200

Table 1: Disk geometrical dimensions of the compound nozzle

4. Internal flow simulations

The CFD package FLUENT 6.2 [9] was used to simulate the internal flow of the compound nozzle whose internal dimensions are given in Table 1. In the present investigation, internal flows are steady, incompressible and the segregated-implicit solver is chosen. According to this method the governing equations

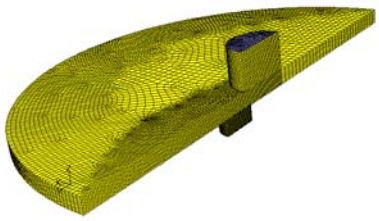


Figure 4: Computational mesh.

are solved sequentially; each equation is implicitly linearized respecting the equation's dependent variable. This technique requires a lower memory than the coupled-implicit solver. The coupling between the velocity and the pressure is strong for incompressible flows; the simple algorithm is then employed to relate velocity and pressure corrections to enforce mass conservation. The turbulence model is the RNG k-ε model in which equations for k and ε are derived from the application of the renormalization group method to the instantaneous Navier-Stokes equation. Although this model is similar in form to the standard k-ε model, it includes additional terms in the equation for ε that are expected to improve the simulation of rapidly strained flows [8]. This modified k-ε model is recognized as being more appropriate than the standard k-ε model to simulate flows with great streamline curvatures and strain rates.

All the calculations are performed with a double precision and numerical convergence is achieved when the relative residuals that are summed over all cells are smaller than 10^{-5}.

Figure 4 shows the meshing of the computational domain. As the flow characteristics of the liquid flow are of main interest, disk 3 was meshed with a higher refinement and all cells have a typical length equal to 5 µm.

As far as boundary conditions are concerned, first the symmetric plane of the nozzle allows the numerical simulations to be performed on one half only. Second a constant normal injection pressure is imposed on the nozzle inlet section. The pressure is set equal to zero at the exit plane; as the flow is subsonic, this condition forces the static pressure to be zero on all cells belonging to the nozzle outlet. Furthermore, a turbulent intensity and a characteristic length scale have to be given at the nozzle inlet. It must be noticed that the inlet turbulent characteristics do not affect the outflow characteristics and that the choice of these initial characteristics is not critical in the present investigation. Thus, it was decided to impose a quiescent upstream flow with a turbulent intensity of 2% and a characteristic length scale of 10 % of disk 1 diameter. A no slip condition is imposed at walls. Finally, a symmetry boundary condition is imposed on the symmetrical plane.

5. Jet break-up simulations

Two phase flows remain a wide field of research. In the particular case of jet simulations, very far from the injector the generated spray can be considered in the dilute regime and classical Eulerian or Lagrangian methods have been extensively developed to describe the spray behavior. When going up to the nozzle injector, the volume loading increases and drop interactions can occur leading to possible collisions, coalescence or secondary break-up. Mass loading is also increased and interaction between phases (two way coupling) is observed. Eventually with empirical correlation, this dispersed regime of the jet is also quite well predicted with classical methods. To go further on in numerical simulations, the main challenge is obviously to capture the interface behavior in the nozzle vicinity with enough accuracy to get a description of the jet primary break-up.

Front tracking methods (Nobari and Tryggvason [10]), Volume of fluid methods (Gueyffier et al. [11]) and level set methods (Sethian [12]) are the most common numerical strategies used to predict interface motion. Font tracking methods, either with moving grids or marker particles, are very accurate but very complex in 3D configuration and when lot of interface breaks occur. Volume of Fluid methods are very accurate for mass conservation but interface smoothing can induce some uncertainties on surface tension forces. Level set method is accurate, quite simple and allows curvature to be easily obtained but mass losses are often observed for under resolved domain. A specificity of the liquid/gas interface simulation is how to handle the discontinuities (variable jumps) across the interface. Two methods can be used: smoothing the interface on 2 or 3 nodes around the interface (Continuum Surface Force), or taking the jumps through the Ghost Fluid method. As the objective of the present study is to deal with the primary break-up of jets, a lot of topological changes occur (interface pinching or merging, droplet coalescence or secondary break-up) and the numerical method must describe the interface motion accurately. We thus chose to develop a 3D code based on the level set method. The ghost fluid method is used to take into account sharp discontinuities at the interface in order to avoid artificial smoothing of the interface and a coupling with the VOF method ensures mass conservation (Sussman and Puckett, [13]). A projection method is used to solve incompressible Navier–Stokes equations. Specific care has been devoted to improve simulation capabilities with MPI parallelization.

We briefly recall the level set method, the coupling between the level set and VOF techniques and the ghost fluid method..

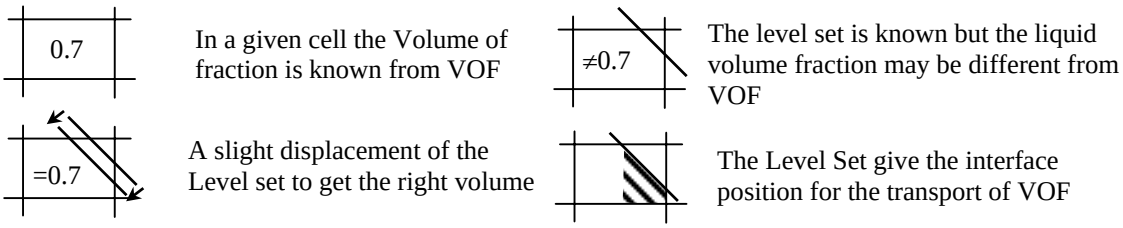
5.1 Level-Set / VOF / Ghost Fluid methods

The overall coupling between Level Set, VOF and Ghost Fluid is extensively presented and discussed in Ménard et al [8] with test case validations and jet primary break-up simulations. A brief overview is presented here.

Level Set methods are based on the transport of a continuous function ϕ which describes the interface between two media. The interface is described by the 0 level of the level set function.
Three main steps are involved:

- Define the function as the algebraic distance between any point of the domain and the interface $\Phi=0$ on the interface ($\Phi<0$ outside , $\Phi>0$ inside),
- Solve a convection equation to follow the evolution of the interface in a given velocity field
- Apply a re-distancing algorithm to keep ϕ as the algebraic distance to the interface

To ensure mass conservation different strategies can be applied. First method is modifications of the reinitialization algorithm by adding a constraint to help in mass conservation. But a major limitation is that they are global and when many liquid parcels are generated these corrections are quite impossible. The second strategy is to couple the level set method with conservative algorithms. We then deal with « mixed » methods, such as the particle level set or a coupling between VOF and Level Set.
In jet atomization, many break-ups are initiated and coupling the Level set method with the VOF technique is much better adapted for our purpose than the particle level set method. The main idea is to benefit from the advantage of each strategy: mass conservation from the VOF and fine description of the interface with the level set and Ghost fluid methods. A very crude overview of the coupling is:



In the Ghost Fluid Method (GFM), Fedkiw et al [14] respect jump discontinuities across the interface and avoid an interface thickness. Discretization of discontinuous variables is more accurate, and spurious currents in the velocity field are thus much lower than with CSF methods. The main idea is to define ghost cells on each side of the interface and following the jump conditions, the discontinued functions are extended continuously and then derivatives are estimated. More details can be found in Liu et al [15] on implementing the Ghost Fluid Method to solve the Poisson equation with discontinuous coefficients.

5.2 Simulation

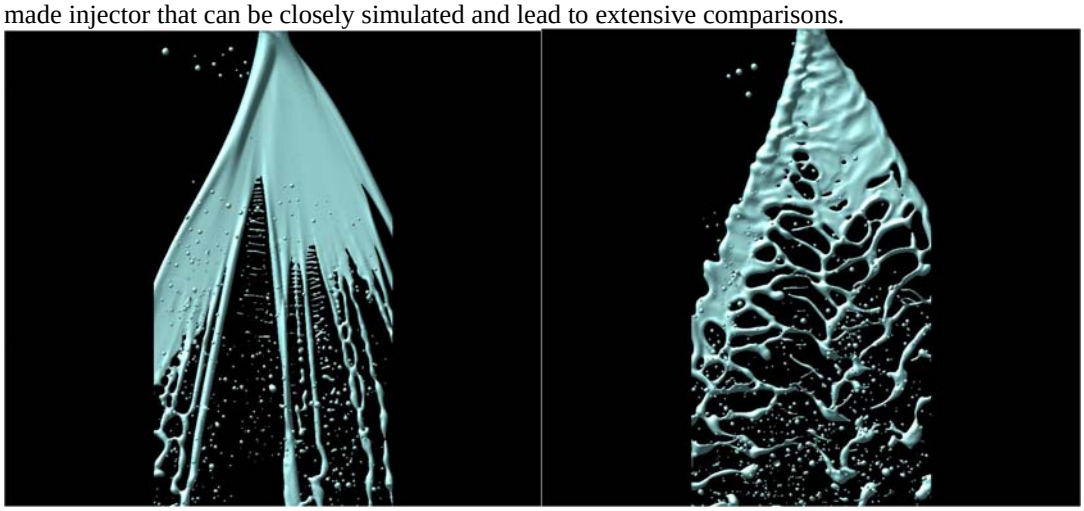
The radius of the issuing liquid jet is R=90 μm and the size of the domain is (16R, 4R, 32R) i.e. (0.00144 m, 0.00036 m, 0.00288 m) in the (x,y,z) directions. The uniform grid is 256x64x512 nodes, which leads to 200 grid nodes on the (half) jet exit. Symmetry boundary condition is applied on y axis and free outlet conditions are set on x and z axis. Inlet velocity profiles are interpolated on the grid nodes inside the liquid jet exit from the above predicted (RNG k-ε) predictions. Calculations are carried out for two cases, with or without turbulent inflow boundary conditions. When turbulence is introduced, we use the method derived by Klein et al. [16], which consists in generating correlated random velocities with a prescribed length scale. In our computation, that scale is approximated by the turbulent integral scale from the inflow predictions and it is set to 0.1 R.

6. Results

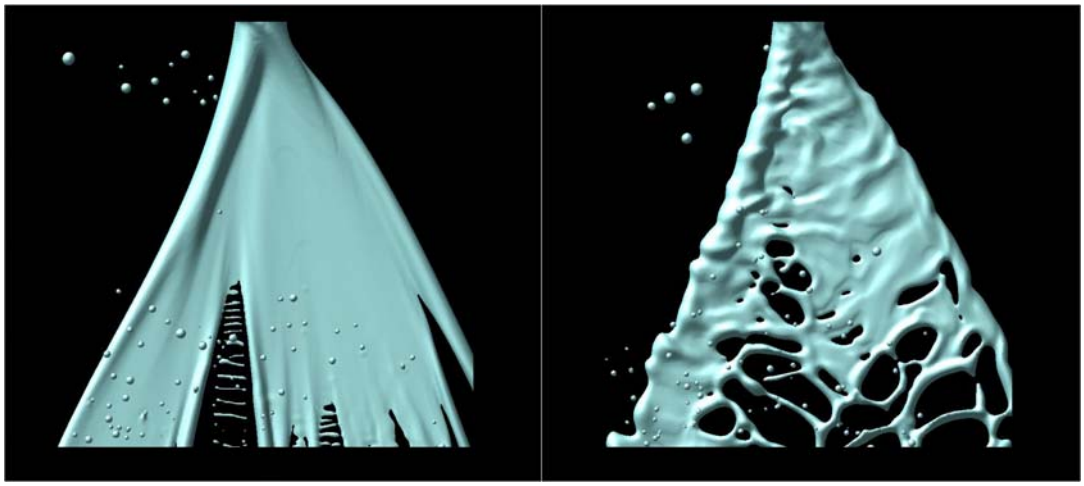
The so-called primary break up is the first step of the atomization. It takes place in a zone where the spray is very dense. In this area the liquid volume fraction is close to one and the liquid surface topology is very complex. As a consequence it is very difficult to get experimental results in order to characterize this zone. The comparisons are thus quite qualitative by comparing simulations and experimental images. We first compare on figures 5 the simulations with or without turbulence at the inlet, and we made a zoom on the jet break-up on the figures 6: the height of the images is 8 nozzle diameters. In both cases, the initial round jet is converted into a liquid sheet with thick edges on both sides as observed in experiments. We clearly observe that the turbulence induces much more perturbations on the liquid interface, both on the edges and on the liquid sheet; the liquid surface topology becomes much wrinkled and the whole flow appears very turbulent and chaotic. The break-up of the liquid sheet arises at a time shorter and closer to the injector nozzle when turbulence is included and it also arises nearer to the injector nozzle when it is compared to experiments (figure 7). It can be due to under resolved simulations (mesh size is 5μm) but the initial conditions at injection are also quite difficult to estimate from experiments. The total angle of the jet exit are of the same order (roughly 46° without turbulence and 41° with turbulence) while it is less in the experiment. Note that a slight dissymmetry is observed in the simulations for the jet angle, which is less pronounced in the experiment.
When turbulence is included, we observe that the liquid sheet break-up exhibits the same behavior in simulations and experiments. Perforations occur in the sheet and ligaments are formed, they reorganized into a network and

then break to generate droplets. This is presented on figures 8 and the same behavior is observed on the simulations and the experiments. It is obvious that the ligament break-up appears to be a major mechanism in the droplet formation in the jet that is considered here.

Comparisons between simulations and experiments can be carried out on ligament lengths or droplet sizes. The main difficulty is to be free of not enough precise inlet conditions in the simulations when compared with experiments. That would lead to unfruitful discussions and that is the reason why a next step is to set up a home made injector that can be closely simulated and lead to extensive comparisons.



Figures 5: Jet break-up –left: without turbulence; right with turbulence



Figures 6: Zoom (0<z<8D) on jet break-up –left: without turbulence; right with turbulence

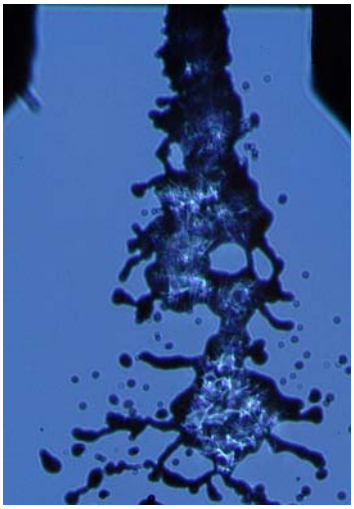


Figure 7: Experimental image

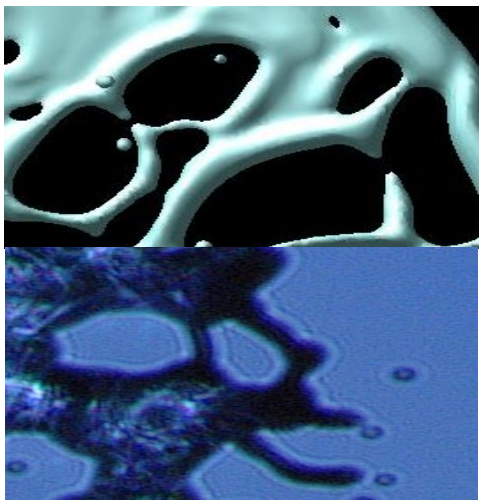


Figure 8: Ligament network

7 Conclusion

A coupling between internal flow and primary breakup simulations for a compound nozzle is carried out. Internal flow simulations are achieved thanks to a RANS approach and DNS approach is used for the primary break-up, where interface tracking is ensured by Level Set method, Ghost Fluid Method is used to capture accurately sharp discontinuities, and coupling between Level Set and VOF methods is used for mass conservation. Specific care has been devoted to improve computing time with MPI parallelization.
The turbulence influence is clearly demonstrated. The interface becomes much wrinkled and some break-up are initiated, ligament formations are observed and drops are generated from ligaments break-up. The simulations are compared with experimental visualizations and a qualitative good agreement is observed. These results are a first step before extensive comparisons with LES simulations for the internal flow that will be used as input data for DNS simulation of the atomization process. Computational cost will be subsequently increased due to LES simulations inside the injector but one could expect more reliable injection conditions for the DNS simulations of the jet break up.

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