2017 WJTA-IMCA Conference and Expo
October 25-27 ● New Orleans, Louisiana

Paper

LES-VOF SIMULATIONS OF A PURE WATER JET DEVELOPING INSIDE AN AWJC NOZZLE: PRELIMINARY OBSERVATIONS AND GUIDELINES

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ABSTRACT

In this work, a numerical approach to predict the behavior of a pure water jet developing inside a nozzle for Abrasive Water Jet Cutting (AWJC) is investigated.
In a standard AWJC configuration, the water jet carries the major energy content of the entire system, and is responsible for accelerating abrasive particles that will perform the cutting action of hard materials. Therefore an accurate simulation of a pure water jet can bring significant insight on the overall AWJC process. Capturing the behavior of a multiphase high-speed flow in a complex geometry is however particularly challenging.
In this work, we adopt a combined approach based on the Volume of Fluid (VOF) and Large Eddy Simulation (LES) techniques in order to respectively capture the water/air interface and to model turbulent structures of the flow. The aim of this contribution is to investigate how the two techniques apply to the specific problem, and to offer general guidelines for practitioners willing to adopt them. Costs considerations will be then presented with particular reference to the usage of the OpenFOAM® environment. The reported results are meant to provide guidance for AWJ applications and future developments of AWJ nozzles.

1. INTRODUCTION

Abrasive Water Jet Cutting (AWJC) is a widespread technology that allows cutting many different materials. An AWJC system embodies a pumping system that makes available water at pressures usually ranging from 500 to 6000 bar. The pressurized water is accelerated through a diamond/sapphire orifice producing a high-velocity water jet. The jet passes through a mixing chamber creating a partial vacuum and stabilizing. In order to cut hard materials, abrasive particles are usually inserted in the chamber, accelerated by the jet and carried outward.

The resulting three phase flow jet, consisting of water, entrained air, and accelerated particles, has been proven an excellent tool to cut materials, due to the low cutting force involved and the negligible thermal effects (Hashish 1984). These characteristics can significantly improve the weldability of the piece and eliminate the need of post-cut treatment. At the same time, they eliminate the logistic disadvantages caused by melting and vaporization of thermally attacked working pieces, like, for instance the necessity for air filtering systems.

In AWJC the characteristics of the three phase jet can deeply influence the quality of the kerf and the time required for the cut, therefore an understanding of the dynamics of air and particle entrainment in the pure waterjet, as well as a study on the stability conditions of the system can be of high interest for the research and development in this field (H. Liu 2004). In the standard AWJ configuration, the pure waterjet formed in the orifice creates a local depression that entrains the particle into the mixing chamber-nozzle focusing tube. This component is responsible for the formation and stabilization of the jet that will be delivered on the working piece. Within the nozzle, the jet undergoes some of the most critical steps for its development. It must be noted that in the nozzle and mixing chamber the main kinetic energy content stays within the pure water jet, which can be considered the core of the abrasive water jet (M. Annoni 2014). This environment is very hard to explore with purely experimental studies since the high velocities and energies involved make accurate observation unfeasible in most cases. Therefore a rising attention has been posed in recent years on numerical simulation of this process (M. Annoni 2014) (H. Liu 2004) (D. Deepak 2012) (Rongguo Hou 2014). Despite the relevant findings in the field, the development of a stable and reliable numerical method able to describe the complexity of the AWJ with affordable computational costs remains extremely challenging. This constitutes a major limitation to the adoption of CFD techniques in this specific branch of research and development.

As pointed out in (H. Liu 2004) (Rongguo Hou 2014) (Md. G. Mostofa 2010) (Gabriele Pozzetti 2017), the complexity of the interactions rising within the turbulent three phase flows developing in the nozzle imposes to adopt some simplifications, in order to make a numerical simulation affordable. A first approach to understand the dynamics is to start with an accurate simulation of the structures holding the higher energy content, namely, the pure water jet. One may assume that if the stability of the pure water jet cannot be granted within a set of geometrical and operational parameter, the resulting particle laden jet would hardly be stable. It is of note that even the simulation of a high-velocity pure water jet developing a complex geometry remains challenging and must be carefully addressed. In particular, the complexity of the phenomena and the limitation of the adopted computational methods must be clearly understood before approaching the numerical simulation. The air-water environment is a high density, high viscosity ratio multiphase flow traveling at high speed through a complex geometry.

Due to the highly different kinetic content of water and air within the nozzle, it is important to be able to accurately track the interface between them. This is mandatory in order to correctly predict the local energy content of the flow. Various numerical techniques have been developed for this purpose, and are usually referred to as interface capturing methods. Those methods aim to identify a two-dimensional interface between the phases as an analytical function or isosurface of a volume fraction. The interface will be moved according to the flow profile determining and evolving configuration. Among the interface capturing methods, the Volume of Fluid (VOF) technique is adopted in multiphase contest and has been proven capable of addressing complex problems in an efficient way (Edin Beberovic 2009) (Tryggvason 2011). It is based on the definition of a scalar function indicating the local fluid phase. This function, when integrated over a control volume, provides information regarding the volume fraction of the phase itself. Generally, a VOF scheme consists of two steps. Firstly, the position of the interface

is reconstructed from the information about the volume fraction field. There are several different possibilities in order to do so and one can refer to (Tryggvason 2011) and citations within for a more exhaustive description. Secondly, the volume fraction field is transported from the velocity and therefore defines a new interface location. In this contribution, we refer in particular to the algebraic VOF scheme presented in (Edin Beberovic 2009) and aim to investigate its capabilities in dealing with the simulation of the water jet developing inside an AWJ nozzle.
Depending on the specific material that is meant to be cut, its thickness and the future application, different pressure of the water are normally adopted (Hashish 1984). The latter translates in different velocities of the jet that can vary from some hundreds up to one thousand meters per second. Within this range of high velocities, the flow regime is far from laminar, as typically, Reynolds numbers of 10^5 or higher can be achieved. The numerical simulation of turbulent flows is a particularly complex subject as their behavior is determined by very small structures whose dynamics occur in an extremely short time scale (Piomelli 1999). Hence, a direct numerical approach aiming to completely resolve these structures is never adopted for the solution of industrially scaled problems. As a matter of fact, resolving all the relevant structures of the flow would imply a prohibitive computational burden, furthermore a detailed information to initialize the problem at that scales range is unlikely to be available. Therefore, numerical methods that try to convey information on averaged quantities of the flow while simply modeling the effect of the small and rapidly decaying scales, are the most commonly adopted for engineering problems (Pope 2000).
A common approach consists of averaging the equations over a period of time comparable to the one interesting for the macroscopic observation of fluid action. In this way, one will not have to resolve the rapid changes of the small and big fluid structures, but a steadier and uniform equivalent flow (Pope 2000). This is the main concept behind the RANS (Reynolds Averaged Navier Stokes equations), that represents the most economic alternative to address the turbulence problem. On the other hand, the modeling effort required to define a RANS scheme is very significant, and that is why RANS models often lack generality. In particular for complex flows, as the multiphase ones, RANS models are not generally validated, and the brute application of mono phase RANS could suffer from this lack of generality. Another approach to deal with the over mentioned problem is to try to simulate the unsteadiness of the flow while filtering its smallest structures. In this way, the big fluid Eddies would be computed exactly, while the effect of the small eddies modeled (Piomelli 1999). This is the approach on which Large Eddy Simulations (LES) are based. Despite being generally more computationally expensive, LES schemes are acquiring popularity over the RANS in several applications (Piomelli 1999). This is due to the fact that LES models are simpler, involve fewer assumptions, and are therefore often more general. Also, LES simulations are able to capture the unsteady behavior of turbulent flows, and this is extremely important in addressing problems that are affected by instabilities.
This contribution aims to investigate the feasibility of simulations of a pure water jet developing inside an AWJ nozzle with a numerical method combining LES and VOF. The paper is organized as follows: firstly, a description of the governing equations of the system is proposed and the model adopted described. Secondly, a consideration on the setup of the numerical problem in terms of mesh generation and boundary conditions is performed. Thirdly the numerical solution is analyzed, with reference to the influence of the main numerical parameter on the outcome. Finally, a cost consideration is proposed and scalability performances of the solver are observed.

2. METHOD

Unfiltered governing equations of the continuum phases
In this work, an unsteady incompressible, immiscible, two-fluid system is considered, which is governed by the Navier-Stokes in the form:

$$\frac{\partial \rho_f \mathbf{u_f}}{\partial \tau} + \nabla \cdot \left(\rho_f \mathbf{u_f}\, \mathbf{u_f}\right) = -\nabla p + \nabla \cdot \left(\mu_f (\nabla \mathbf{u_f} + \nabla^T \mathbf{u_f})\right) + \boldsymbol{T_\sigma} + \boldsymbol{F_b}, \tag{1}$$

with $\boldsymbol{T_\sigma} = \sigma k\, \mathbf{n}\, \delta_\sigma$ the surface tension force, $\mathbf{F_b}$ a body force. The choice of treating the two phases as incompressible represents a critical aspect of the present work. This is motivated by the assumption that, after passing through the sapphire, the water has undergone the main acceleration-decompression process and, while in the mixing chamber, its flow can be considered as non-compressible. For what concerns the gas phase, this assumption is clearly much stronger, as the air is known to undergo significant compression within the focusing tube. Nevertheless, the choice of considering both fluids as incompressible highly simplifies the numerics, allowing a better conservation of the phase fraction and momentum. It is important to remember that for what concerns the air, the obtained numerical results will refer to an equivalent incompressible fluid. Due to this choice, the incompressibility constraint must be fulfilled in the form

$$\nabla \cdot \mathbf{u_f} = 0\,. \tag{2}$$

Local density and viscosity change with the fluid phase and can be written in the form

$$\begin{aligned} \rho_f(\mathbf{x}) &= \rho_1 \alpha(\mathbf{x}) + \rho_2 \left(1 - (\mathbf{x})\right), \\ \mu_f(\mathbf{x}) &= \mu_1 \alpha(\mathbf{x}) + \mu_2 \left(1 - (\mathbf{x})\right), \end{aligned} \tag{3}$$

with α a volume fraction defined by

$$\chi = \begin{cases} 1, & if\ first\ fluid \\ 0, & if\ second\ fluid \end{cases} \tag{4}$$

$$\alpha = \frac{1}{V} \int_V \chi(\mathbf{x}) d\mathbf{x}.$$

The volume fraction is considered as a scalar transported by the fluid flow, for which

$$\frac{\partial \alpha}{\partial \tau} + \nabla \cdot (\alpha \mathbf{u_f}) + \nabla \cdot (\alpha(1-\alpha)\mathbf{u_c}) = 0, \tag{5}$$

must hold, with $\mathbf{u_c}$ indicating the relative velocity between the two phases, referred as compression velocity. This term is introduced in order to avoid an excessive numerical dissipation. The computations of the fluid fields are performed using OpenFOAM® (H. G. Weller 1998), an extensively used open source library for field operation and manipulation and in particular the interFoam solver. Finally, the VOF scheme described in (Edin Beberovic 2009) is adopted in this work.

The finite volume method (FVM) is used to discretize the conservation equations. For the source terms as well as the transient term the midpoint rule is adopted and an integration over the cell volume is performed. An implicit Euler scheme is used to discretize temporal derivatives. Convective and diffusive terms are treated by converting the volume integrals into surface integrals, followed by an integration over these surface values.

LES approach to the turbulent scale

LES schemes aim to compute exactly the large, energy-carrying structures of the flow, while modeling the smaller scales whose behavior is accepted to be less local (Pope 2000). This is obtained by a filtering operation applied on every field variable

$$\overline{\boldsymbol{y}}(\mathbf{x}) = \int_{\boldsymbol{D}} \boldsymbol{y}(\boldsymbol{x}')\boldsymbol{\Phi}\left(\mathbf{x}, \boldsymbol{x}', \widetilde{\boldsymbol{\Delta}}\right)\boldsymbol{dx}', \tag{6}$$

where **D** is the simulation domain, $\boldsymbol{\Phi}$ is a generic filter, $\widetilde{\boldsymbol{\Delta}}$ is the filter width. When the filtering operation is applied to the Navier-Stokes equations the nonlinear advection term becomes

$$\nabla \cdot \overline{\mathbf{u_f}\mathbf{u_f}}\,, \tag{7}$$

that cannot be directly expressed in terms of filtered velocity. When this operation is applied to the governing equations of a multiphase flow, further terms generally arise, and in particular (M. C. A. Toutant 2009)

$$\begin{aligned}
\boldsymbol{\tau_{interf}} &= \overline{\mathbf{u_f} \cdot \nabla\alpha} - \overline{\mathbf{u_f}} \cdot \overline{\boldsymbol{\nabla}\alpha}, \\
\boldsymbol{\tau_{temp}} &= \overline{\rho_f \mathbf{u_f}} - \overline{\rho_f}\ \overline{\mathbf{u_f}}, \\
\boldsymbol{\tau_{diff}} &= \overline{\mu_f(\boldsymbol{\nabla}\mathbf{u_f} + \boldsymbol{\nabla}^T\mathbf{u_f})} - \overline{\mu_f}(\boldsymbol{\nabla}\overline{\mathbf{u_f}} + \boldsymbol{\nabla}^T\overline{\mathbf{u_f}}), \\
\boldsymbol{\tau_{superf}} &= \overline{\sigma k\, \boldsymbol{n}\, \boldsymbol{\delta_\sigma}} - \sigma\bar{k}\bar{\boldsymbol{n}}\overline{\boldsymbol{\delta_\sigma}}
\end{aligned} \tag{8}$$

Toutant et al (M. C. A. Toutant 2009) (E. L. A. Toutant 2008) and Hermann et al (M.Herrmann 2013), proposed approaches to model the terms in (9) respectively for the cases where sub-filter surface tension contributions are negligible and determinant. Those works were focusing on configurations in which the surface tension force was determinant for the global system (static bubble in isotropic turbulence). Several works (Ehsan Roohi 2013) (B Befrui 2008) (A Gosset 2005) (Nai-xian Lu 2010) go in the direction of neglecting those contributes with respect to the convective sub grid term

$$\tau_t = \overline{\rho_f \mathbf{u_f}\mathbf{u_f}} - \overline{\rho_f}\ \overline{\mathbf{u_f}}\ \overline{\mathbf{u_f}}\,. \tag{9}$$

In particular, this approach is generally chosen when the surface force becomes negligible with respect to the fluid inertia. Considering the velocities and shear stresses typical of a very high velocity waterjet, we assumed the term of equation (9) as predominant. This allows us to adopt simple and stable sub grid models. Nevertheless, we acknowledge that the development of an ad-hoc sub-filter model for the specific case could provide important benefits, and represents an interesting field for future studies.

In eddy viscosity models, like the one adopted in this work, this term is expressed through the relation

$$\tau_{t_{ij}} - \frac{\delta_{ij}}{3}\tau_{t_{kk}} = -2\nu_t\, \widetilde{S_{ij}}, \tag{10}$$

where the sub-grid scale stresses are related to the large scale strain rate tensor

$$\widetilde{S_{ij}} = \frac{1}{2}\,\overline{\rho_f}\left(\frac{\partial\overline{\mathbf{u_f}}}{\partial x_i} + \frac{\partial\overline{\mathbf{u_f}}}{\partial x_j}\right). \tag{11}$$

As pointed out in (Piomelli 1999) this scale separation makes LES very promising and in particular, it provides interesting advantages over the Reynolds Averaged Navier-Stokes (RANS) approach.

Subgrid models

Several models have been presented in the literature for the treatment of the sub grid scales effects on the resolved wavelengths, namely models for the calculation of $\mathbf{\nu_t}$. In general LES equations tend to use simpler and more general models for the equation closure than the RANS schemes. The Smagorinsky model (Smagorinsky 1993) is often considered the progenitor of the subfilter-scale stress models. It is based on the hypothesis that the production of turbulent kinetic energy is equal to its dissipation. In this model, the turbulent viscosity ν_t is expressed as

$$\nu_t = \left(C_s\overline{\Delta}\right)^2\left(2\,\overline{S}_{ij}\overline{S}_{ij}\right)^{\frac{1}{2}}, \tag{12}$$

with C_s a real constant that makes, therefore, the model absolutely dissipative. This implies that the model is not able to tackle phenomena of back-scattering, or the transfer of energy from the sub-grid scale to the resolved one. This will make this model less suitable to study instabilities at frequencies close to the sub-grid scale. Considering once again the high velocity regime, typical of the flow in an AWJC nozzle, one may claim that the back-scattering could indeed be negligible. The model is rather stable but often over-dissipative (Piomelli 1999). Despite this, the Smagorinsky model is still widely used today.

Another standard approach to the sub grid contribute calculation is via the usage of one extra equation. This obviously introduces extra computational burden with respect to the simpler Smagorinsky model, yet it allows to introduce less artificial dissipation. One equation models are becoming quite popular in LES, in this work we use a one-equation eddy viscosity model that solves a transport equation for the turbulent kinetic energy.

$$\nu_t = \Gamma_\nu \boldsymbol{k}^{\frac{1}{2}}\boldsymbol{\Delta}, \tag{13}$$

$$\frac{\partial \boldsymbol{k}}{\partial \boldsymbol{\tau}} = +\nabla\cdot(\mathbf{k}\,\overline{\mathbf{u_f}}) = \nabla\cdot\Psi - \frac{\Gamma_\epsilon \mathbf{k}^{\frac{2}{3}}}{\widetilde{\Delta}} - \boldsymbol{\tau_f}:\overline{\mathbf{u_f}}$$

$$\Psi = \left[\left(\Gamma_k \boldsymbol{k}^{\frac{1}{2}}\,\widetilde{\Delta} + \nu\right)\nabla\boldsymbol{k} + \boldsymbol{\tau}_f\cdot\overline{\mathbf{u_f}}\right]$$

with $\boldsymbol{k}$ the turbulent kinetic energy, Δ the grid size, $\widetilde{\Delta}$ the filter size, Γ_ν , Γ_e , Γ_k suitably defined constants.

Mesh generation

The mesh generation for a the LES-VOF simulations of the flow inside the nozzle is particularly delicate. In this work, we addressed the problem of the mesh generation with the software Salome (Caremoli 2007), an open-source platform that offers a drawing and meshing module allowing to mesh complicated geometry starting from basic entities.

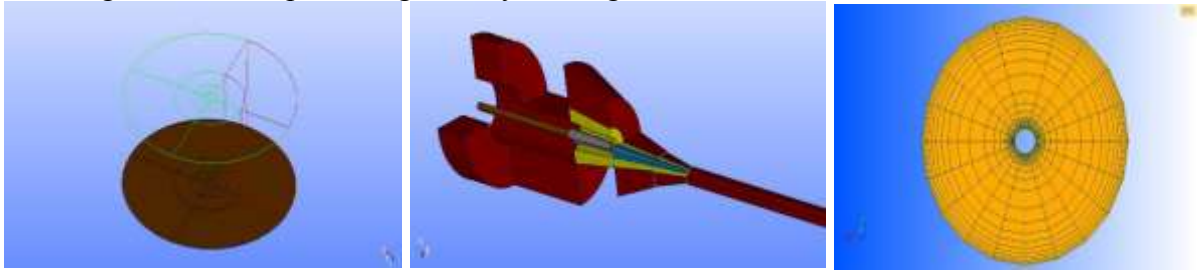

Figure 1 *Structured mesh generation with Salome: Single block definition (Left), Block assembly (center) and mesh refinements (right)*

In **Figure 1** we propose an example for the geometry generation of the focusing tube starting from elemental blocks.

In particular significant sections of the piece are identified. From those sections, basic blocks will be reconstructed, and then re-assembled to form the complete geometry. This strategy allows us to have a better control on the mesh size within the geometry, as the number of elements in every single block can be controlled. Therefore, the mesh quality can be granted and local refinements along critical areas can be performed.
This is important as the overall numerical scheme will present nonuniform requirements in terms of mesh refinement. For instance, the area near the water-air interface will undergo complex interface dynamic, and high shear-stress induced turbulence. Therefore being able to locally control the mesh size is of high importance. For the same reason, hexahedral elements are used. Different mesh refinements have been adopted and will be referred to in section **3.**

Boundary Conditions
The boundary conditions adopted for the simulation are described hereafter. We will focus separately on the variable of velocity, pressure, and volume fraction. Four different boundary areas are distinguished as water inlet, air inlet, wall, and outlet. For the velocity field, we impose a non-slip boundary condition at the wall. At the water inlet, a uniform Dirichlet boundary condition is imposed. This is done to focus on the solution of a reference state, in which primary perturbations of the jet are not occurring. Two main considerations that led to this choice are the small ratio between the jet inlet diameter and the mixing chamber, and the assumption that the main turbulent structures will arise from the interaction between the jet and the surrounding environment. At the outlet, convective boundary condition has been imposed along with a local coarsening of the grid in the flow main direction in order to create a sponge-like region. For the pressure, a Neumann Boundary condition is applied at the wall and at the inlet region. At the outlet atmospheric pressure is imposed. For the volume fraction, a uniform Dirichlet condition has been imposed at the inlet, since the water compression ensures the presence of only water at the sapphire outlet. A Neumann boundary condition for the volume fraction is imposed at the walls of the nozzle. At the outlet, a switch is imposed according to the flow direction. When the velocity is directed in the outlet direction, Neumann boundary conditions are imposed, while when the flow is directed inward, a Dirichlet condition holds forcing the phase to be air. This is done under the assumption that in any condition water cannot enter back through the nozzle exit. The latter assumption is reasonable considering the outlet velocities of the jet and highly simplifies the numeric.

3. RESULTS

Flow Regimes
It is possible to distinguish between two different flow regimes, the first dominating the jet formation across the focusing tube, and the second featuring the dynamic of the already formed jet. In **Figure 2** characteristic moments of the jet formation are shown. In particular, the interface between liquid and gas phase is shown along with streamlines of the velocity field. Three simulation snapshots have been chosen in different regimes of the jet formation.

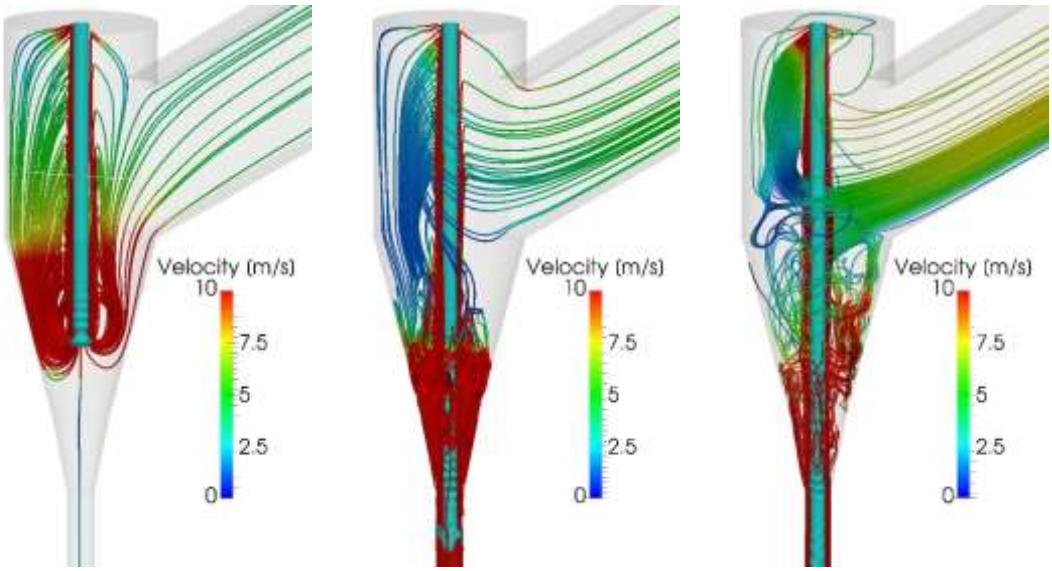

Figure 2 *Characteristic moment on the jet formation. Jet forming in the mixing chamber (left), Jet entering the tubular part (center), and fully developed jet (Right). The jet is colored in blue, streamlines of the velocity field are present*

A scale between 0 and 10 meters per second has been chosen for the streamlines for visualization purposes. This was done in order to better capture the velocity gradient in the gas phase, as it is observed that the high velocity area (hundreds of meters per seconds) is limited to the region close to the jet. For the first regime, the jet is forming within the mixing chamber inducing recirculating structures in the second fluid phase. One can here observe a classical structure of the jet head due to the local deceleration of the fluid. When the jet head leaves the mixing chamber the velocity profile tends to stabilize.

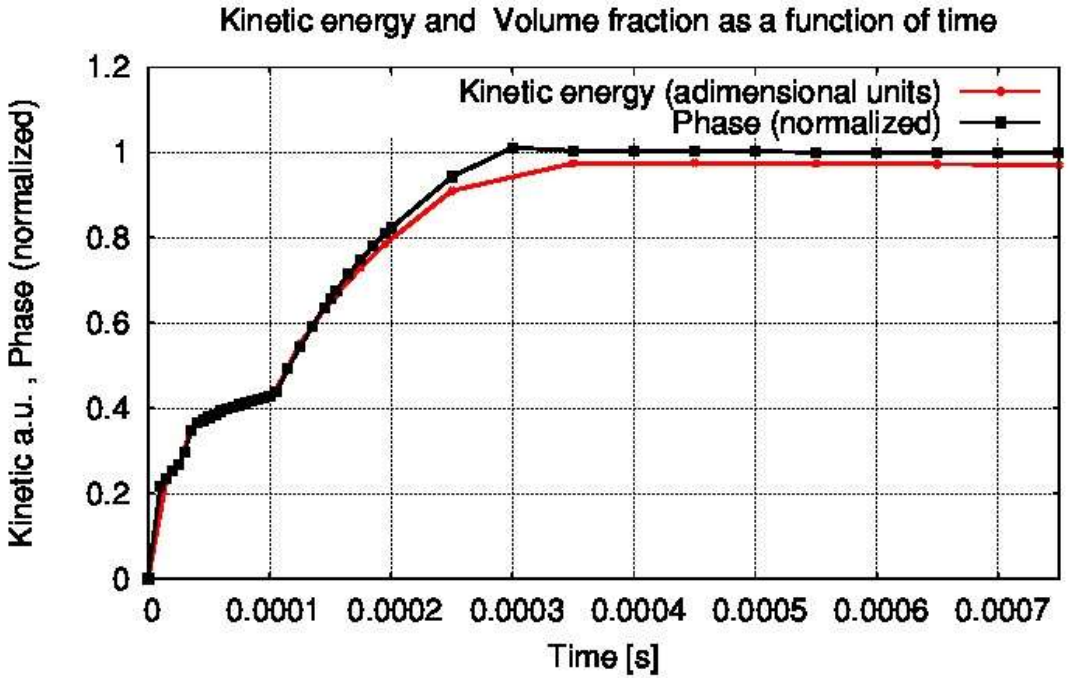

Figure 3 *Kinetic energy and volume fraction as functions of time during the simulation. During the Jet development, the kinetic energy of the system increases, until reaching a stable value when the jet stabilizes.*

It is interesting to identify those two regimes by observing the total kinetic energy of the flow.

As shown in **Figure 3** the first regime is characterized by an increase in the kinetic energy of the system due to the entrance of the high density-high velocity phase. When the jet reaches the exit, the average total kinetic energy remains constant.
In **Figure 3** a non dimensional kinetic energy was defined as the ratio between the kinetic energy at a specific time and the one after 0.0008s. The same is done for the volume fraction or (liquid) phase content that is additionally multiplied by a factor 0.99 in order to be observable. This is done in order to make the two quantities comparable. From such a comparison one can notice how the two profiles have the same behavior. This was expected since, as introduced in section 1, the water phase retains most of the kinetic energy of the system.

Mesh-Time independence analysis during the jet formation
Capturing the jet formation in the first regime is a very delicate computational task that requires particular attention on the choice of the timestep and mesh discretization, as these represent a critical factor for the correct phase advection and therefore surface reconstruction. A mesh/time step independence analysis is, therefore, highly recommended for the study of this first regime.

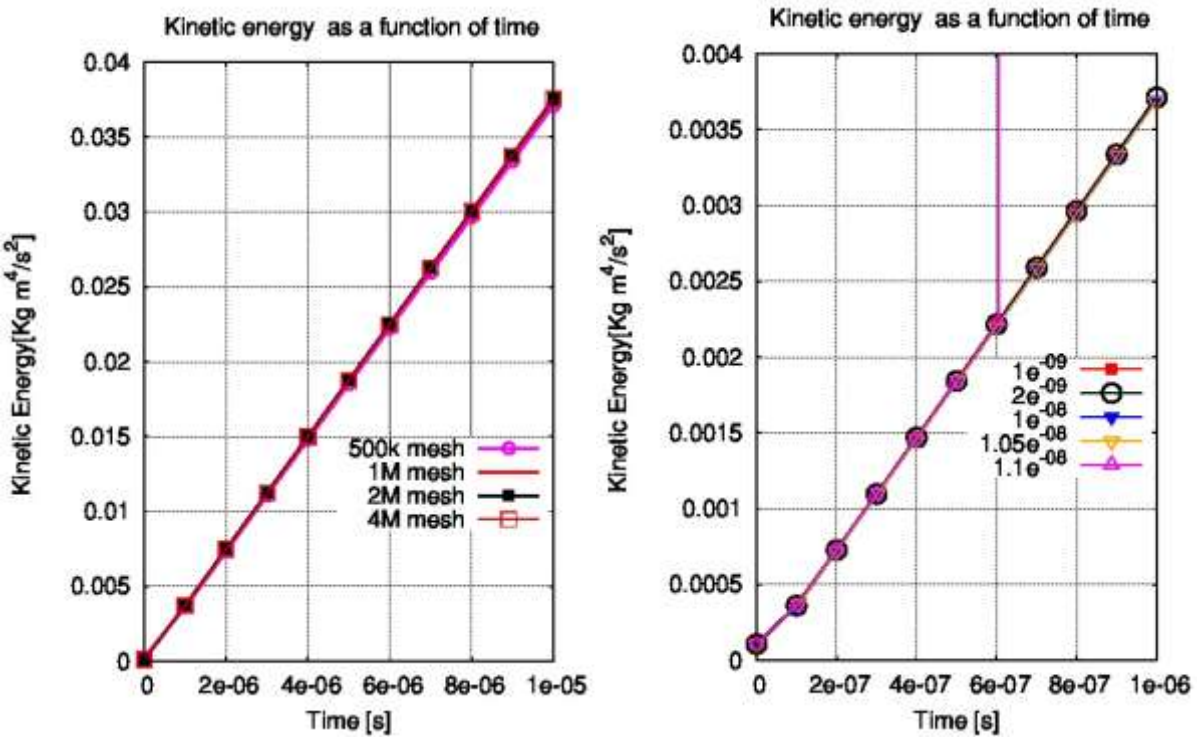

Figure 4 *Dependency of the Kinetic energy from the grid and time step resolution.*

In **Figure 4** we propose a comparison between the kinetic energies for the first stages of the developing jet, obtained using different mesh discretization and time steps. It can be clearly seen how the simulation is mesh sensitive. While simulations performed using 1, 2 and 4 millions of grid points show mesh independent results, discretization of less than 1 million of points are not convergent. The reported results refer to a limited time range in which the jet is still in the first formation regime. Furthermore, looking at the comparison between the different time discretization for a mesh of 4 millions of points, one can observe that the choice of coarse timestep quickly leads to instability of the solution. This can be observed in **Figure 4** as time step values of 10^-8 seconds lead to an unstable behavior of the solution. In particular, while small differences can be observed between a time discretization of 10-8 and 10-9 sec, using a slightly coarser timestep leads to a divergence of the kinetic energy which can numerically result in a floating point exception.

With reference to the mentioned setups, we, therefore, recommend performing a mesh and time step analysis, and as a general guideline, using a time step of 10^-9 for the first regime.

Mean profiles of the formed Jet

The jet reaches the outlet region in approximatively 0.0003 s, from this point (that determines the second flow regime) larger time step can be adopted. As shown in **Figure 2** in this configuration, the waterjet is traveling across the mixing chamber through the focusing tube and exiting the nozzle. It is possible to observe how in the main part of the mixing chamber the fluid profile is more homogeneous, while in the converging part more chaotic and turbulent structures are observed. In **Figure 2** the scale of the velocity norm has been chosen in order to make observable the difference in the velocity of the gas phase which, within the mixing chamber and the converging part of the focusing tube, remains significantly lower than the jet velocity.

In these regions, the highest velocity gradients can be observed in proximity of the jet interface, and this region can benefit from a grid refinement as the reconstruction of both the interface within the VOF scheme, as well as the turbulent structures generated by shear, perform better on finer meshes. Those high velocity gradients around the surface of the mesh are also the reason why the problem of the initial condition for the simulation was not addressed here. As a matter of fact, within the first regime, generating syntetic turbulence within the static mixing chamber is not expected to affect the results of a simulation that is dominated by shear stresses of a velocity field with a norm several orders of magnitude higher than the initial one. For what concerns the simulation of the second regime we advise to use velocity fields obtained from the simulation of the first regime rather than generating syntetic, isotropic oscillations. This is because the velocity field is observed to be highly anisotropic and geometry dependent.

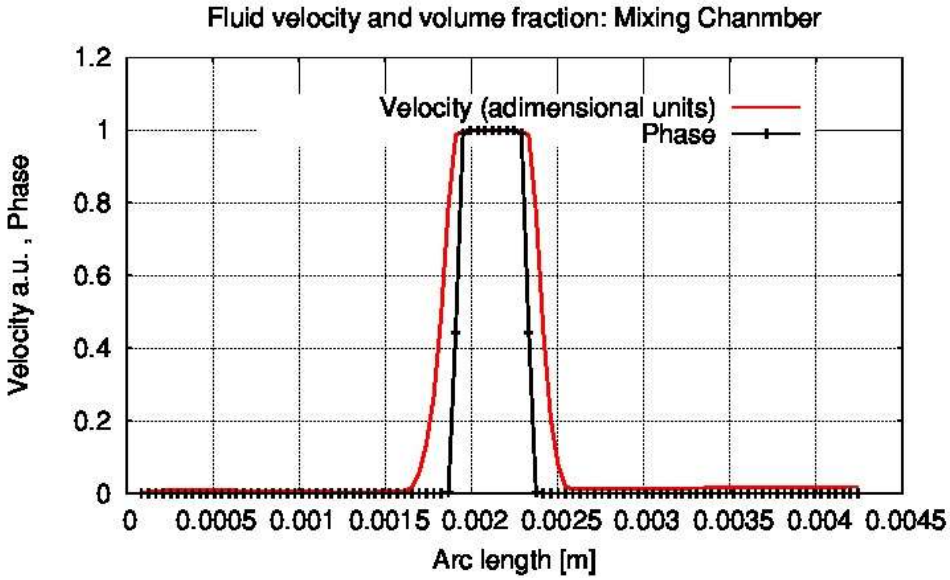

Figure 5 *Stabilized jet: velocity and volume fraction profiles in the mixing chamber*

The fluid solution in the second regime shows markedly different behavior in different regions of the nozzle. In particular, as shown in **Figure 5**, the velocity profile is not uniform within the mixing chamber, with high velocity focusing in an area close to the heavy phase and significantly low velocity for the rest of the volume. In **Figure 6** the same variable plotted along a line crossing the converging part of the nozzle are proposed.

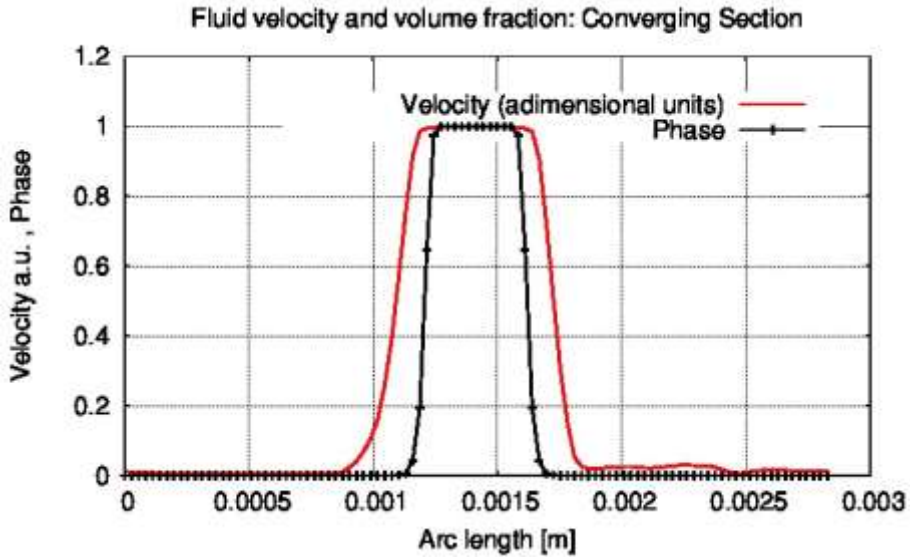

Figure 6 *Fluid solution: velocity and volume fraction profiles along the converging nozzle section.*

A non-dimensional velocity defined as the ratio between the local fluid velocity and the velocity of the fluid at the inlet, is adopted in order to observe velocity and phase fraction on a comparable scale.It is possible to observe how the profile in the converging nozzle is similar to the one observed in the mixing chamber with high velocity region focusing around the jet. Some more marked oscillations in the gas phase can be observed, still featuring velocities below the one percent of the one of the jet.
This once again, remarks how important is to correctly capture the interface between the two fluids as almost all the kinetic energy is contained within the heavy one. The profiles within the tubular part of the focusing tube are instead more homogeneous.

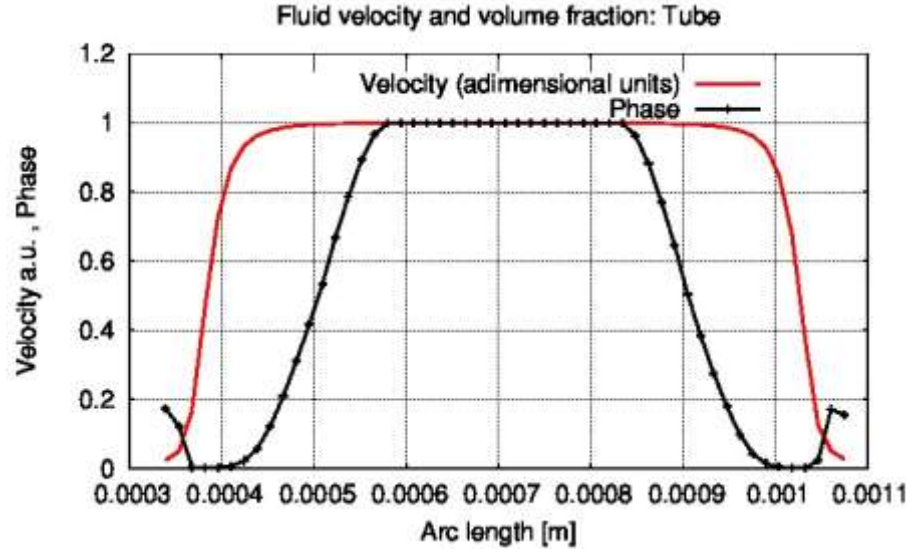

Figure 7 *Fluid solution: velocity and volume fraction profiles along a section of the focusing tube.*

Firstly, as shown in **Figure 7**, in the tubular region the jet occupies a larger part of the cross section. Secondly, the gas phase is characterized by velocities of the same order of magnitude as the jet, and high velocity gradients can be here observed at the wall boundary layer more than at the jet surface.

Oscillating Structures

As shown in **Figure 2**, some surface perturbation of the jet can be observed at the junction between the converging part of the nozzle and the tubular part, but they don't lead to the jet rupture. The air phase is characterized by lower velocities and a more chaotic behavior and in particular one can observe a recirculation trend pushing the entering air to the water inlet region, where a local depression is present due to the expansion of the jet.

As mentioned in the previous paragraph, in the proximity of the junction between the converging part of the nozzle and the tubular part, some oscillating structures can be observed. Those structures could potentially lead to the jet rupture. Jet rupture represents one of the main interesting phenomena that a numerical simulation attempts to predict, as it will induce completely different flow patterns inside the nozzle. Therefore, it is interesting to study the influence of different numerical parameters on those structures, in order to understand how predictive a simulation can actually be.

We here focus on the influence of the turbulence model and the mesh refinement on the prediction of those structures.

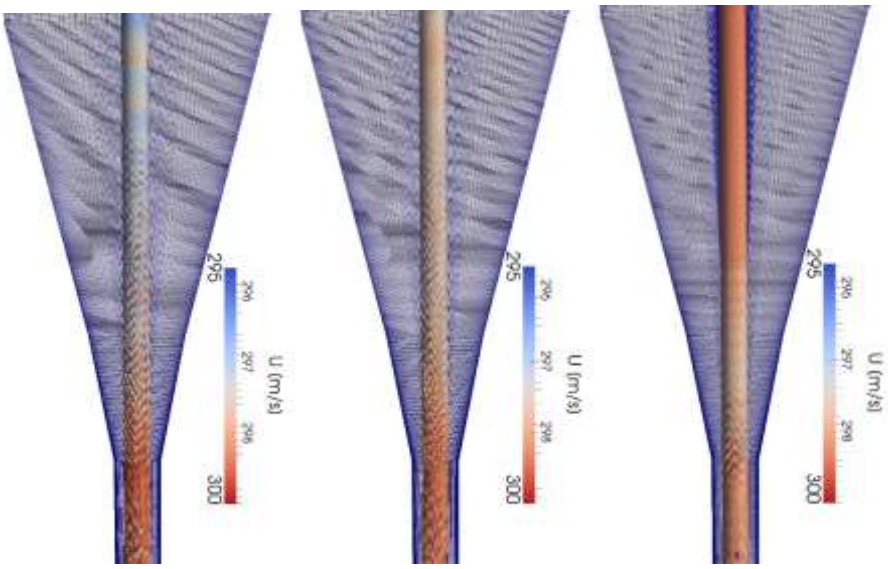

Figure 8 *Different surface structures obtained with Smagorinsky model (Left) One equation model (Center) One equation model and mesh refinement around the jet (Right)*

In **Figure 8** Different surface structures obtained with Smagorinsky model (Left) One equation model (Center) One equation model and mesh refinement around the jet (Right) a comparison between the air-water interface obtained employing respectively the Smagorinsky model, the one equation eddy viscosity model, and the one equation eddy viscosity model with a mesh refinement around the nozzle is proposed.

One can notice how both the jet structure and the local velocity at the interface are influenced by the model as well as the grid refinement, in particular, using a less dissipative model along with a local refinement of the mesh significantly reduces the dimension of the surface oscillation.

This might be linked to the interface advection scheme which is known to generate spurious currents. An investigation of the influence of the advection scheme on those structures is an interesting topic for future studies.

Costs and scalability properties

In order for numerical simulations to be routinely used as predictive tools, the issue of their

computational cost must be addressed. Hence, the scalability of a numerical algorithm is a crucial aspect for its applicability to real case scenarios.
Some works are available in literature assessing the scalability properties of OpenFOAM against relatively simple case scenario (Culpo 2012). Nevertheless, it is interesting to take track of the performance of the interFoam solver when operated in more complex setups, as this can represent an important bottleneck in the usability of the software.

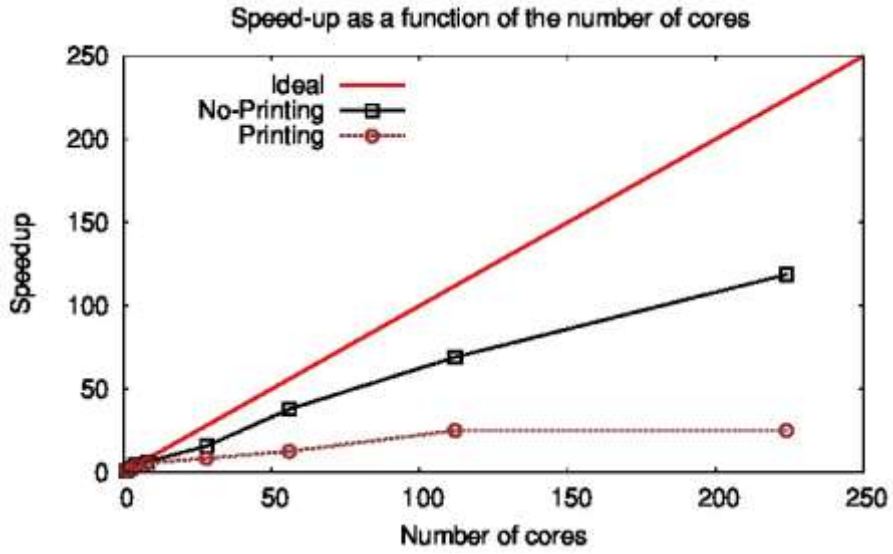

Figure 9 *Speedup as a function of number of cores with a printing rate of 1/100 step (Printing) and 1/1000 step (No-printing)*

Subsequently, we report scalability performances which are defined by investigating the ratio between the time required by the sequential job versus the time required by the job when the computation is distributed in N nodes

$$S_N = \frac{t_{clock_{seq}}}{t_{clock_{Nprocesses}}} \tag{14}$$

This is done in order to give a global indication about the cost of a simulation as the one described above, rather than to specifically analyze the parallel performances of the code, for development purposes.
The scalability tests were conducted with the iris cluster of the University of Luxembourg, consisting of 100 *DellC6320* nodes (2800 Intel Xeon E5-2680 @ 2.4 GHz, 128 GB RAM) interconnected through Infiniband EDR (100Gb/s) Network.
In **Figure 9** the speedup obtained with different printing rates are proposed. The results refer to the first 10^-6 seconds of simulation on a mesh with 4 millions hexahedral cells. Using 200 cores a speedup of approximatively 100 times can be achieved. Conversely, a single core computation of this first moments requires around three days, while the same job distributed over 224 cores, requires around 25 minutes.
It can also be observed how the input-output operation deeply affects the scalability properties of the code, therefore, reducing the output at the minimum is mandatory for this kind of simulation. These results are in accordance with the general guidelines of OpenFOAM that refers to simpler geometries. The latter recommend performing partitions featuring at least 20000 cells in order to optimize the parallel performances.
The cost considerations provided above confirm the consensus in the literature concerning both LES and VOF simulations. The computational burden of such a simulation is surely intensive, and should be generally limited to cluster computation. Nevertheless, when this is an option, combined LES and VOF simulation may represent a competitive tool to tackle very complex

flow regimes.

4. CONCLUSIONS

In this work, the capabilities of a numerical approach based on a combination between LES and VOF, for the numerical simulation of a pure water jet developing inside an AJWC nozzle have been analyzed. The basic equations and assumption of the approach have been presented, and their solution discussed with the particular reference to the OpenFOAM environment.
The influence of some basic numerical parameters, and different models on the simulation outcome has been investigated and a setup proposed for the simulation. Cost considerations have been proposed in order to investigate the feasibility of the approach and general guidelines and caveat for practitioners willing to adopt it, offered.

ACKNOWLEDGEMENTS

This project was done in collaboration with CERATIZIT Luxembourg s.a.r.l. The authors gratefully acknowledge in particular Ralph Useldinger and Michael Droeschel for providing the nozzle geometric parameters and for their thoughtful help in understanding the main problematics related to the industrial development of the nozzles. The authors gratefully acknowledge André Wilmes for his invaluable help in the revision of the manuscript.
The experiments presented in this paper were carried out using the HPC facilities of the University of Luxembourg (S. Varrette 2014). The authors gratefully acknowledge Alban Rousset for the continuous and tireless support regarding the scalability tests on the iris cluster.

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