

# Explicit calculation of natural aeration using a Volume-of-Fluid model

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## Abstract

Accurate prediction of the air-entrainment process in air-water two-phase turbulent flows is one of the most computationally challenging subjects under current investigation in hydraulic engineering. An ideal numerical model for air-entrainment needs to be accurate and fast in the definition of a macroscopic interface and simultaneously precise enough to take into account the formation of bubbles through the free-surface, their transport and their natural interactions: bubble-bubble and bubble-fluid. The problem is made more complex by the strong coupling between mesh and solution exhibited by interface capturing schemes which are commonly used for such problems. This paper examines numerical and modelling aspects of the entrainment process for two canonical cases; the 2D dam break and 3D circular plunging jet cases. We start by investigating the capacities of a Volume-of-Fluid based model to detect the free-surface and predict the velocities inside the water phase, examining the effect of coarsening and refining the mesh on the prediction of the interface location. A reformulated explicit term is used to detect bubble formation and air-entrainment at the free-surface, without the need of a calibration process and adapted to run together with Volume-of-Fluid models. The results obtained with this new approach are further compared with similar cases in the literature in terms of bubble formation and free-surface wave's amplitude. The correct definition of the free-surface was found to be strongly dependent on the mesh refinement in a way that has very significant implications for the development of air-entrainment modelling.

*Keywords:* Air-entrainment, Air-water two-phase flow, Sub-grid explicit model, Volume-of-Fluid

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## 1. Introduction

Air-entrainment occurs in most turbulent free-surface flows in nature resulting in a dispersed two-phase flow below the surface with a complex turbulent mixture structure, where compressibility and density are important physical properties affecting the air-entrainment and transport characteristics. The accurate prediction of air-entrainment is a very ambitious goal for most Computational Fluid Dynamics (CFD). The air-water interface is very unstable and the length scales of turbulence range from those influenced by the bubbles and surface tension (order from microns to

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1 millimetres) to those of the mean flow (order of meters). The simulations should be able to work on a coarse grid  
2 in order to simulate the mean flow behaviour, the free-surface position and all the similar large length scales (LLS),  
3 whilst at the same time being sufficiently detailed to model the transport of the bubbles of gas within the flowing  
4 fluid and simulate important phenomena as bubble formation, breakup, coalescence and collision, which take place  
5 on small length scales (SLS).

6 In CFD, Volume-of-Fluid (VOF) [16] and Level-Set (LS) [32] based models are typically used to capture the  
7 interface between two fluids, solving a single set of Navier-Stokes equations representing both air and water, together  
8 with an indicator function propagated by an advection equation. These interface models are widely used for many  
9 free-surface flows with macroscopic interfaces and LLS systems, as in vertical plunging jets [17, 24, 28]. Direct  
10 Numerical Simulations could simulate all aspects of the entrainment process right down to the subsequent dynamics  
11 of the bubbles; however this would be incredibly time-consuming and, in some cases, the application of VOF method  
12 to dispersed phases could lead to a non-physical interpretation of bubbles or droplets [7]. Instead, for a realistic mesh  
13 resolution the representation of the entrained air (SLS system) can be accomplished by the inclusion of an Eulerian  
14 dispersed phase model with a second set of equations representing the dynamics of the bubbles. Different approaches  
15 that follow this idea can be found in the literature. The model of Cerne et al. [7] blends the VOF interface tracking  
16 with a two-fluid model formulation [11]. In this model, in zones where the phase separation are clear and where  
17 just one fluid is present, the two-fluid model is switched off and a single set of Navier-Stokes equations together  
18 with the VOF method is solved instead. A criterion based on the local dispersion of the interface is used to switch  
19 between the two formulations, however, the accuracy of the results has exhibit a strong dependence on the value of  
20 this threshold which goes against the essence of a blending model. To overcome the dependency of the dispersion  
21 threshold, Yan and Che [39] introduced a unified solution framework for coupling VOF with a two-fluid model. The  
22 idea was to blend the two formulations ensuring the conservation of all three phases; i.e. when the LLS of air are  
23 present (phase2), the interface tracking model is activated; then when the LLS are absent from the cell, the two-phase  
24 model is used to solve for the local characteristics of the fluids (phase1 for water and phase3 for bubbles). The model  
25 shown to be efficient for the simulation of a rising bubble and a swarm of bubbles in a vertical pipe. However, volume  
26 fraction conservation when the three phases are present is not guaranteed, with particular losses occurring for phase2.  
27 Wardle and Weller [36] introduced in OpenFOAM® a hybrid formulation based on the combination of an Eulerian  
28 multifluid framework (to solve the SLS) with an interface capturing method using VOF (to solve the LLS), along with  
29 a switching function based on the work of Cerne et al. [7]. Shonibare and Wardle [33] extended this hybrid model to  
30 deal with variable bubble size using the reduced population balance method and applied it to a vertical plunging jet. A  
31 similar conceptual approach to the last was implemented by Marschall and Hinrichsen [25] in OpenFOAM® for solely  
32 two-phase flows. Hänsch et al. [14] extended the inhomogeneous Multiple Size Group (MUSIG)-approach by adding  
33 a continuous gas phase in order to solve simultaneously in the same domain, dispersed and continuous gas phases.  
34 The transition between the two was modelled by the "clustering method" that utilises an additional interfacial force  
35 applied to the Eulerian multifluid framework. The solutions were verified for the case of plunging jets. Yet another

1 type of subgrid models combine an interface model (VOF/LS) with the two-phase flow formulation by including a  
2 source term to detect the air formation at the free-surface [15, 22, 23]. Source terms at the interface relate the rate of  
3 bubble formation to surface flow properties such as local turbulence and the size of interface waves.

4 A typical experiment in which air-entrainment has been observed and extensively studied is the plunging jet  
5 [1, 2, 4, 8, 10, 18, 29, 31]. Plunging jets are efficient mechanisms to dissipate energy, and in doing so produce  
6 and transport significant quantities of bubbles through the body of the water. Practical examples of plunging jets  
7 include dam spillways and plunge pool stilling basins, waste-water treatment, oxygenation of bioreactors and river  
8 re-oxygenation. Air-entrainment in the pool depends upon the jet impact, the physical properties of air and water, the  
9 jet diameter, the free falling distance between the jet and the pool, and the jet turbulence. At the intersection point of  
10 the jet and the water, free-surface instabilities are the reason for air-entrainment when the jet impact velocity exceeds a  
11 characteristic velocity or onset velocity [8]. Slightly above the onset velocity, the air entrains in the form of individual  
12 bubbles and small pockets. At the impact point, the free-surface is observed to assume a shape which balances the  
13 forces between both sides of the interface. With increased liquid velocity at the jet impact zone, the local stress  
14 is increased, and small cavities are formed and pulled bellow the free surface. Deeper into the pool, these cavities  
15 decrease in radius but continue balancing the surface forces. A critical condition is reached where either (a) a steady  
16 balance of forces can no longer be maintained or (b) the inferior end of the cavity or the free-surface is disrupted by  
17 disturbances at the free jet stream and/or on the pool. The result is the sequential generation of small bubbles or air  
18 pockets below the free surface. In this case, the rate of air-entrainment is very small and challenging to measure with  
19 common intrusive probes. At higher jet velocities, a substantial air pocket or sheath is formed at the periphery of the  
20 jet below the free surface; this air pocket is unstable and its breakup forms the entrained air bubbles which are then  
21 the subject of transport within the body of the water [4].

22 This paper proposes a reformulated explicit term for bubble formation that is independent of calibrating factors  
23 by using a renewed formula for surface wave's amplitude. The explicit term was included in the well validated  
24 *interFoam* VOF solver from the OpenFOAM® toolkit to accurately predict the interface position [19, 20, 21]. An  
25 interface location coefficient is necessary for this coupling. This study represents a starting point for the development  
26 of a VOF-based model with a modelled closure to represent the entrained air. Section 2 develops the equations behind  
27 the numerical model along with the interface location technique and the air-entrainment term. Section 3 presents the  
28 results and their discussion for two canonical test cases; a 2D dam break case and a 3D plunging jet. Finally, section 4  
29 presents conclusions.

## 30 2. Numerical Model

### 31 2.1. General concepts

32 Interface capturing models such as the VOF model (implemented in the OpenFOAM® toolkit as *interFoam*) rep-  
33 resent the free-surface dynamics of the two phases in terms of single phase-weighted velocity and pressure fields,

1 governed by a single set of mass and momentum equations. For a system of isothermal, incompressible and im-  
 2 miscible two-phase flow, the Reynolds averaged equations for mass conservation and momentum are written in their  
 3 conservative form:

$$\nabla \cdot \mathbf{U} = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) = -\nabla p^* + \mathbf{g} \cdot \mathbf{x} \nabla \rho + \nabla \cdot \boldsymbol{\tau} + \mathbf{f} \quad (2)$$

4 where  $\rho$  ( $kg\ m^{-3}$ ) is the fluid local density,  $\mathbf{g}$  ( $m\ s^{-2}$ ) the gravitational acceleration,  $\mathbf{U}$  ( $m\ s^{-1}$ ) the velocity vector,  
 5  $\boldsymbol{\tau}$  ( $Pa$ ) the shear stress tensor,  $p^*$  ( $Pa$ ) a modified pressure adopted by removing the hydrostatic pressure ( $\rho \mathbf{g} \cdot \mathbf{x}$ )  
 6 from the total pressure and  $\mathbf{f}$  ( $kg\ m^{-2}\ s^{-2}$ ) the volumetric surface tension force. It is important to note that in interface  
 7 capturing models, the velocity vector  $\mathbf{U}$  acts as a shared velocity of the two fluids, i.e.  $\mathbf{U} = \mathbf{U}_{f1} = \mathbf{U}_{f2}$ , rather than in  
 8 mixture models where  $\mathbf{U}_{fk}, k = \{1, 2\}$  can assume different magnitudes.

9 The decomposition of the viscous stress term is given by the Stokes's stress constitutive equation (Eq. 3) where  
 10  $\mu$  ( $kg\ m^{-1}\ s^{-2}$ ) is the dynamic viscosity.

$$\nabla \cdot \boldsymbol{\tau} = \nabla \cdot [\mu(\nabla \mathbf{U} + (\nabla \mathbf{U})^T)] = \nabla \cdot (\mu \nabla \mathbf{U}) + (\nabla \mathbf{U}) \cdot \nabla \mu \quad (3)$$

11 Together with the previous equations, *interFoam* uses the VOF technique [16] to capture the interface between the  
 12 two fluids by solving a transport/advection equation (Eq. 4). Basically, at each cell of the domain we define an alpha  
 13 ( $\alpha$ ) value representing the fraction of the volume of the fluid in that cell [6, 34]. Cells completely filled with fluid  
 14 1 ( $f1$ ) will be represented by  $\alpha = 1$  and cells filled with fluid 2 ( $f2$ ), by a value  $\alpha = 0$ . The interface is localised  
 15 to the cells where  $\alpha$  is intermediate between these two values. The advection equation also includes an interfacial  
 16 compressive term to confine this interface region into as small a region of space as possible (the last term on the l.h.s.  
 17 of Eq. 4) [3, 37], rather than using interface reconstruction schemes [30].

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{U}) + \nabla \cdot [\mathbf{U}_c \alpha (1 - \alpha)] = 0 \quad (4)$$

18 The term  $\alpha(1 - \alpha)$  ensures that the compressive term is calculated just at the interfacial cells of the domain, while  
 19  $C_\alpha$  is a binary coefficient that activates ( $C_\alpha = 1$ ) or deactivates ( $C_\alpha = 0$ ) the interface sharpening term. The source  
 20 term also includes the compressive velocity ( $\mathbf{U}_c$ ) that acts as a velocity perpendicular to the interface and is written as:

$$\mathbf{U}_c = C_\alpha |\mathbf{U}| \frac{\nabla \alpha}{|\nabla \alpha|} \quad (5)$$

21 It is worth emphasising that the interface is merely being localised within the volume of space for which  $0 < \alpha < 1$ .  
 22 For simplicity it is often taken that the interface is represented in post-processing by the isosurface  $\alpha = 0.5$ , but strictly  
 23 speaking this is simply an assumption, one which we wish to explore in the present work.

1 When  $\alpha$  assumes values between 0 and 1, the physical properties of the two-fluid mixture are defined as a weighted  
2 average of two fluid properties:

$$\rho = \alpha\rho_{f1} + (1 - \alpha)\rho_{f2} \quad (6)$$

$$\mu = \alpha\mu_{f1} + (1 - \alpha)\mu_{f2} \quad (7)$$

3 The volumetric surface force function is explicitly estimated by the Continuum Surface Force (CSF) model (Eq. 8)  
4 developed by Brackbill et al. [5] where  $\sigma$  ( $kg\ s^{-2}$ ) is the surface tension and  $\kappa$  ( $m^{-1}$ ) is the surface curvature calculated  
5 as  $\kappa = \nabla \cdot (\nabla\alpha/|\nabla\alpha|)$ .

$$\mathbf{f} = \sigma\kappa\nabla\alpha \quad (8)$$

6 The turbulent kinetic energy ( $k$ ) and rate of energy dissipation ( $\varepsilon$ ) are calculated using the realizable  $k$ - $\varepsilon$  turbulence  
7 model, with the effective dynamic viscosity ( $\mu$ ) being given by a sum of molecular viscosity ( $\nu$ ) and turbulent viscosity  
8 ( $\nu_t$ ) ( $\mu = \rho(\nu_t + \nu)$ ). The choice of the realizable  $k$  -  $\varepsilon$  is based on its known ability to accurately predict the spreading  
9 rate of both planar and round jets [13, 40]. This turbulent model is also superior to the standard  $k$  -  $\varepsilon$  model for the  
10 simulation of flows involving rotation, boundary layers under strong pressure gradients, separation and recirculation.  
11 The realizable  $k$  -  $\varepsilon$  also requires less computational time than Re-Normalisation Group (RNG)  $k$  -  $\varepsilon$  which was  
12 derived to deal with the swirl effect on turbulence [13].

## 13 2.2. Bubble formation

14 The air-entrainment process is described by the inclusion of a function  $E_g$  ( $m^{-3}s^{-1}$ ) which describes the rate of  
15 bubble generation at the free-surface. It is calculated at the end of each time-step and does not change any convergence  
16 process within the standard solver. The formulation of this variable follows closely the work of Ma et al. [23], who  
17 represent it as:

$$E_g = \left\langle \frac{\partial \mathbf{U}_n}{\partial \mathbf{n}} \right\rangle \frac{a}{\phi_{ent} V_g} \quad (9)$$

18 where  $\mathbf{U}_n$  is the normal velocity component to the free-surface,  $a$  ( $m$ ) is the amplitude of the cavities formed at the  
19 free-surface (Fig. 1),  $V_g$  ( $m^3$ ) is the volume of a sphere calculated assuming an averaged bubble diameter and  $\phi_{ent}$  ( $m$ )  
20 is the interface thickness, given by  $\phi_{ent} = 0.05L$ , where  $L$  ( $m$ ) is a characteristic linear dimension (equal to the pipe  
21 diameter for pipe flow or the hydraulic diameter when dealing with river systems). The symbols  $\langle \rangle$  are used to turn  
22 the normal derivative zero if its value is less than zero:

$$\langle f(x) \rangle = \begin{cases} f(x) & , f(x) > 0 \\ 0 & , f(x) \leq 0 \end{cases} \quad (10)$$

1 A rough way to predict the volume fraction occupied by the bubble phase at each cell can be done by  $E_{g,frac} =$   
 2  $E_g V_g \Delta t$ , where  $\Delta t$  (s) is the computational time step. This neglects the advection and diffusion terms of the void  
 3 fraction conservation and transport at the free-surface, however, when the velocities are small, it can provide a good  
 4 first impression of void fraction magnitude.

5 In this work and according to Ervine and Falvey [12], the amplitude of the surface disturbances ( $a$ ) is considered  
 6 as having the same order of magnitude as the radius of the turbulent eddies at the free-surface ( $l'$ ). From here, we  
 7 obtain:

$$a = l' / 2 = C_\mu^{3/4} \frac{k^{3/2}}{2\varepsilon} \quad (11)$$

8 where  $C_\mu$  is a turbulence model constant which in the  $k - \varepsilon$  model theory assumes the value 0.09 [27, 35]. Similar  
 9 criteria is used by Hirt [15] to calculate surface disturbances at free-surface in the CFD commercial code Flow-3D®.  
 10 In the model of Ma et al. [23], the amplitude of the surface disturbances ( $a$ ) is calculated as  $a = C_{ent} k/g$ , where  $C_{ent}$   
 11 is a constant that needs to be calibrated for each case.

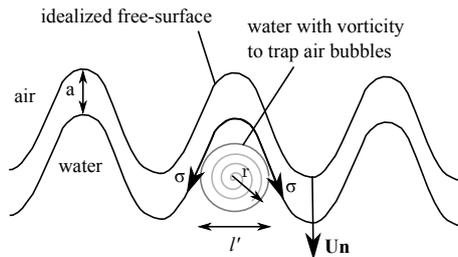


Figure 1. Free-surface with physical parameters used. Adapted from Ervine and Falvey [12].

### 12 2.3. Interface location

13 The location of the air-entrainment in our VOF model does not follow the same criteria as in work from Ma et al.  
 14 [23] (which uses LS methods). In LS, the interface can either be located by assuming a certain threshold for interface  
 15 thickness, or by limiting the velocity to some threshold value. However, in VOF models, the interfacial structure can  
 16 only be detected by the change of volume fraction or by its gradient, as for example in the the algebraic equation  
 17 formulated by Hänsch et al. [14]. In this work,  $E_g$  is calculated using a similar criterion as used for the compressive  
 18 term, i.e. by multiplying the last by the function  $\phi_{FS} = 4\alpha(1 - \alpha)$ . This will work as a masking function, which returns  
 19 0 when calculated in cells away from the free-surface and 1 at the interface. From the fact that this coefficient uses  
 20  $\alpha$  to detect the free-surface, it is fairly essential keep the interface confined to a small number of cells possible, and  
 21 from this we see the need of a mesh dependence study.

### 3. Results: Example cases

#### 3.1. 2D Dam-break

The example presented here is the benchmarking 2D dam-break case without obstacle. This case is used by many other authors to show the capabilities of free-surface models and of interest for this work as it can exhibit several possible zones of natural aeration of the flow and the interface location. A static water column is initially held against the left wall by a vertical gate as shown in Fig. 2. On removing the gate, the water column collapses and the resulting slosh hits the right wall before returning in the form of a small propagating wave.

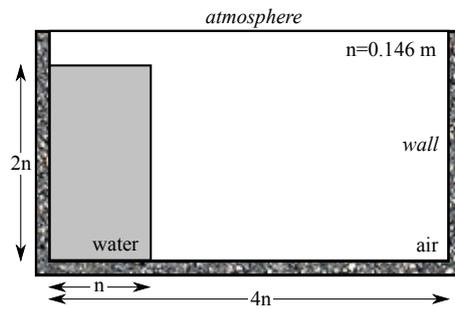


Figure 2. 2D dam-break domain.

Numerical simulations are performed in four different meshes:  $16 \times 16$ ,  $32 \times 32$ ,  $46 \times 46$  and  $64 \times 64$  cells. The fluid properties were chosen to represent the physical values of water and air at  $15^\circ\text{C}$ . Surface tension is set to  $0.072 \text{ kg s}^{-2}$ , the averaged bubble radius ( $r_b$ ) is  $0.002 \text{ m}$  and  $\phi_{ent} = 0.05n = 0.0071 \text{ m}$ , where  $n$  stands for the water column width (Fig. 2). The domain is bounded by walls with the exception of the top one that represents the atmosphere. The pressure at the walls is given by Neumann boundary conditions (BC), whilst the velocity is set to no-slip (Dirichet-BC).

Figure 3 presents snapshots of the free-surface position for  $t = 0.1, 0.3, 0.7$  and  $1.0 \text{ s}$  for finer mesh. Figure 3a shows the  $\phi_{FS}$  function and Fig. 3b the values of the terms  $E_g$  and  $E_{g,frac}$ . Figure 4 demonstrates the influence of changing the mesh size on the free-surface position for  $t = 0.8 \text{ s}$ . Again, Fig. 4a shows the  $\phi_{FS}$  function and Fig. 4b the values of the terms  $E_g$  and  $E_{g,frac}$ .

The function used to detect the free-surface has demonstrated excellent accuracy throughout the simulation time even when a large cavity is formed inside the fluid (Fig. 3a4). One second after the collapse of the water column (Fig. 3b1), due to the friction with the bottom wall, air is forced to enter from the bottom, where the term  $E_g$  assumes high values. High values of air-entrainment can also be seen in the zone where the water collides with the right wall (Fig. 3b2) and on its way back in the area where a small cavity of the breaking wave is formed (Fig. 3b3). The mesh influence study show a large difference between meshes  $16 \times 16$  and  $32 \times 32$  cells both for  $\phi_{FS}$  and  $E_g$  values. The free-surface in the last three finer meshes have a similar shape, whereas the maximum values of  $E_g$  are on the order of  $4 \times 10^7$  in the mesh with  $32 \times 32$  cells (Fig. 4b2) and of the order of  $5 \times 10^7$  for  $46 \times 46$  and  $64 \times 64$  cells (Fig. 4b3 and

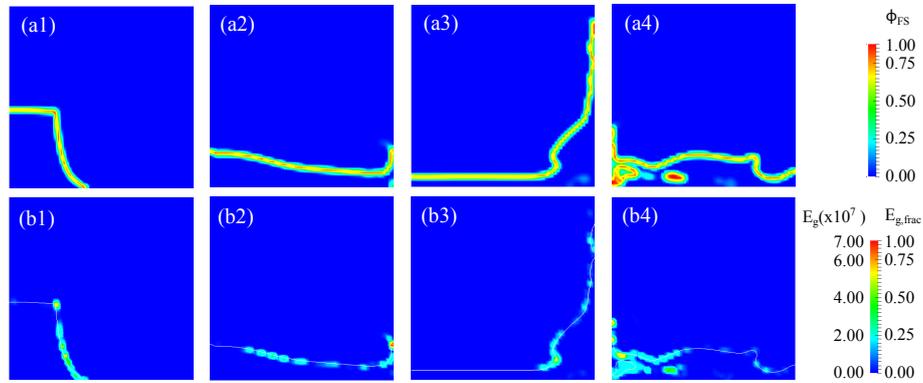


Figure 3. Dam-break process for the time steps  $t = 0.1, 0.3, 0.7$  and  $1.0s$  using the finest mesh ( $64 \times 64$  cells). Top images are photographs of the experiment, middle figures (a) show the function to detect the free-surface position ( $\phi_{FS}$ ) and bottom figures (b) show the bubble formation term ( $E_g$ ) and its volume fraction on the cells ( $E_{g,frac}$ ).

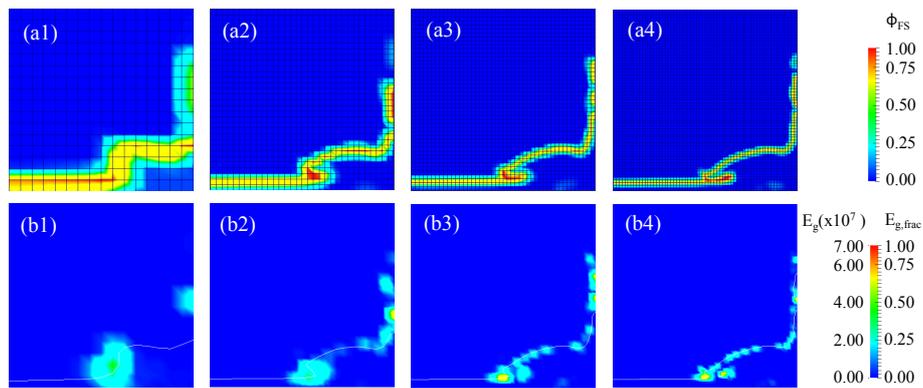


Figure 4. Mesh influence study of dam-break case at  $t = 0.8s$ . From the left to right the meshes are:  $16 \times 16$ ,  $32 \times 32$ ,  $46 \times 46$  and  $64 \times 64$  cells. Top figures (a) show the function to detect the free-surface position ( $\phi_{FS}$ ) and bottom figures (b) show the bubble formation term ( $E_g$ ) and its volume fraction on the cells ( $E_{g,frac}$ ).

1 Fig. 4b4). This shows that, even with the decreasing of the mesh size, the values of  $E_g$  are quasi mesh independent,  
2 although its spacial location is sensible to the grid size.

### 3 3.2. 3D vertical plunging jet

4 The 3D computational domain represents a part of the experimental apparatus used by Chanson and Manasseh  
5 [9], schematically represented in Fig. 5. This experimental work provides extensive data on void fraction and bubble  
6 count rate inside the water, which despite not being relevant in this work, will be useful to compare the results when a  
7 full air-entrainment model is completed. The simulation of a 3D domain rather than a 2D domain allows us to better  
8 represent all the flow structures across the interface which are manifestly 3D structures. Also, comparisons to the 3D  
9 model of Ma et al. [22] in terms of  $E_g$  values and later for void fractions can be done clearly and without constraints  
10 (note that Ma et al. [22] applied their model to the same case in their study).

11 A plunging jet of clean water is ejected from a  $d_0 = 0.025$  m diameter nozzle, into a pool of stationary water. The  
12 distance between the water surface and the nozzle is constant and equal to  $x_1 - x_0 = 0.1$  m. The impact velocity of  
13 the jet at the pool is  $U_1 = 3.5$  m  $s^{-1}$ . Velocity profiles are obtained at different horizontal planes from  $0.8d_1$  (m) to  
14  $10.0d_1$  (m) below the initial pool free-surface, where  $d_1$  is the jet diameter at the impact zone ( $d_1 \approx 0.024$  m) and  
15  $r_1$  the jet radius ( $r_1 \approx 0.012$  m). To investigate the impact of mesh resolution on the solution, three different grids  
16 with different mesh resolutions were generated and their characteristics summarized in Table 1. In order to decrease  
17 the computational time, instead of using spatially uniform meshes, three zones with different grid sizes are created as  
18 defined in Fig. 5.

|                        | cell length, $\Delta x$ (m) |                    |              | N.Cells   | N.Proc. | Time (s) |
|------------------------|-----------------------------|--------------------|--------------|-----------|---------|----------|
|                        | jet and surface (Z1)        | centre-bottom (Z2) | lateral (Z3) |           |         |          |
| Coarse grid (G0.005)   | 0.005                       | 0.005              | 0.005        | 84 192    | 16      | 1963     |
| Medium grid (G0.0025)  | 0.0025                      | 0.0025             | 0.005        | 521 124   | 16      | 39 891   |
| Fine grid (G0.00125)   | 0.00125                     | 0.0025             | 0.005        | 2 104 460 | 16      | 281 073  |
| Finnest grid (G0.0008) | 0.0008 - 0.00125*           | 0.0025             | 0.005        | 2 458 835 | 32      | 284 242  |

Table 1. Grid characteristics to demonstrate the mesh dependency. Zones Z1, Z2 and Z3 are represented in Fig. 5. \*In this case, cells with 0.0008 m edges were placed just on the intersection between jet and pool.

19 The initial conditions are set as represented in Fig. 5. The pool is filled with stationary water ( $U = 0$  m  $s^{-1}$ ) to a  
20 constant depth. A cylindrical column of water with a fixed inlet velocity is used to represent the jet. In order to get fast  
21 convergence of the solution and computational stability the air velocity in the vicinity of the jet is set equal to the jet  
22 velocity. Four different boundary conditions (BC) are used in this simulation as shown in Fig. 5. The velocity at the  
23 inlet is calculated based on the jet impact velocity using Bernoulli's principle,  $U_0 = \sqrt{U_1^2 - 2g(x_1 - x_0)} = 3.21$  m  $s^{-1}$ .  
24 The atmosphere just allows the air to leave the domain by setting  $U$  as dependent on pressure with total pressure set  
25 as zero. The lateral boundaries have Neumann-BC for  $\alpha$ ,  $p$  equal to hydrostatic pressure and non-slip Dirichet-BC  
26 for  $U$ . For the bottom boundary the hydrostatic pressure is set to  $\rho_f 1g(x_{bottom} - x_1) = 3915.2$  Pa and Neumann-BC are  
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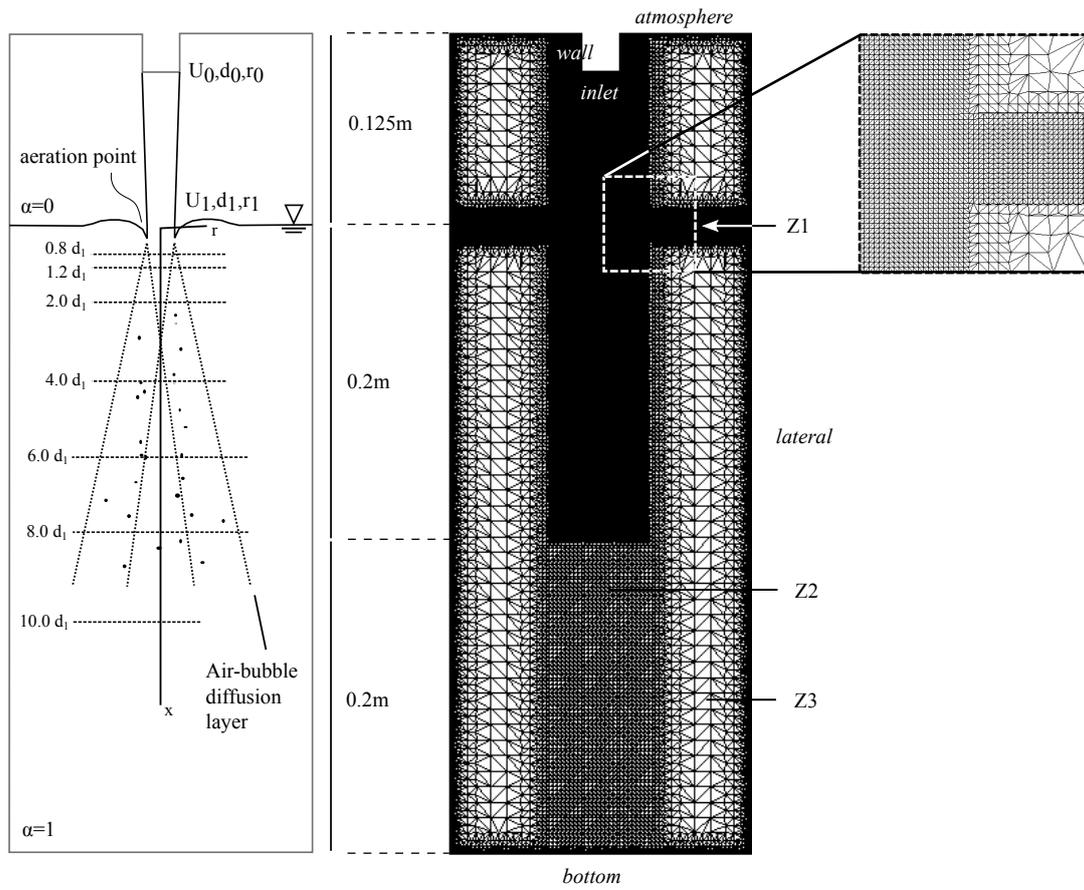


Figure 5. Vertically-centred slice of the computational domain for the 3D circular plunging jet problem. The mesh presented corresponds to G0.00125 (Table 1).

used for the remaining variables. In order to verify the correct application of these boundary condition, we simulated with the coarser mesh the full experimental domain and verified that the results in terms of  $U$ ,  $p$  and  $\alpha$  in the zone close to the jet agreed with those calculated on the smaller domain.

The  $k$ ,  $\varepsilon$  and  $\nu_t$  variables at the *inlet* are calculated by:

$$k_0 = \frac{3}{2}(U_0 I_0)^2 = 0.000235 \text{ m}^2 \text{ s}^{-2} \quad (12)$$

$$\varepsilon_0 = C_\mu \frac{k_0^{3/2}}{l_0} = 0.000371 \text{ m}^2 \text{ s}^{-3} \quad (13)$$

$$\nu_{t,0} = C_\mu \frac{k_0^2}{\varepsilon_0} = 1.3416 \times 10^{-5} \text{ m}^2 \text{ s}^{-1} \quad (14)$$

where  $U_0$  ( $\text{m s}^{-1}$ ) is the mean flow velocity at jet inlet;  $I_0$  (%) the turbulent intensity at jet inlet, set as 0.39 % (value from the experiment of Chanson and Manasseh [9]) and  $l_0$  ( $\text{m}$ ) the length scale at jet inlet, in this study calculated as  $l_0 = 0.035 d_0$  ( $\text{m}$ ). On the remaining boundaries  $k_0$ ,  $\varepsilon_0$  and  $\nu_{t,0}$  are defined as Dirichlet-BC. The fluid properties were chosen based on the physical values of water and air at 15°C. Surface tension is set to  $0.072 \text{ kg s}^{-2}$ , bubble radius ( $r_b$ ) is  $0.00175 \text{ m}$  and  $\phi_{ent} = 0.0012 \text{ m}$ . The simulation ran with the extra term activated from the beginning. A steady-state solution was acquired after 6500 time iterations with an averaging time step of  $0.0001 \text{ s}$  for the simulation with coarser mesh, which gives a final time of about  $0.65 \text{ s}$ . This state was identified from the criteria that the residuals of  $k$ ,  $\varepsilon$  and  $p$ , and the volume fraction on the domain were constant in time. The averaged values from the last  $0.1 \text{ s}$  were used to plot the results. Maximum Courant number and maximum Courant for  $\alpha$  are both defined to 0.5.

### 3.2.1. Radial velocity profiles

The liquid velocity plays a key role in the transport of bubbles into the fluid. This therefore represents a good variable with which we can validate the solution and demonstrate grid independence. In order to prove this, in this section, the computed radial distribution of liquid velocity is presented. Figure 6 shows the dimensionless radial velocity profiles ( $U/U_1$ ) on the pool depths of  $x = 0.8d_1$ ,  $1.2d_1$  and  $2.0d_1$  for the four meshes presented. These three profiles were chosen here because these were the positions where Chanson and Manasseh [9] measured experimentally the air concentration profiles.

From the data in Fig. 6, it can be seen that the velocity has the maximum value at the jet centreline and tends to zero away from the centre. For a free jet in air, the greater the distance from the jet inlet, the lower and wider the velocity profile becomes, eventually assuming the universal shape of a Gaussian curve [26]. However, for a jet impacting a pool it is also known that the profiles closer to jet impact zone are affected by the abrupt decreasing of the velocity from its maximum value to zero. This situation is clearly visible in the results of the finer mesh (Fig. 6). The velocity on the jet axis was equal to  $3.5 \text{ m s}^{-1}$  ( $U/U_1 = 1.0$ ), and this value remained constant until a distance equal to the radius of the jet. After reaching a distance of  $1.0r/r_1$ , the velocity passed from this maximum to roughly zero in about  $0.25r/r_1$ . On the coarser meshes, numerical viscosity smooths the profile; the axis velocity remains correct

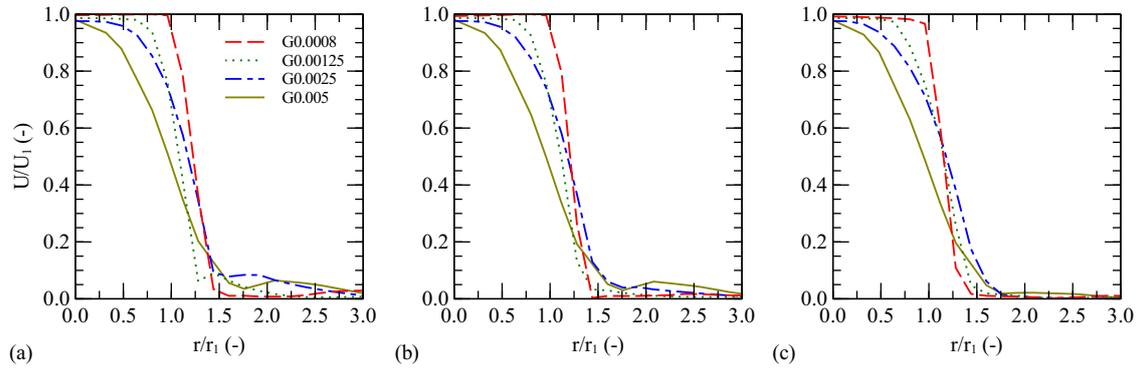


Figure 6. Liquid velocity for pool depths (a)  $x = 0.8d_1$  (m), (b)  $x = 1.2d_1$  (m) and (c)  $x = 2.0d_1$  (m).  $U_1 = 3.5 \text{ m s}^{-1}$ ,  $d_1 = 0.024 \text{ m}$  and  $r_1 = 0.012 \text{ m}$ .

1 and the curves tends to zero velocity at similar values of  $r/r_1 \approx 1.5$ , but the shape of the curve between these extremes  
 2 is significantly affected, with a smoother shape for the coarser meshes indicating a reduction of velocity inside the jet  
 3 ( $r/r_1 < 1.0$ ). On the finest mesh the jet flow remains as a plug flow and the variation in velocity is restricted to the air  
 4 region around it. From these results we can also assume that we reach a mesh independent solution for the grid with  
 5  $\Delta x = 0.0008 \text{ m}$ .

6 More interesting results are obtained when the profiles are plotted in a different dimensionless form. In a developed  
 7 flow region the curve must present an self-similar shape in all the sections and it can be compared with the solutions  
 8 of Wilcox [38](Fig. 7a) and Tollmien [1, 29](Fig. 7b). On both, the local velocity  $U$  is divided by the velocity on  
 9 the jet axis  $U_x$ . The radial distance  $r$  is rendered dimensionless by dividing it by the vertical distance  $x$  for Wilcox  
 10 profile and by dividing  $r$  by  $b$  for Tollmien solution, where  $b$  represents the value of  $r$  where the velocity is half of the  
 11 velocity on the jet axis. Note that in a developing flow region  $U_x = U_1$ .

12 Figure 7 presents the fluid velocity profiles for horizontal profiles at distances  $x = 0.8d_1$  to  $x = 10.0d_1$  from the  
 13 beginning of jet impact zone and the comparison with the solutions of Wilcox and Tollmien using mesh G0.0008.  
 14 Since these solutions were derived to predict the velocities in the fully developed flow region [1], we must keep in  
 15 mind that they will not necessarily correctly predict the flow at the jet beginning, and this is indeed what we find.  
 16 From the analysis of Fig. 7a and Fig. 7b it can be noted that the profiles are converging to a self-similar solution,  
 17 however, the first three profiles are quite a long way away from the fully developed solution, indicating that those are  
 18 within the developing flow region and can not be used as a comparison. The true convergence and self-similarity was  
 19 achieved slightly after  $4.0d_1$ , as is better shown in Fig. 7a. The profile at  $x = 10.0d_1$  is shown not to converge on the  
 20 approximation to the Tollmien solution at distances to the axis of the jet lower than  $1.0r/b$  (Fig. 7b). At this depth the  
 21 mesh is coarser and consequently the results are less accurate. The velocities plotted at profiles  $x = 0.8d_1$  to  $8.0d_1$   
 22 were evaluated in the refinement zone Z1 – Z2, whereas  $10.0d_1$  were evaluated further down in the zone just covered  
 23 by the refinement Z2 (Fig. 1).

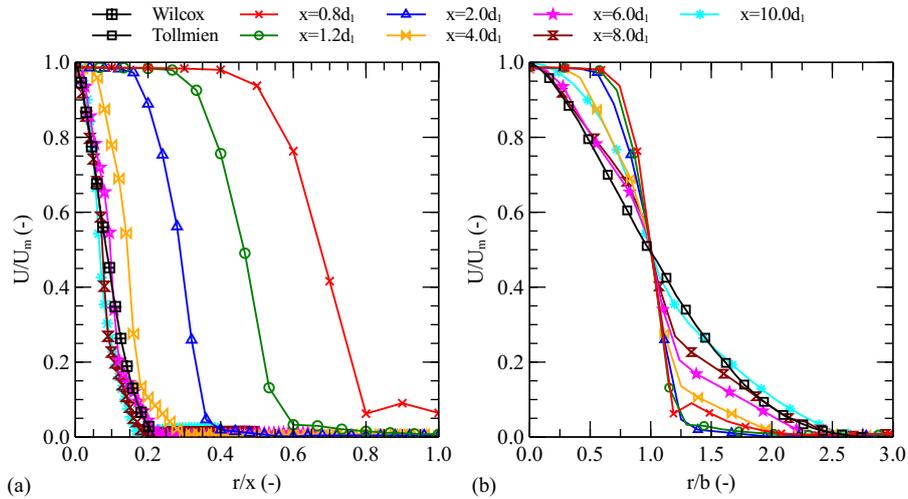


Figure 7. Liquid velocity profiles for some horizontal profiles along the pool depth ( $x = 0.8d_1$  to  $10.0d_1$ ).  $U_x$  is the velocity on the jet axis,  $x$  is the vertical direction and  $b$  the value of  $r$  where the velocity is half of the velocity on the jet axis. The profiles are compared with the solutions of (a) Wilcox and (b) Tollmien using mesh G0.0008

1 3.2.2. Free-surface detection and bubble formation

2 The dependence of the free-surface location on the  $\alpha$  value and on the mesh refinement is shown in Fig. 8.  
 3 Figure 8a shows the variation of the free-surface shape with  $\alpha$  values on the finest mesh (G0.0008). Figure 8b shows  
 4 the free-surface for different meshes keeping the value of alpha constant to 0.3.

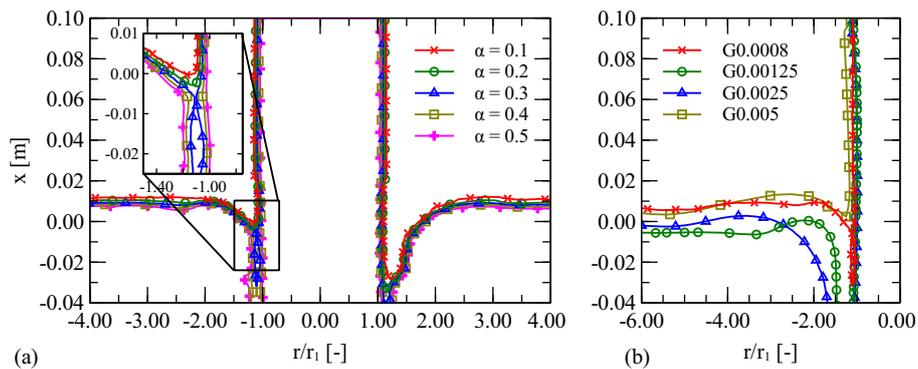


Figure 8. Temporal-averaged free-surface and air-cavity determined by: (a) keeping the finer mesh (G0.0008) and changing  $\alpha$  value and (b) keeping  $\alpha = 0.3$  and changing the mesh refinement. The  $x$  (m) axis is the vertical direction and  $r_1$  (m) the jet radius at impact zone ( $r_1 = 0.012$  m).

5 In a VOF simulation, the value of  $\alpha$  that correctly represents the interface is not clearly defined; the interface  
 6 is instead captured in the values between 0 and 1. Although some authors use a value of 0.5, the appropriate value  
 7 should be subject of an analysis depending on the case under consideration. The  $\alpha$  isosurface is strongly influenced

1 by turbulence at the free-surface and by what value of  $\alpha$  we wish to consider as a threshold for the interface. Figure 8  
2 shows the temporally averaged shape of the free-surface and the air cavity for various values of  $\alpha$ . The overall shape  
3 of the free-surface (Fig. 8a) seems insensitive to the value of  $\alpha$  used, however the cavity shape increases substantially  
4 in volume with increasing values of  $\alpha$ . In fact, the interface fluctuations are higher in the air-cavities of the jet than in  
5 the remaining free-surface, making the value of  $\alpha$  much more important in those regions.

6 Figure 8b presents the shape of the interface for the different levels of mesh refinement. The lack of cells in the  
7 coarser mesh produces a smoother connection between the pool free-surface and the jet, and neglects the creation of  
8 air cavities. In the other hand, the medium and fine mesh are able to generate and detect the cavities, however due to  
9 the lack of mesh resolution to calculate correctly the forces acting on the interface, the air cavity may not be formed  
10 correctly and closed, although we can see on the fine grid a smaller gap between the jet and the surface. At the end,  
11 the finest mesh has sufficient resolution to generate and close the cavities.

12 The effect of changing the mesh resolution is highly significant for the overall modelling of the entrainment  
13 process. As mentioned in the introduction, the whole entrainment process could be simulated by resolving the free-  
14 surface all the way to the scale of the entrained bubbles, however doing so would be phenomenally expensive and  
15 inappropriate for an engineering simulation. A more cost-effective approach would be to model the large scale shape of  
16 the free-surface on a relatively coarse mesh, with modelled entrainment into an Eulerian two-fluid model representing  
17 the statistical propagation of subgrid scale entrained bubbles. Technically speaking, for the Eulerian two-fluid model  
18 to work the bubble size should be substantially smaller than the cell size; however since the process of air-entrainment  
19 is a continuous one which is having to be truncated at some intermediate scale, it is likely that this constraint is being  
20 violated at some point.

21 The function  $E_g$ , representing the number of bubbles formed at the free-surface, is also presented in this section.  
22 Figure 9 shows the time-averaged values of  $E_g$  for the four meshes used and the free-surface position, delimited by  
23  $\phi_{FS}$  isolines of 0.1, 0.5 and 0.9. As mentioned before, a sharp interface is very important in order not to spread the  $E_g$   
24 term over a large number of cells. In the first instance, observing Fig. 9, just the meshes G0.0008 and G0.00125 show  
25  $E_g$  values calculated at the intersection of the jet with the pool, which is indeed the position where bubble formation  
26 was observed experimentally. However, our concern is also about the accuracy of  $E_g$ , and in these terms, G0.0008  
27 mesh generates closest values when compared with the work of Ma et al. [23] and a more precise location of the zone  
28 of aeration – it can be noticed the generation of bubbles exactly inside of the air cavity, whereas in remaining meshes,  
29  $E_g$  is spread all over the free-surface.

30 Figure 10 shows the comparison between the values of free-surface wave amplitude ( $a$ ) using (a) the formulation  
31 of Ma et al. [23] and (b) the concept proposed in the current paper. Around the jet impact zone and inside the air  
32 cavity, the values are reasonably similar in both cases ( $a \approx 0.001 m$ ). These places, out of all the area occupied by the  
33 free-surface, are exactly the zones where the comparison should be made. The differences found at the centre of the  
34 jet has no importance for the calculation of  $E_g$  term and can be ignored.

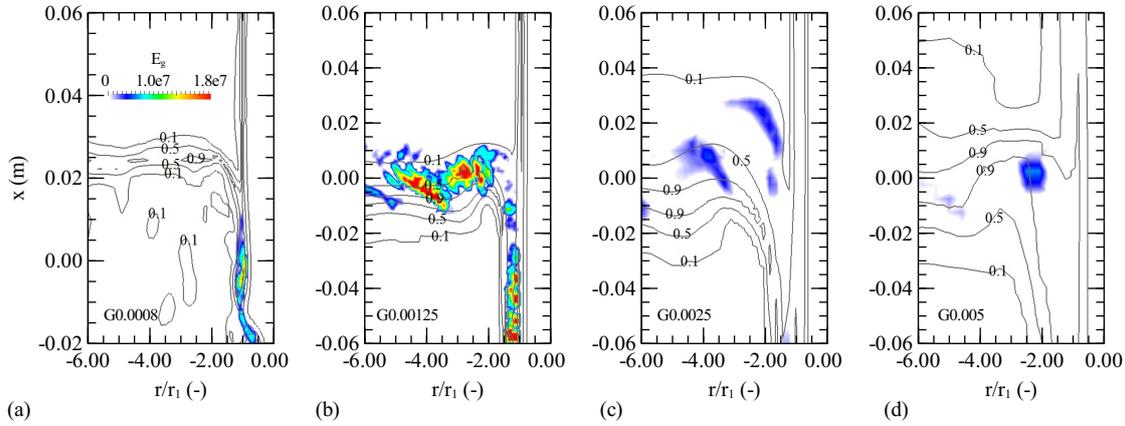


Figure 9. 2D centre-slice profiles of the free-surface and bubble formation term using the meshes: (a) G0.0008, (b) G0.00125, (c) G0.0025 and (d) G0.005. Isolines correspond to  $\phi_{FS} = 0.1, 0.5$  and  $0.9$ . The axis  $x$  is the vertical direction and  $r_1$  the jet radius at impact zone ( $r_1 = 0.012\text{ m}$ ).

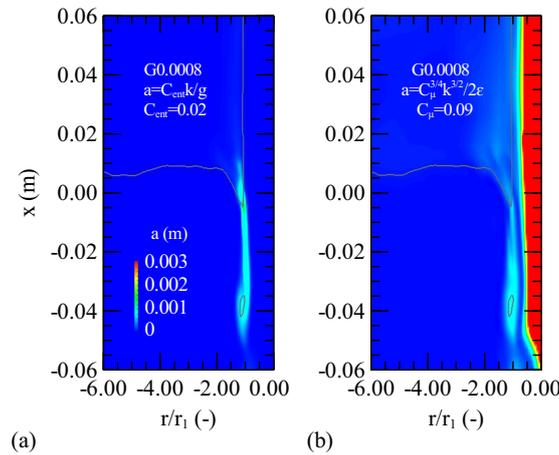


Figure 10. Comparison between the value of free-surface wave amplitude ( $a$ ) using (a) the formulation of Ma et al. [23] and (b) the concept proposed in this paper. The location of the free-surface is represented by  $\alpha = 0.3$ .

1 **4. Conclusions**

2 The present work attempts to numerically simulate air entrainment in two canonical cases; a 2D dam break and  
 3 3D circular plunging jet using Computational Fluid Dynamics. We investigate the interplay of numerical factors such  
 4 as mesh resolution with the modelling processes of surface capturing and entrainment modelling. The VOF interface  
 5 model as implemented in the code *interFoam* from the open-source OpenFOAM® toolkit was used to reproduce the  
 6 interface between the water and air. In addition, an explicit term for air-entrainment detection was adapted to run  
 7 with VOF models without a need of a calibration process. This was done by implementing a factor for free-surface  
 8 detection and new concept of surface wave’s amplitude based on the turbulent length scales.

The 2D dam break case was used to ascertain the influence of mesh size in the definition of free-surface position and aeration zone. The magnitude of air-entrainment term does not suffer much variation with the grid size, which let us believe that the new concept for wave's amplitude also improved the model on its independence of mesh size. The free-surface position is in contrast, much more sensible to the grid size and consequently a responsible to the accuracy of the aeration zone.

In the case of the 3D plunging jet, the free-surface shape was plotted using different mesh refinements and alpha values. The mesh refinement is shown to significantly affect the definition of the air cavities. The radial liquid velocity in the fully developed zone of the jet was found to be in reasonable agreement with analytical solution found on the literature. The term  $E_g$  for bubble formation reaches its maximum value in the intersection between the free-surface and the jet interface. This result is in agreement with visual descriptions of the air-entrainment process found in the literature. The term was successfully adapted to run within VOF based models and to be independent of user-calibration, by setting the free-surface wave's amplitude to be equal to the radius of the turbulent length scales. The results shown here prove that we might be optimistic about the applicability of this new concept, however, some other test cases are needed to validate the data as well as the conclusion of the air-entrainment model to compare the values of transported air.

## 5. Nomenclature

|                        |  |
|------------------------|--|
| <b>f</b>               | volumetric surface tension force, $kg\ m^{-2}s^{-2}$                         |
| <b>g</b>               | gravity vector, $m\ s^{-2}$  |
| <b>n</b>               | free-surface normal vector, –  |
| <b>U</b>               | velocity vector, $m\ s^{-1}$   |
| <b>U<sub>c</sub></b>   | compressive velocity, $m\ s^{-1}$  |
| <b>b</b>               | value of $r$ where the velocity is half of the velocity on the jet axis, $m$ |
| <b>C<sub>α</sub></b>   | binary coefficient, –  |
| <b>C<sub>μ</sub></b>   | turbulence model constant, –   |
| <b>C<sub>ent</sub></b> | constant for air-entrainment model, –  |
| <b>d</b>               | jet diameter, $m$  |
| <b>E<sub>g</sub></b>   | number of bubbles formed at free-surface, $m^{-3}s^{-1}$                     |
| <b>g</b>               | gravity, $m\ s^{-2}$   |
| <b>I</b>               | turbulent intensity, %   |
| <b>k</b>               | turbulent kinetic energy, $m^2s^{-2}$  |
| <b>l'</b>              | turbulent length scale, $m$  |
| <b>p*</b>              | dynamic pressure, $Pa$ or $kg\ m^{-1}s^{-2}$                                 |
| <b>r</b>               | radial direction, jet radius, $m$  |

|    |                      |   |
|----|----------------------|---|
| 1  | $t$                  | time, $s$   |
| 2  | $U$                  | mean velocity, $m s^{-1}$                                     |
| 3  | $V_g$                | volume calculated assuming an averaged bubble diameter, $m^3$ |
| 4  | $x$                  | vertical direction on pool, $m$                               |
| 5  | $Z1, Z2, Z3$         | refinement zones of the mesh, –                               |
| 6  | <i>Greek Symbols</i> |   |
| 7  | $\alpha$             | volume fraction, –  |
| 8  | $\Delta t$           | computational time step, $s$                                  |
| 9  | $\kappa$             | surface curvature, $m^{-1}$                                   |
| 10 | $\mu$                | dynamic viscosity, $kg m^{-1} s^{-2}$                         |
| 11 | $\nu_t$              | turbulent viscosity, $m^2 s^{-1}$                             |
| 12 | $\phi_{ent}$         | interface thickness, $m$                                      |
| 13 | $\phi_{FS}$          | interface location function, –                                |
| 14 | $\rho$               | density, $kg m^{-3}$  |
| 15 | $\sigma$             | surface tension, $kg s^{-2}$                                  |
| 16 | $\tau$               | shear stress tensor, $Pa$ or $kg m^{-1} s^{-2}$               |
| 17 | $\varepsilon$        | turbulent dissipation, $m^2 s^{-3}$                           |
| 18 | $n$                  | water column width, $m$                                       |
| 19 | <i>Subscripts</i>    |   |
| 20 | 0                    | inlet position  |
| 21 | 1                    | jet impact position   |
| 22 | $f1$                 | fluid 1   |
| 23 | $f2$                 | fluid 2   |

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