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KINEMATICS OF A FLUID AT REST WITHIN A RESERVOIR AND OF THE FLOW DUE TO THE DAM BREAKING USING THE LAGRANGIAN SMOOTHED PARTICLE HYDRODYNAMICS MODEL

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Abstract. *The Lagrangian modelling technique for understanding problems of fluid mechanics with heat and mass transfer is gaining the attention of the researchers. In particular, the particle method named Smoothed Particle Hydrodynamics (SPH) is used in fluid mechanics, for both in hydrostatic and hydrodynamic, in order to address the fluid flow with free surface or interfaces, producing consistent results with those obtained by analytical and experimental techniques. The focus of this work is to apply the SPH methodology to analyze the water flow in a reservoir and the fluid flow that occurs after the dam break. The concepts of modified pressure (in hydrostatic) and artificial viscosity (in hydrodynamics) are used to develop the mathematical and numerical models. The inconsistency found in the value of the interpolated function near the boundary is corrected by introducing a correction factor. To prevent the fluid particles pass through solid contours is used the concept of elastic reflection, with full restitution of kinetic energy. A code written in Fortran language is designed to solve the system of algebraic equations. Numerical results are compared with those obtained by analytical solutions and experiments in the laboratory. In the fluid at rest case, the results reported in the literature using Lagrangian SPH modelling show a change in position of the fluid particles over time. This paper presents numerical results identical to the analytical solution. In the dam breaking, numerical results concur with those obtained in laboratory experiments, with a maximum difference of 17.86%.*

Keywords: *Lagrangian SPH model, reservoir, fluid at rest, modified pressure, dam breaking*

1. INTRODUCTION

Originally developed for modeling astrophysical phenomena (Lucy, 1977; Gingold and Monaghan, 1977). The Smoothed Particle Hydrodynamics (SPH) is one of the Lagrangian numerical methods that have been increasingly used in flow problems with free surface and / or interfaces. As in any Lagrangian method, the SPH does not use meshes, easily discretizes complex geometries, refines more easily, easily capture domain and free surfaces and their topological changes. Amongst the difficulties of this method, it can be cited an appropriate implementation of boundary conditions, the inconsistencies found in physical quantities interpolated for particles close to the boundaries and agglomeration of particles in certain regions of the domain.

Hydrostatic of an incompressible and isothermal fluid in a reservoir is a well-known problem, where each fluid particle obeys the equation of mass conservation and momentum balance. Using the Lagrangian SPH method and different formulations for the viscous terms, the results of simulations showed the appearance of oscillations in the particles positions, which will increase in time (Vorobyev, 2013). SPH was employed to study this problem, the fluid inside a rotation tank, and dam breaking (Goffin *et al.*, 2014). The numerical results found presented unwelcome effects. In dam breaking, a particle agglomeration has been observed on the tank walls, an effect that was reduced from the use of a symmetry condition. Still in 2014, two solutions were proposed for the problem of the particle agglomeration in certain domain regions, caused by the decrease of the kernel gradient for small distances between particles (Korzilius *et al.*, 2014). In their work, results were presented to the problem of reservoir filled with water at rest. The oscillations of the particles has become smaller over time and converged to a steady state system, however divergent of the correct state.

In the literature, several research works have been carried out to address the boundary conditions to be imposed on fluid flow, regarding the particle-boundary interaction. The repulsive forces and the Lennard-Jones method were proposed by Monaghan (1992). Following the same idea and using variational calculus, has introduced the concept of contact force in the boundaries to address the interaction between the particles and rigid solids contours (Kulasegaram *et al.*, 2004). Subsequently, in 2013, the renormalization factor (that depends on the shape of the wall and the particles ' positions on the wall) was introduced. An improvement to the contact force model on the boundaries presented by the previous researcher was also developed (Ferrand *et al.*, 2013). To reduce processing time, a new way to calculate the renormalization factor in the wall was proposed and presented a unified semi-analytical boundary conditions (Leroy *et al.*, 2014). In 2015, an extension to the "virtual particles modified method" in which the wall is discretized by a set of virtual particles and simulated by the local symmetry approach was performed (Fourtakas *et al.*, 2015). It has achieved an improvement in the zero-th and first orders consistency in SPH. Although the first case results show an improvement over conventional techniques that use virtual particles in treatment of contours, when the method was applied in the study of hydrostatic fluid within the reservoir was still noticed the change in position of the particles in time.

This paper presents a proposal for the study of hydrostatic problems using the concept of the modified pressure in SPH (Batchelor, 2000). To study a fluid at rest within a reservoir, using the modified concept pressure and the solid wall boundary conditions with the use of virtual particles, provided numerical results coincident with the analytical solution. The application of the SPH in the dam breaking study is also presented. Considering the geometric boundary conditions (with fixed geometric planes at the solid boundaries) and a kinetic energy coefficient of restitution for collisions between fluid particles and boundaries, the numerical results are promising when compared with experimental results.

2. MATHEMATICAL MODELLING

The flow mathematical modelling in viscous and incompressible fluids is performed by the equations of mass conservation and momentum balance – Eqs. (1) and (2), respectively.

$$\frac{D\rho}{Dt} + \rho\nabla.\vec{\mathrm{v}} = 0 \tag{1}$$

$$\frac{D\vec{\mathrm{v}}}{Dt} = \frac{1}{\rho}\left(-\nabla P + \mu\nabla^2\vec{\mathrm{v}} + \rho\vec{g}\right) \tag{2}$$

where $\vec{\mathrm{v}}$ is the velocity, t is the time, ρ is the density, ∇ is the nabla mathematical operator, P is the absolute pressure, μ is the dynamic viscosity, $\vec{g}$ is the gravitational acceleration.

The fluid dynamic pressure is calculated by Eq. (3), known as Tait equation, suggested in (Batchelor, 2000):

$$P_{\mathrm{dyn}} = B\left[\left(\frac{\rho}{\rho_0}\right)^{\gamma} - 1\right] \tag{3}$$

where P_{dyn} is the dynamic pressure, B is the term associated with fluctuations in the fluid density, ρ_o is the fluid density at rest and $\gamma = 7$.

For the Tait equation could be applied in predicting the dynamic pressure, it must be ensured that the Mach number is not greater than 0.1.

The modified pressure concept is used in this research (Batchelor, 2000), which is defined by Eq. (4):

$$P_{\mathrm{mod}} = \left(P - P_0\right) + \rho g(H - \mathrm{y}) \tag{4}$$

where P_{mod} is the modified pressure, P_0 is the reference pressure, H and y are the ordinates of the free surface and fluid, respectively (with the referential fixed at bottom).

In this work, the concept of the modified pressure was implemented to study an incompressible, uniform, viscous and isothermal fluid at rest inside a reservoir. This concept can be applied to cases of hydrostatic or fluid dynamics. In hydrostatic cases, the modified pressure is zero.

3. NUMERICAL MODELLING

The mathematical identity is valid for a scalar function defined and continuous $f\left(X\right)$, given by Eq. (5):

$$f\left(X\right) = \int f\left(X'\right)\delta\left(X - X'\right)dX' \tag{5}$$

A smoothing function, or kernel, is used to calculate the interpolated value of the function. The interpolated value of the function at the position X can be calculated by Eq. (6):

$$\left\langle f\left(X\right)\right\rangle = \int f\left(X'\right)W\left(X - X',h\right)dX' \tag{6}$$

where $f\left(X\right)$ is the value of the scalar function at the fixed point X, $f\left(X'\right)$ is the value of the scalar function at the variable point X', $\delta\left(X - X'\right)$ is the Dirac delta function, dX' is the infinitesimal volume element, $\left\langle f\left(X\right)\right\rangle$ is the approximated value of the scalar function at the fixed point X, $W\left(X - X',h\right)$ is the smoothing function or kernel, h is the support radius.

Expanding the Taylor series for the function $f\left(X\right)$ around the fixed point, can be shown that the function value approximation $\left\langle f\left(X\right)\right\rangle$ presents a 2nd order error, $O(h^2)$.

In Figure 1, the particles disposition is show in a schematic representation within influence domain.

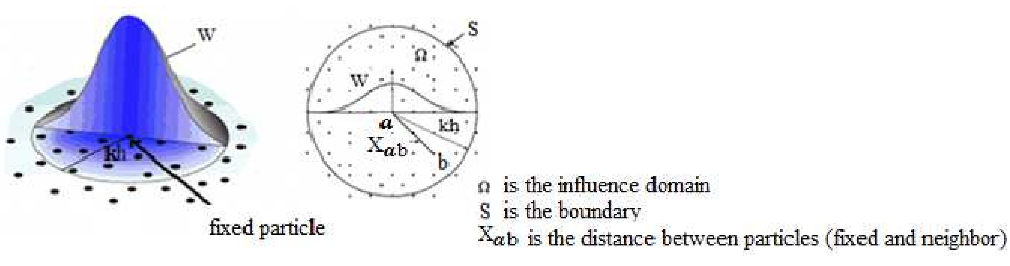


Figure 1. Graphical representation of the influence domain. The fixed particle a has as neighbors all particles within the influence domain (particles b), k is a scale factor which depends of the used kernel.

In Equation (6), the infinitesimal volume element is replaced by the mass of the element by the relation:

$$dX' = \frac{dm'}{\rho'} \tag{7}$$

where dm' is the mass of the infinitesimal volume element of the fluid and ρ' is the fluid density.

The Lagrangian SPH method is based on the representation of continuous spatial domain by discrete material particles. The interpolated value given by Eq. (6), after substitution of the infinitesimal volume, showed in Eq. (7), can be calculated by the discrete material form as:

$$f_a = \sum_{b=1}^{n} m_b \frac{f_b}{\rho_b} W(X_a - X_b, h) \tag{8}$$

where f_a is the approximate value of the function in the fixed particle's position, f_b is the approximate value of the function in the neighboring particle position, X_a is the fixed particle's position, X_b is the neighboring particle's position, m_b is the mass of neighboring particle, ρ_b is the density of the neighboring particle, n is the number of neighboring particles.

The approximations for the divergent, gradient and Laplacian of the function are presented in Eqs. (9) to (11).

$$\nabla . f_a = \frac{1}{\rho_a} \sum_{b=1}^{n} m_b (f_b - f_a) . \nabla W(X_a - X_b, h) \tag{9}$$

$$\nabla f_a = -\rho_a \sum_{b=1}^{n} m_b \left(\frac{f_a}{\rho_a{}^2} + \frac{f_b}{\rho_b{}^2} \right) \nabla W(X_a - X_b, h) \tag{10}$$

$$\nabla^2 f_a = 2\sum_{b=1}^{n} \frac{m_b}{\rho_b}(f_a - f_b) \frac{X_a - X_b}{\left|X_a - X_b\right|^2} . \nabla W(X_a - X_b, h) \tag{11}$$

where ρ_a is the reference particle density, held fixed during the interpolation calculation.

In the literature, kernels as the quartic (Lucy, 1977), quintic spline (Morris, 1997) and new quartic (Liu and Liu, 2003) are used to solve physical problems by SPH method. In this work, the kernel cubic spline is used to solve problems of hydrostatic and dam breaking, in 2-D (Liu and Liu, 2003).

Applying the approximations of Eq. (8), (9), (10) and (11) in Eq. (1) and (2) are obtained discrete forms of SPH for the equations of mass conservation and momentum balance.

$$\frac{D\rho_a}{Dt} = \frac{1}{\rho_a} \sum_{b=1}^{n} m_b (\vec{v}_b - \vec{v}_a) . \nabla W(X_a - X_b, h) \tag{12}$$

$$\frac{D\vec{v}_a}{Dt} = -\sum_{b=1}^{n} m_b \left(\frac{P_a}{\rho_a{}^2} + \frac{P_b}{\rho_b{}^2} \right) \nabla W(X_a - X_b, h) + 2\upsilon_a \sum_{b=1}^{n} \frac{m_b}{\rho_b} (\vec{v}_a - \vec{v}_b) \frac{X_a - X_b}{\left|X_a - X_b\right|^2} . \nabla W(X_a - X_b, h) + \rho \vec{g} \tag{13}$$

where $\vec{v}_a$ is the fixed particle velocity, P_a is the absolute pressure in the fixed particle, P_b is the absolute pressure in the neighboring particle, $\vec{v}_b$ is the neighboring particle velocity and υ_a is the fixed particle kinematic viscosity.

By application of the modified pressure concept, the momentum balance equation will be written as follows:

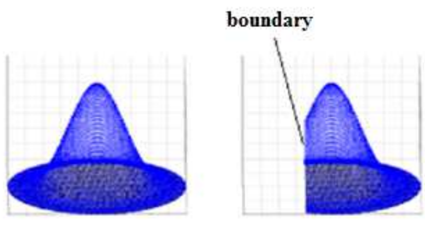
$$\frac{D\vec{v}_a}{Dt} = -\sum_{b=1}^{n} m_b \left(\frac{P_{\text{mod}(a)}}{\rho_a{}^2} + \frac{P_{\text{mod}(b)}}{\rho_b{}^2} \right) \nabla W(X_a - X_b, h) + 2\upsilon_a \sum_{b=1}^{n} \frac{m_b}{\rho_b} (\vec{v}_a - \vec{v}_b) \frac{X_a - X_b}{\left|X_a - X_b\right|^2} . \nabla W(X_a - X_b, h) \tag{14}$$

where $P_{\text{mod}(a)}$ and $P_{\text{mod}(b)}$ are the modified pressures on the fixed particle and neighboring particle, respectively.

The support domain length influences the accuracy of the calculations directly. Guaranteeing respect for the kernel properties and its gradient (antisymmetry and non-standardization), numerical tests showed that a greater number of particles that 21 within the influence field does not change the results significantly (Fraga Filho, 2014) but it affects the time spent in the simulation. In order to keep the number of particles near a constant value, it was used the correction to the support domain length (Liu and Liu, 2003).

The dam breaking problem involves a shock wave propagation that needs to be measured. To avoid numerical instabilities in the model, it is introduced the concept of artificial viscosity (Liu and Liu, 2003). The term related to artificial viscosity is added to the terms of pressure (Fraga Filho, 2014).

The consistency of SPH is guaranteed if the values of the moments of zero-th and first orders are respectively one and zero. When the reference particle is sufficiently far from the contour, the influence domain is complete, as shown in Fig. 2(a). If the influence domain is complete, there is a sufficient number of particles inside it (without clustering in certain regions) and the support radius has been properly defined, it can be found the conditions for the consistencies of zero-th and first orders, due to the properties of the kernel normalization and symmetry. This will not happen if the reference particle is close to the border and has an incomplete or truncated influence domain, as shown in Fig. 2(b). This truncated domain produces the phenomenon known as particles inconsistency, which is a particle imbalance inside the incomplete influence domain.



(a) (b)

Figure 2. The influence domain. (a) Complete and (b) Incomplete or truncated (the kernel is not defined in the entire influence domain).

In this work, the CSPM method is used for the particles inconsistency treatment, by introducing a correction factor (Chen *et al.*, 1999). The particle density is corrected from the use of given expression in Eq. (15):

$$\rho_a^{\ *} = \sum_{b=1}^{n} m_b W(X_a - X_b, h) \Big/ \sum_{b=1}^{n} W(X_a - X_b, h) \frac{m_b}{\rho_b} \tag{15}$$

where $\rho_a^{\ *}$ is the corrected particle density. Similar expressions are obtained for the pressure gradient Cartesian components (Fraga Filho, 2014).

In this paper, the boundary treatment in the hydrostatic problem is performed using virtual particles. In dam breaking, geometric reflections of particles against the countours are implemented and the energy losses during the collisions are considered by a coefficient of restitution of kinetic energy (Fraga Filho, 2014).

4. RESULTS AND DISCUSSION

A numerical code written in FORTRAN language was developed to solve Eqs. (12), (13) and (14). Numerical simulations has been carried out for the fluids static problem and dam breaking. The results for these simulations are compared with results available in the literature, analytical or from experiments.

4.1 Fluid at rest in a reservoir

This hydrostatic problem consists of an uncovered reservoir filled by an incompressible and uniform fluid at rest. The physical laws of mass conservation and momentum balance are obeyed for the studied case. The solution consists from obtaining a solution to the momentum balance equation, while using incompressible particles.

The analysis was performed to a 2D domain. The particles have been regularly distributed in the reservoir with dimensions 1.00 x 1.00 m. 50 particles per side were employed, totaling 2500 fluid particles. The number of particles within the influence domain was twenty-one. The boundary treatment has used virtual particles. Three rows and three columns of this particle type have been added to the regular distribution of fluid particles, totaling 636 virtual particles. A complete influence domain has been guaranteed for all fluid particles, avoiding the particle inconsistency next to the boundary regions (Liu and Liu, 2003). The zero-th and first orders of consistency of SPH method have been assured because there was no kernel truncation.

The modified pressures for all particles (fluid and virtual), at rest, were initialized to zero. The used time step was 1.00×10^{-4} s and was obeyed the Courant-Friedrichs-Lewy convergence criterion (Courant, Friedrichs and Lewy, 1967). The temporal integration of the positions and velocities have been done by the Euler method (first-order Runge-Kutta).

After the solution of Eq. (14) and updating from the particles positions and velocities by the temporal integration, for each numerical iteration, those remained unchanged, and the hydrostatic equilibrium have been maintained. The modified pressures field were restored with zero at the start of each new iteration, since the particles were at rest.

In the approximations taken by the SPH method to a function and its derivatives there are errors (Fraga Filho, 2014; Vaughan *et al.* 2008). When the SPH was applied without the use of the modified pressure to the obtaining of approximations for the pressure and viscosity forces, terms which were present in the momentum balance equation and which were added to the gravitational force, made small mistakes appear. Despite of the small orders of magnitude from these errors, they have spread and increase during the numerical simulation. It has resulted in the appearance of particles movement, as shown in the recent studies (Vorobyev, 2013; Goffin *et al.*, 2014; Korzilius *et al.*, 2014); Fourtakas *et al.*, 2015). Using the modified pressure, the addition of the terms approximate by the SPH for surface forces to the gravitational force has been avoided. Thus, the errors have been eliminated and a consistent solution to the physical problem has been obtained. It was verified the coincidence between the initial positions of the particles and the positions obtained by SPH at time 5.00 s, as shown in Fig. 3.

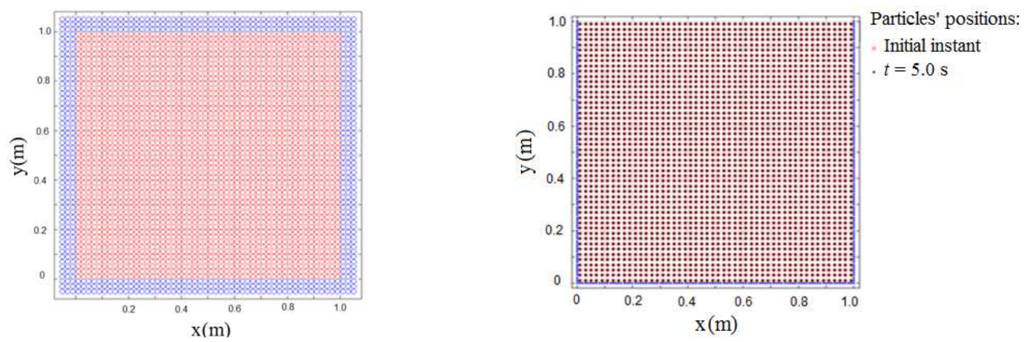


Figure 3. On the left, the initial distribution of fluid particles (red) and virtual particles (light blue). On the right, the coincidence between the inicial positions of the particles (red circles) and at time instant 5.00 s (black dots).

4.2 Dam breaking

In the dam breaking modelling, the obedience to the laws of mass conservation and momentum balance was guaranteed. Numerical simulations were performed for two different heights of dammed water (H), and the results were compared to the results of experiments (Cruchaga *et al.*, 2007). The 2-D computational domains simulated were: (1) square area with height and width of 0.114m, discretized by 1296 fluid particles; (2) rectangular area with height of 0.228m and width of 0.114m, discretized by 2556 fluid particles. The experimental apparatus is schematically shown in Fig. 4.

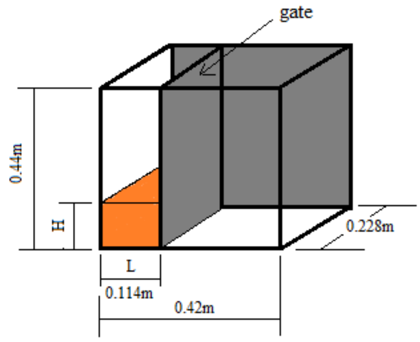


Figure 4. Experimental apparatus used in the dam breaking experiments.

The parameters used in the simulations were: mathematical modeling of laminar viscous stress, estimate the dynamic pressure field with the use of the Tait equation (term B with the value of 0.85×10^5 Pa), variation of support radius, use of CSPM method for correcting density and pressure gradients near the contours, boundary treatment with the use of fixed planes (against which there was totally elastic particle collisions), temporal integration by Euler method and time step of 1.00×10^{-5} s. The simulations were made to the physical time 0.50 s (50000 numerical iterations). For both geometries simulated, the artificial viscosity has been implemented (Fraga Filho, 2014). The coefficient α_π received the values 0.20 and 0.30, and the β_π received the value 0.00. The sound velocity in the fluid was 62.60 m/s. The free surface particles were marked and the constant pressure condition (zero) was first applied, and renewed every numerical iteration (Fraga Filho, 2014).

Figures 5 to 7 show the experimental and numerical results for both simulated domains.

Table 1 shows the percentage differences between the abscissa of the wave fronts obtained by SPH and experimentally, calculated from the expression:

$$\Delta x_p = \frac{(x_{\exp} - x_{SPH})}{x_{\exp}} 100 \tag{16}$$

where $x_{\exp}$ and x_{SPH} are the abscissas of the wave fronts obtained by experiments and SPH, respectively, and Δx_p is the percentage difference between the abscissas of the wave fronts.

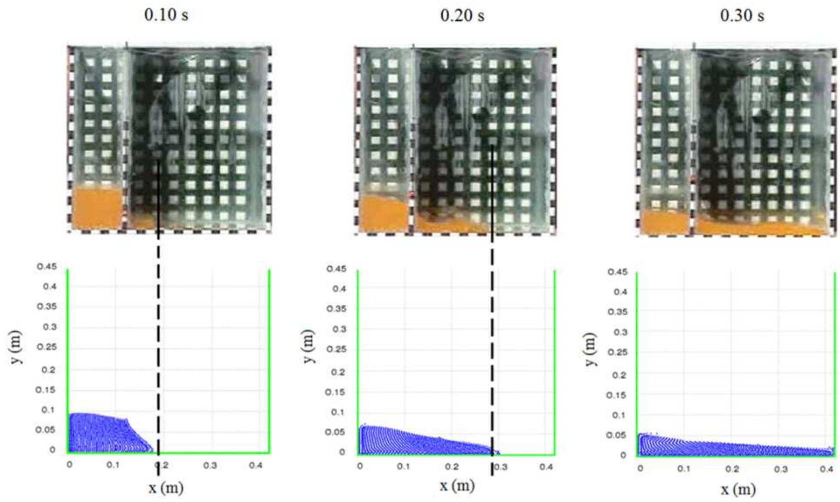


Figure 5. Experimental and numerical results for the first simulated geometry, with the implementation of the artificial viscosity (α_π = 0.20).

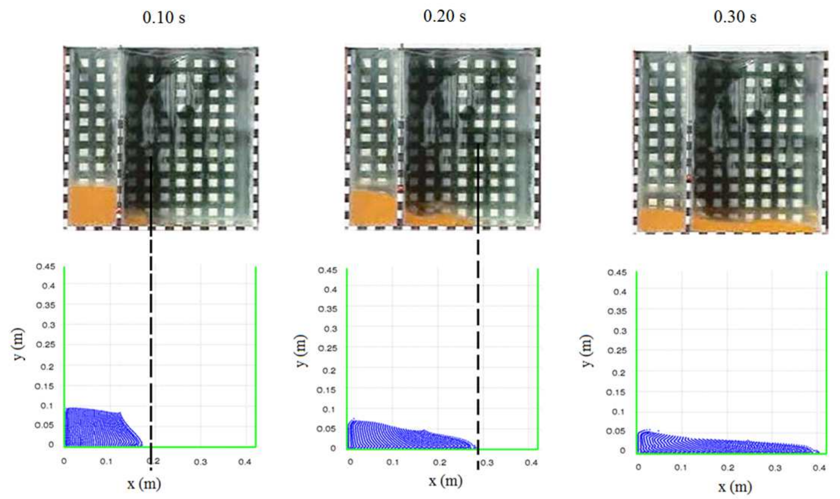
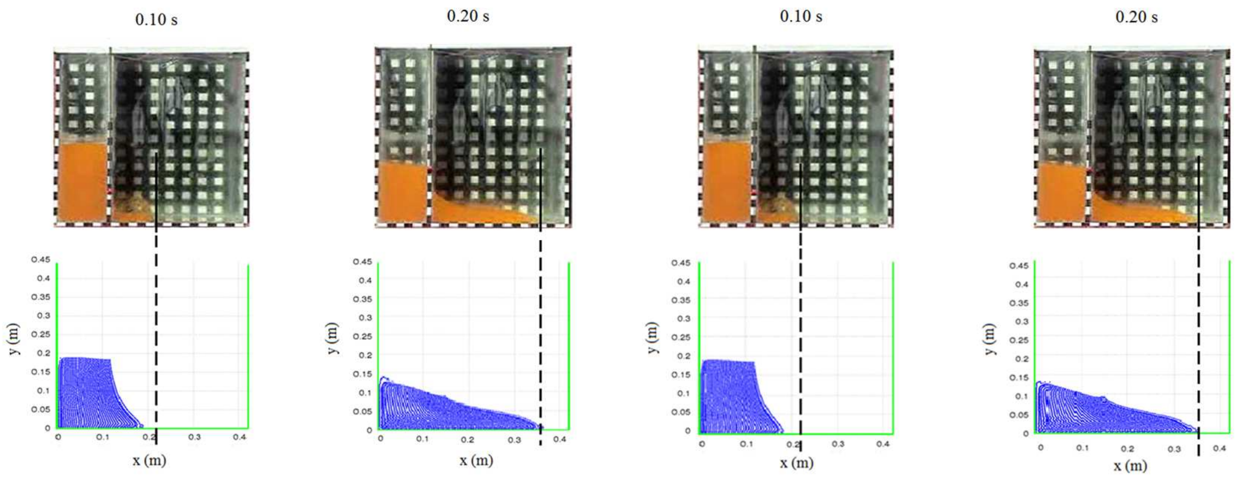


Figure 6. Experimental and numerical results for the first simulated geometry, with the implementation of the artificial viscosity (α_π = 0.30).



(a) (b)

Figure 7. Experimental and numerical results for the second simulated geometry, with the implementation of the artificial viscosity. In (a), α_π = 0.20 and in (b), α_π = 0.30.

Table 1. Percentage differences between abscissas of wave fronts (comparison between experimental and numerical results)

First domain simulated					Second domain simulated				
α_π	t (s)	x_{exp} (m)	x_{SPH} (m)	Δx_p (%)	α_π	t (s)	x_{exp} (m)	x_{SPH} (m)	Δx_p (%)
0.20	0.10	19.00	18.07	4.89	0.20	0.10	22.00	19.00	13.64
	0.20	29.00	30.28	-4.41		0.20	36.00	37.00	-2.78
0.30	0.10	19.00	17.58	7.47	0.30	0.10	22.00	18.07	17.86
	0.20	29.00	28.70	1.03		0.20	36.00	35.16	2.33

From the analysis of the Tab. 1, the largest differences between the positions of wave fronts have been seen in the early stages of dam breaking (7.47% in the first and 17.86% in the second geometry), when the coefficient α_π received the value 0.20. With the time progress, the differences decreased, as shown at time 0.20 s. The smaller differences between wave fronts (1.03% in the first and 2.33% in the second geometry) have occurred when it was used the coefficient α_π with the value 0.30.

5. CONCLUSION

With the implementations of the modified pressure concept, regular distribution of particles at domain and boundary treatment using virtual particles (in an extended area of the domain, ensuring no kernel truncation) the numerical results obtained are in agreement with the analytical solution to the hydrostatic problem of a uniform, incompressible and viscous fluid within a reservoir, which had not yet been satisfactorily solved with the use of SPH method. It has been found that there was no change in the positions of the fluid particles throughout the simulated time, with the complete exclusion of any oscillatory movement seen in previous studies, even after steady state is reached.

The dam breaking case study was performed to the time before the first collision of the fluid against the wall of the reservoir. In the boundaries treatment, fixed geometric planes were used at the walls, against which the fluid particles were elastically reflected in the collision moment. Restorations of the consistencies of zero-th and first-orders have been implemented to the densities and pressure gradients, respectively. The artificial viscosity was added to the pressure terms. The numerical results obtained were consistent with the results of the experiments (Cruchaga *et al.*, 2007).

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