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COMPARATIVE STUDY OF CONVERGENCE OF CFD COMMERCIAL CODES WHEN SIMULATING DENSE UNDERFLOWS

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Abstract. *In this paper, we present numerical simulations of saline, discontinuous density currents, in two and three dimensions. The simulation of these flows poses a severe challenge for all codes. In fact, the currents present characteristic flow instabilities at the interface which are constituted by small spatial scales. A very fine resolution of these scales is needed to adequately capture the instabilities.*

The two-dimensional simulations reported herein were performed with two CFD codes. The first one is a comprehensive finite-element platform, whereas the other one is a commercial code. The runs were undertaken under quite similar conditions. Simulations show that only when the mesh employed in the commercial code is strongly refined a convergent solution is attained, which is similar to the solution obtained with the finite-element CFD code. This result would warn about the indiscriminate use of commercial codes with supposedly "fine" meshes when simulating complex underflows. The solution with the finite-element code, in turn, shows the shedding of large vortices containing salt. These vortices do not have a physical basis, but they correspond to the true solution of the two-dimensional Navier-Stokes Equations.

1 INTRODUCTION

Density currents are one of the most beautiful flows that Nature has to offer. They can be broadly defined as flows driven by density differences. As such, they can be encountered in a host of natural conditions.

For instance, they can manifest themselves as dust storms and snow avalanches in the atmosphere. In addition, sudden, cold down flows can generate atmospheric micro-bursts that have been dubbed as the source of accidents of airplanes[1]. The scales of these atmospheric flows can be really large: dust storms can reach velocities of tens of meters per second, and heights of hundreds of meters. Volcanic eruptions also promote the formation of density currents, since heavy material ejected up by the volcano can then move down to spread as an underflow. Lava flows constitute another expression of atmospheric density currents.

In water environments, density currents appear in the form of saline intrusions in estuaries, and as sediment pulses in rivers, among other kinds of flow.

Density currents may be initiated by diverse mechanisms, such as inflow of turbid water to ponds, sub-aqueous slumps, discharges of mining tailings, temperature gradients, or dredging operations. *The relevance of density currents consists in that they are capable of transporting contaminants for very long distances.* Therefore, their motion can underscore a severe pollution problem. Typically, tiny density differences can produce relatively important flows.

The heavier constituent of density currents could be dissolved (salinity type), or it could be formed by solid particles in suspension ("turbidity current"). The currents could also be continuous or discontinuous, depending on whether or not there is constant supply of heavier material from the source.

One of the characteristics of these underflows is that they present Kelvin-Helmholtz instabilities at the interface of the two fluids (see Fig. 1). These instabilities are the result of the motion of masses of fluid of different density at different velocities. Clearly, the instabilities possess length scales much smaller than the size of the body of the density current.

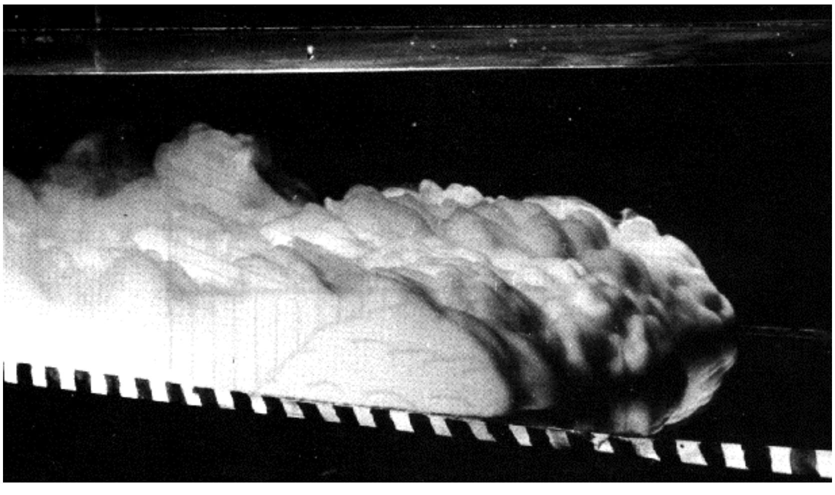


Figure 1: View of a density current in a laboratory water environment moving in an incline (towards the right).

An accurate simulation of these instabilities is needed for the precise determination of the current location. The underflow is powered by the density difference, which determines how far the current goes. This difference in turn decreases as the current moves downwards, due to dilution promoted by water entrainment. In fact, in the tail of the current, vortices shed from the front break down, mixing the entrained water with the heavier water in the current. This process leads to the formation of a well-mixed layer as the front passes by.

In order to correctly simulate those instabilities by numerical means, i.e., in order to be able to adequately capture all the spatial scales of the phenomenon, a very fine resolution in the region in which the instabilities are expected to occur becomes necessary. Since this region can be approximated in principle, but it is a priori unknown, the zone of refined mesh must of necessity cover a larger portion of the domain. Oftentimes, the available computer resources do not allow for such a refined solution, and issues of convergence appear. Furthermore, issues associated with numerical diffusion when using commercial codes may very likely appear.

In a pioneering paper, Straka et al.[2] presented a decade ago the results of a workshop aimed at studying better ways to simulate dense atmospheric underflows. The simulations were performed with the supercomputers of the time. Those simulations showed that when the flow is “adequately resolved,” the high-order and spectral methods perform better in describing the flow instabilities. Obviously, discerning the exact meaning of what is “adequately resolved” in each application implies some careful analysis. Overall, the results of that workshop could be summarized in that care must be taken when interpreting the physics described by simulations with resolutions that might be considered “marginal.”

In addition to the flow instabilities at the interface, the base of the head of density currents also poses a challenge for modeling. In fact, the base of the head possesses sharp gradients of concentration. Some numerical codes may produce “over-shooting” at those locations, if the numerical scheme does not handle appropriately sharp fronts. An adequate description of this zone of density currents becomes instrumental for a correct prediction of sediment entrainment to the current from movable beds. This has in turn important implications on erosion processes of the bed, and potential pollution of the water body, if the sediments are contaminated.

This paper reports a comparison of two-dimensional numerical results obtained with two Computational-fluid-dynamics (CFD) codes, when simulating dense underflows originating in a lock-exchange operation. One of the codes is a finite-volume commercial code, and the other one is a finite-element, open-source code. Convergence tests were performed with both codes, addressing their different response to mesh refinement.

2 PREVIOUS NUMERICAL EFFORTS RELATED TO DENSITY CURRENTS

One-dimensional (1D) numerical solutions for density currents have been presented by Bonnecaze et al.[3] (two-layer fluid solution for particle-driven gravity currents), and Choi & García[4] (turbidity currents). The balance equations solved in the above efforts were those for fluid mass, streamwise momentum and suspended-sediment mass. Bradford & Katopodes[5, 6] presented a depth-averaged, two-dimensional (2D) solution for turbid underflows in the sea.

In general, 2D numerical simulations in vertical planes have been directed to atmospheric, large-scale flows (of the order of several kilometers in length and height), and viscous-flow models have been employed in these large-scale numerical computations.

The first numerical efforts can be traced back to the classic paper by Daly and Pratch[7] (laboratory scale). Similarly, interesting studies were presented by Mitchell and Hovermale[8], Thorpe et al.[9], Crook et al.[10], Haase and Smith[11], and Straka et al.[2] (all of them related to atmospheric phenomena). Some authors have presented a 2-D solution based on multiple layers[12]. Chen and Lee[13] added a RNG k-ε turbulence closure model in their 2-D study. Pacheco et al.[14] presented a simulation of the collision of two unequal gravity currents through a viscous-flow model. In turn, De Cesare[15], and De Cesare et al.[16] employed a commercial code to implement a 3-D, two-phase model for the study of density currents in a reservoir, and used the k-ε turbulence closure in the solution.

In addition to the numerical issues discussed in Section 1, there is another issue associated with the simulation of turbulence. Several papers have presented simulations with turbulence closure (typically with the k-ε model) but others have used a viscous model. Recent papers have been devoted to the Direct Numerical Simulation (DNS) of density currents (see for instance Hartel et al.[17], Necker et al.[18], and Cantero et al.[19]).

3 TEST CASE AND THEORETICAL MODEL

The tests we selected for our analysis correspond to an unpublished set of measurements performed by Prof. M. H. García at the University of Minnesota. They correspond to a lock-exchange device (see Fig. 2). Denser fluid consisting of a salt-water mixture was placed in an almost square box on the top of a flume. This denser fluid was separated from fresh water laying in the rest of the flume by a thin gate. This gate was released at time $t = 0$, allowing for the motion of the denser fluid as a discontinuous underflow. Several tests were developed for different densities of the salty fluid, and for different sizes of the box (the size of the box determines an initial length scale that characterizes the flow).

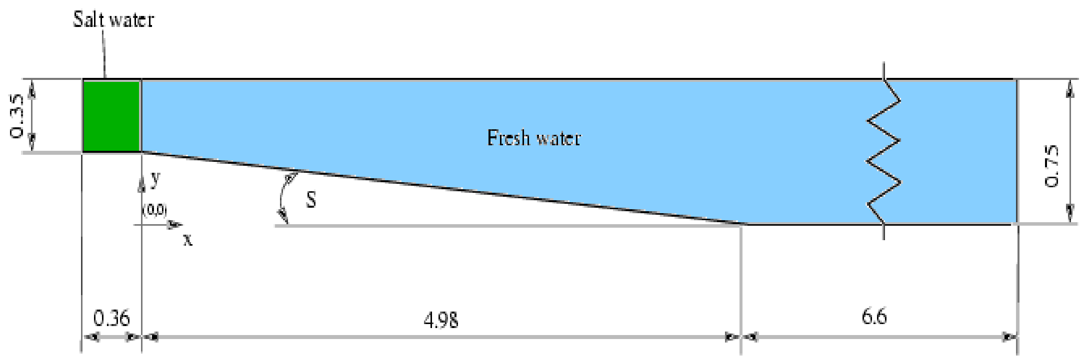


Figure 2: Schematic of the experimental device numerically simulated. Distances are expressed in meters.

The motion of the discontinuous current was video recorded. Snapshots of the front of the current in the sloping part of the flume showed the presence of lobes and clefts, whereas the instabilities dominated the interface, very much as shown in Fig. 1.

The *initial* condition of lock-exchange flows has the interesting, unique property of a distinct direction of the gradients of pressure and density. In fact, meanwhile the pressure gradient is vertical, the gradient in density is horizontal. Vertical density gradients appear later as the current moves.

In order to simulate this flow, a relatively simple theoretical model was adopted. Since the salt is dissolved in the water and the concentration diminishes when the current moves downwards, a *viscous*, single-phase, continuously-stratified-fluid model was adopted, as follows:

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x_i} + \frac{\rho}{\rho_0} g_i + \frac{1}{\rho_0}\frac{\partial}{\partial x_j}\left(\tau_{ij}\right) \tag{2}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(u_j \rho\right)}{\partial x_j} = 0 \tag{3}$$

where u_i denotes the velocity component in the i-th direction (i goes from 1 to 3), x_i is the spatial coordinate in the i-th direction, p is the pressure, ρ the local density, and τ_{ij} denotes the viscous stresses. For the viscous stresses, the Newtonian model was employed. The standard incompressible form of the mass balance equation was used in (1), whereas the Boussinesq approximation has been used in the momentum conservation equation (2). Eq. (3) is often called the "density equation," in order to distinguish it from the mass conservation equation. Eq. (3) allows for the transport of a scalar; this scalar was the density for the commercial code and a saline concentration for the finite-element code. Since the differences in density are driven by differences in salt content, Eq. (3) comes from $DC/Dt = 0$ and, therefore, both approaches are formally equivalent.

The soundness of a viscous model for a salty density current in laboratory conditions, when low concentrations of suspended sediment are present and the bed is not erodible, is supported by observations made by Lin & Mehta[20] and several other comparisons (see Daly and Pratch[7]).

4 OVERVIEW OF THE NUMERICAL MODELS

The first code we used in this research corresponds to the three-dimensional (3D) platform BUCHESS. The theoretical model presented above was implemented in BUCHESS through the addition of suitable subroutines. This platform represents a long-term development of the Grupo de Mecánica Computacional del Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, CNEA, Argentina. Early versions of the platform can be found in

Buscaglia[21], Buscaglia et al.[22], Lew[23], and Cantero[24]. We have extended the scope of the model to simulate two-phase flows (see Buscaglia et al.[25], Bombardelli[26], and Cantero[27]). It runs in a cluster of PCs.

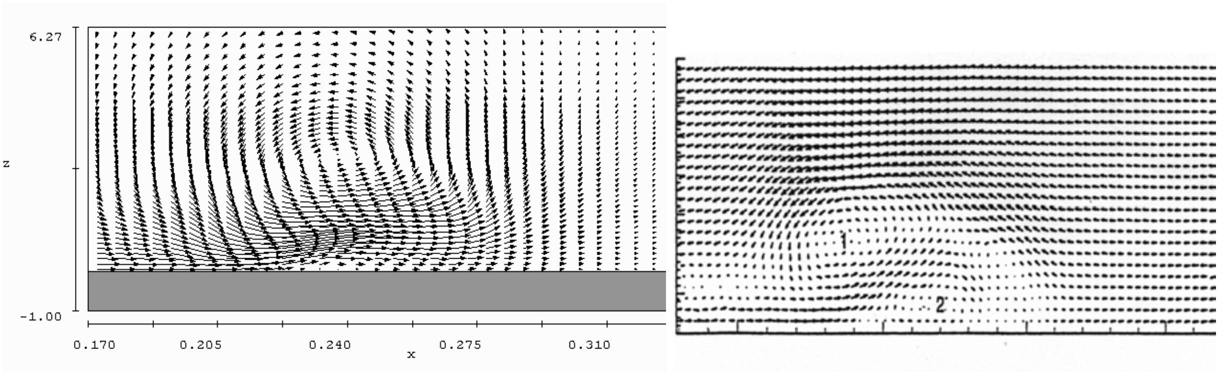
The code is based on the finite-element method, and uses equal-order interpolation. Several choices for numerical stabilization of the equations are available: SUPG, SGS, and GLS. In addition, a discontinuity-capturing technique has been implemented for the adequate description of the sharp gradients at the base of the head[27, 28]. The technique introduces numerical diffusion in the direction parallel to the concentration gradient. Several elements in 2D and 3D are available in the platform.

The commercial code, although not originally devised for hydraulic problems, is being increasingly used in the civil engineering community. The code is based on a quite standard finite-volume formulation, so that we believe the results reported herein are representative of a wide class of available commercial software. It incorporates partially blocked volumes to account for the solid obstacles, which marks a clear difference with BUCHESS. The commercial code is explicit.

5 PRELIMINARY NUMERICAL TESTS

The commercial code was first employed to test the theoretical model in 3D under an axisymmetric lock-exchange device. The flow field associated with a density current corresponding to this case was obtained by Alahyari and Longmire[29], via the use of Particle Image Velocimetry (PIV) in a circular sector of 55°. The purpose of this test was to initially address the concept of "adequate resolution" by Straka et al. The 3D device of Alahyari and Longmire was set up in a rectangular Eulerian grid. A dense mesh of 130x90x70 (radial, tangential, and vertical directions) was used in the computations, for a domain of 0.90 m in the radial direction and 0.26 m in the vertical. The initial denser region was a circular sector of 13 cm in height and 8 cm in radius. Thus, more cells were located below 13 cm in height (60 cells). In the radial direction, 120 cells were included in the first 68 cm. Based on the almost 700,000 open cells used, this mesh was judged as an important resolution according to Straka et al.'s concepts.

A rigid-lid boundary condition at the free surface was adopted. Figures 3 show measured and computed vector fields for a time of 2.5 seconds after the gate release, at the center plane, for this numerical test. It can be seen that the model can predict satisfactorily the presence of two vortical structures, denoted by 1 and 2 by Alahyari and Longmire. Vortex 1 is generated by the relative motion between the current head and the surrounding fluid, and vortex 2 is the result of the boundary-layer separation induced by the adverse pressure gradient ahead vortex 1. From the simulations, it can be seen that both vortices are located in similar positions with respect to the measured ones. However, the boundary layer appears to be *less* pronounced in the simulations than in the experiments. Also, some other local discrepancies are identified. Same results were observed for smaller and larger times, not reproduced herein. This means that, despite the important number of cells devoted to capture the current, and the intrinsic issues associated with the measurements (accuracy, averaging, etc.), the comparison of the above figures reveals some discrepancies at several scales.



(a) ➔ : 0.15 m/s (b) 0.15 m/s: ▼

Figure 3: Modeled (left) and measured (right) flow field associated with a density current in an axysimmetric device.

6 NUMERICAL IMPLEMENTATION OF THE 2D TESTS AND RESULTS

6.1 Numerical implementation

Runs *in two dimensions* based on the experiments explained in Section 3 were defined. These runs can be dubbed as “mathematical,” in the sense that 3D physical effects are not accounted for (we are not solving the third dimension). Since it is well-known that the behavior of these currents is fully 3D even in relatively-narrow flumes, we expect to address to what extent 2D simulations can capture the main features of the flow.

A condition corresponding to an initial density for the salty water of 1007 kg/m^3 was implemented in both codes. For the finite-element code, quadrilateral elements were employed, to make the comparison rigorous. (It is fair to point out that the comparison is not totally rigorous because of the inherent nature of the codes; however, the comparison can be considered fair enough for the purpose of extracting valuable conclusions.) The time step for the finite-element run was fixed in 0.01 s. (For the commercial code, the time step is controlled automatically.) A second-order, monotonicity-preserving method was selected for the solution of the density equation in the commercial code.

In both cases, the boundary at the top was considered as a symmetry plane. Also, a symmetry plane was imposed on the downstream boundary.

The initial conditions for the codes were defined specifying initial regions of density (commercial code) or concentration of the dissolved phase (finite-element code). In this way, solutions differ quantitatively but the distributions of values should be the same.

In the following comparisons, we quote number of nodes for the finite-element code, and number of “open cells” for the commercial code, in an attempt to offer comparative measures of the computational effort.

In Fig. 4 and 5, blue-like colors indicate concentrations close to zero, while reddish colors denote larger concentrations.

6.2 Numerical results

Fig. 4 shows the evolution in time of contours of salinity/density for the current every 10 s, up to 50 s, obtained from the numerical simulations with the two codes. The run with

BUCHESS has been obtained using about 20,500 nodes while the run with the commercial code was produced using 58,500 open cells.

It is possible to see in first place that both runs are quite different. Whereas the run with the commercial code shows the density current falling in a drop-like manner along the slope, the results with BUCHESS reveal a very rich structure of salty vortices in the tail. This is a significant qualitative disagreement that we sought to analyze.

For this purpose, we refined the meshes for both runs. Results with BUCHESS proved to be independent of mesh refinement in its qualitative features (see Fig. 5, left). Results with the commercial code, on the other hand, revealed more and more features as the mesh was refined. This mesh-convergence process was, however, extremely slow. In Fig. 5 (right) we show the results of the commercial code using 630,000 open cells. It is evident there that both codes predict the same type of instabilities and global behavior, but the commercial code requires an enormous amount of cells to arrive to a qualitatively-correct result. This is quite striking for a formally second-order-accurate method. We believe the explanation comes from numerical limiters added in commercial codes to "increase robustness," which end up yielding "numerically over-damped" methods that are inadequate for instability-driven flows such as the tail of the density current considered here.

7 DISCUSSION

To address whether or not a 2D, mathematical solution can reproduce the basic aspects of the current motion, we plotted in Fig. 6 the evolution in time of the current front. We have used the results of the commercial code, for the run with 58,500 open cells, to that end. We see from the comparison between modeled and measured non-dimensional values that the 2D solution can capture the front motion at the beginning, with reasonable accuracy. One may think that this solution with the commercial code is “correct,” based on this “good agreement” with experiments.

The runs presented above are essentially mathematical. It is well known that the evolution of vorticity in 2D is completely different to that in 3D, because vortex-stretching and self-induced velocity both contribute to the “dissipation” of eddies in 3D.

In the solution with the finite-element code, the vortices shed by the current remain in the flume during an exaggerated long period, because the mechanisms for their dissipation (vortex-stretching and self-induction velocity) are not present in the simulation. This result is clearly unphysical, but we think that it corresponds to the true solution of the *2D* Navier-Stokes Equations, given the sources of instability through the Kelvin-Helmholtz structures, and the weak mechanisms of eddy dissipation in 2D. Several solutions of density currents in 2D in papers described in Section 2 do not show this vortex shedding.

In comparison, the tail obtained with the commercial code seems to be more physically “correct,” but this is just an artifact. The tests indicate that the commercial code spuriously damps the instabilities for a moderate number of cells and, although some aspects of the flow show an apparently “better” agreement with experiments, in reality there is an erroneous description of the flow dynamics. This is explained by the fact that, when we refine the mesh using a very large number of cells in the commercial code, the structures predicted with the finite-element code do appear. Commercial codes need to offer the users numerical answers in most of the cases the users attempt to obtain a solution. This means that they often pay a great deal of attention to the robustness of the code at the expense of numerical accuracy. Stability is gained at the price of a large numerical diffusion, one of the well-known quandaries in Numerics. This fact calls for a careful analysis of convergence of the numerical solutions obtained with commercial codes when simulating underflows. Fig. 4 is a remarkable example on how over-diffusive codes may offer a solution that may look as "better" compared with other solutions in some aspects, a solution that may not show any indication of sub-resolution (i.e., wiggles, etc.), but in the end a solution which may be far from being converged!

The finite-element code, which due to the stabilization with an equal-order formulation and first-order interpolation can have the reputation of being "over-diffusive," has proved to be more accurate than the implemented method in the commercial code. This fact is even more relevant considering that a second-order scheme was selected in the commercial code.

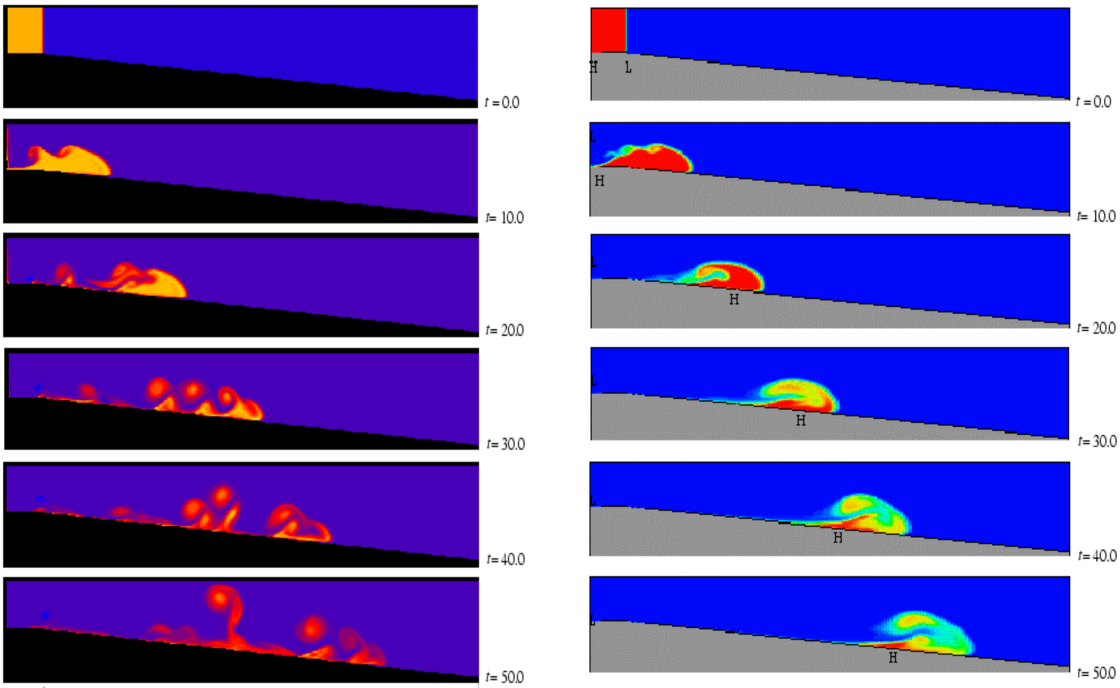


Figure 4: Numerical results obtained with the two codes. Left: BUCHESS solution with 20,451 nodes. Right: solution with the commercial code with 50,500 open cells.

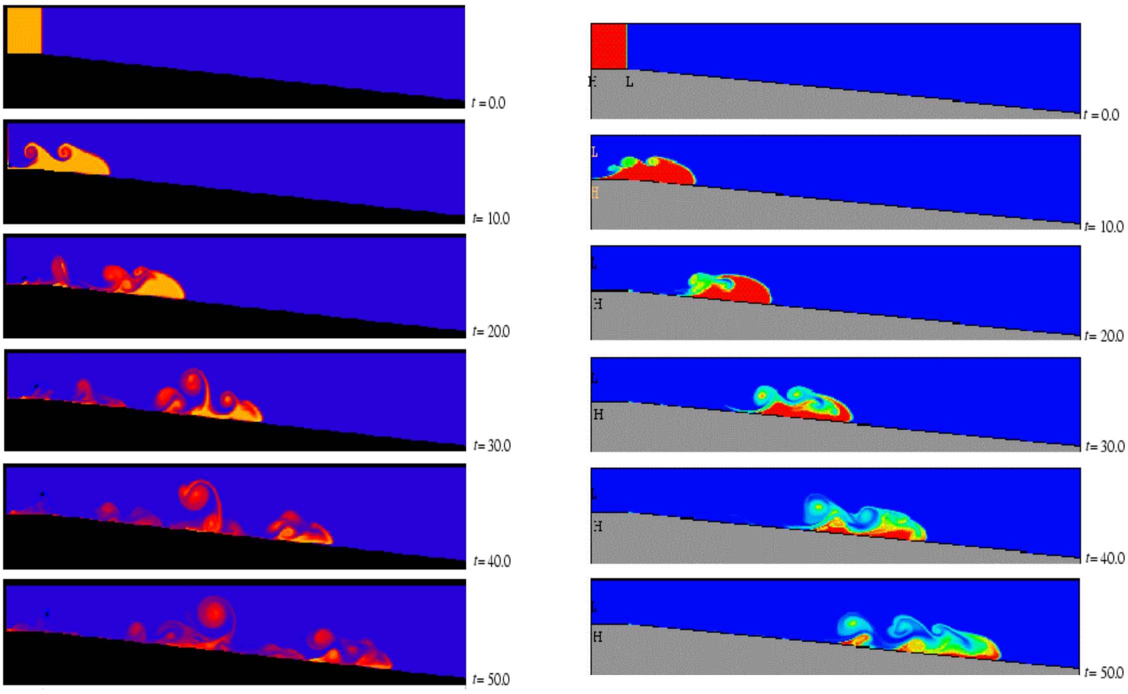


Figure 5: Numerical results obtained with the two codes. Left: BUCHESS solution with 45,676 nodes. Right: solution with the commercial code with 630,000 open cells.

8 CONCLUSIONS

The presented numerical results show that:

a) The issue of "adequate resolution" put forward by Straka et al. is clearly dependent on the numerical code employed, as expected, but it is especially critical with commercial codes. In this sense, meshes for numerical solutions that would be judged as "fine" in some cases, need to be carefully tested as producing converged results when simulating dense underflows. This is due to the fact that the small scales in the instabilities are really smaller than what can be anticipated with a simple computation. In complex flows, the "formal" order of certain schemes may be lost due to implementation details of commercial codes included to make them robust.

b) Two-dimensional solutions of density currents present shedding vortices that are not shown in solutions found in the literature. These vortices correspond to the true solution of the 2D Navier-Stokes Equations, and they do not appear in the experiment. In some published numerical solutions, we believe that they have been damped by a "global numerical error." This error may arise from the (usually small) discretization errors introduced in each equation, amplified by the different stabilizing tricks usually included in commercial codes. The net effect, for density currents, appears as a strong over-damping of the tail's dynamics and mixing.

c) We believe to have shown a good example in which a "good agreement with experiments" can be misunderstood. When we used a 3D solution with the finite-element code, the tail has the adequate shape and the shed vortices decay, showing that the exaggerated vorticity in the current's tail in the finite-element code is not an artifact from the method but, rather, is a result of the 2D approximation (see Cantero et al.[28]).

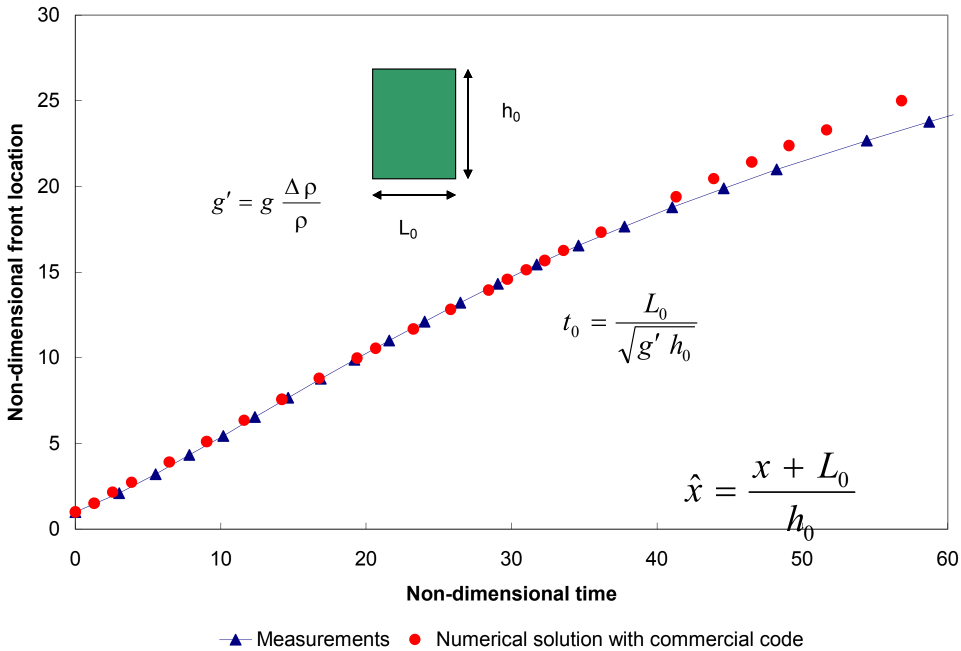


Figure 6: Comparison between measured and modeled position of the front of density current.

9 ACKNOWLEDGMENTS

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