Large-eddy simulation of pyroclastic density currents

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Summary. We investigate the dynamics of turbulent pyroclastic density currents (PDCs) by adopting a 3D, Eulerian-Eulerian multiphase flow model, in which solid particles are treated as a continuum and the grain-size distribution is simplified by assuming two particulate phases. The turbulent sub-grid stress of the gas phase is modelled within the framework of Large-Eddy Simulation (LES) by means of a eddy-viscosity model together with a wall closure. Despite the significant numerical diffusion associated to the upwind method adopted for the Finite-Volume discretization, numerical simulations demonstrate the need of adopting a Sub-Grid Scale (SGS) model, while revealing the complex interplay between the grid and the SGS filter sizes. We also analyse the relationship between the averaged flow dynamic pressure and the action exerted by the PDC on a cubic obstacle, to evaluate the impact of a PDC on a building. Numerical results suggest that the average flow dynamic pressure can be used as a proxy for the force per unit surface acting on the building envelope (Fig. 5), even for such steeply stratified flows. However, it is not possible to express such proportionality as a constant coefficient such as the drag coefficient in a steady-state current. The present results indeed indicate that the large epistemic and aleatory uncertainty on initial and boundary conditions has an impact on the numerical predictions which is comparable to that of grid resolution.

Key words: Large-Eddy Simulation, pyroclastic density currents, numerical simulation, multiphase flows

1 Introduction

Pyroclastic density currents (PDCs) are high-temperature, high-velocity particle-laden flows that propagate along the flanks of a volcano under the effect of their density contrast with respect to the atmosphere. They are made up of volcanic gases and fragments of magma and rocks, ranging in size from a few microns to several decimeters, with variable density and shape, which are the

product of the *fragmentation* of the liquid magma during its decompression along the volcanic conduit. PDCs can be generated by the instability and collapse of a volcanic jet (pyroclastic flows and surges), by the collapse and crumbling of a lava dome (block-and-ash flows) or by the lateral explosion of a pressurized magma body (directed blasts). Solid particles within the current tend to segregate leading to a steep density stratification, with solid concentrations ranging from dense packing at the base (volume fraction $> 50\%$) to very dilute (volume fraction $<< 1\%$) on the top boundary [1, 9, 16]. PDCs dynamics are controlled by the competing effects of sedimentation and turbulent mixing. Particles are suspended by turbulence in the more diluted part of the current, whereas in the basal layer they are mainly supported by fluid pressure and particle collision, since the increasing solid concentration dampens turbulent fluctuations [2].
PDCs are among the most hazardous volcanic phenomena, due to their fast emplacement and destructive nature. One of the main objectives of volcanology is therefore to make a quantitative assessment of their dynamics, in order to mitigate their impact on the inhabited areas around active, explosive volcanoes. Unfortunately, PDCs are difficult to measure, even indirectly, and most of the information on their dynamics is related to the study of their deposits. On the other hand, analogue experiments are only partially useful, because of the difficulty of scaling. Theoretical and computational models thus represents a unique opportunity to deepen our knowledge of the fluid dynamics of these volcanic flows.
In the last years, thanks to the rapid development and availability of parallel supercomputers, 3D multiphase flow simulation of volcanic plumes and PDCs have become a viable tool for volcanological research [4, 10, 15]. Numerical results demonstrated the ability to catch the intrinsically 3D dynamics of the turbulent mixing, the instability of the gas-particle volcanic plume and the complex interaction of PDCs with 3D topographic features [5].
The need of simulating such non-steady-state processes over a wide range of spatial scales (from a few metres up to tens of km) and the difficulty of increasing the number of discretization elements to directly simulate all turbulent scales, make the Large Eddy Simulation (LES) approach promising [7, 12]. Nevertheless, the highly polydisperse nature of volcanic flows and the coexistence of several dynamic regimes (from dense to dilute, from high to low Mach number, from turbulent to granular flows), increases the complexity of the model and makes it difficult to achieve a high numerical accuracy. The estimate of the uncertainty associated to the numerical discretization and to the physical modeling becomes thus important to assess the quality of the results and the reliability of hazard estimates. The present work intends to give a contribution to this issue by investigating the role of grid resolution and of SGS modeling in the LES simulation of PDCs and of their impact on buildings.

2 Overview of the physical and numerical model

The dynamics of the eruptive mixture is modelled by adopting an Eulerian-Eulerian multiphase flow model. Accordingly, gas and particulate phases are treated as continua and balance equations for mass, momentum, and energy are solved accounting for advective transport, viscous dissipation, body forces and interphase momentum and energy transfers. An equation of state and a Newtonian stress tensor are prescribed for each phase in order to close the set of coupled partial differential equations (PDE). More details about the physical model can be found in [9].

A LES approach to turbulence is adopted where the Sub-Grid Scale (SGS) stresses for the gas phase are modeled through the Smagorinsky closure [13]. At the wall boundary, a roughness closure for the filter length is specified [7]. For solid particles, physical and rheological properties, as well as interactions between them, are described by using semi-empirical correlations validated in the laboratory, and no SGS model is imposed.

The transport equations are solved by a Finite-Volumes (FV) technique on a 3D, staggered grid in Cartesian coordinates. Convective fluxes are discretized through a second-order upwind method, based on MUSCL reconstruction of fluxes at the cell boundaries. Diffusive fluxes are computed explicitly by a second-order centered scheme. The non-linear system of discretized PDEs is solved by applying an iterative procedure based on the Implicit Multi Field (ICE-IMF) algorithm [3]. Mass and momentum equations and the interphase coupling are solved through a semi-implicit (predictor-corrector) algorithm, by adopting a point-relaxation (SOR) technique. Energy equations are solved explicitly by a first-order Euler scheme. Although it is well known that upwind FV schemes are affected by a considerable numerical diffusion [12], a cheap and robust numerical technique is required for the study of the dynamics of both subsonic and supersonic multiphase flows, with a low to high degree of phase coupling, such as those encountered in volcanic phenomena.

The numerical algorithm is parallelized by adopting a domain-decomposition strategy and the Message Passing Interface (MPI) [4].

3 3D simulation of a stratified PDC

The model above is applied to the numerical simulation of the propagation of a PDC in a rectangular box of size $L_x = 5$ km, $L_y = L_z = 1$, with steady-state inlet conditions on the left (x=0) boundary (Fig. 1a). Initial PDC thickness is equal to 100 m. In this application, the grain-size distribution is approximated with two particle phases of 30 and 500 μm, with densities of 2500 and 1000 kg/m^3, representative of volcanic ash and pumice, respectively. Initial conditions are comparable with those occuring in Plinian eruptions and derive from the large-scale simulations of the collapse of a volcanic jet [5], resulting in an estimated bulk Reynolds number of the current exceeding 10^7. The initial

velocity of both gas and particulate phases is 25 m/s and temperature equals 573 K. The flow pressure at the inlet is equal to the atmospheric pressure, so that it must adjust to balance the mixture hydrostatic load immediately after the injection in the domain. The inlet volumetric fractions of particles of 30 and 500 μm are, respectively, 0.65×10^{-3} and 1.625×10^{-3}, corresponding to solid bulk densities of 1.625 kg/m^3 for both particulate and about 0.6 kg/m^3 for the gas. The resulting flow dynamics pressure $P_d = 0.5\rho_m v_m^2$ is about 1.25 kPa.
We analyze hereafter the influence of the computational grid size (dx, dy, dz), of the Smagorinsky coefficient (C_s) and of the filter width (Δ). The values of these parameters considered herein are summarized in Table 1.

Run name	dx=dy [m]	dz [m]	C_s	Δ [m]
A1	10	2-20	0.1	[5.8:12.6]
A2	10	2-20	0.0	[5.8:12.6]
A3	10	2-20	0.1	10
A4	20	2-20	0.1	[9.3:20.0]
B1	20	4-40	0.1	[11.7:25.2]
B2	20	4-40	0.0	[11.7:25.2]
B3	20	4-40	0.2	[11.7:25.2]
C1	10	10	0.1	10

Table 1. Grid and turbulence model parameters adopted in 3D simulations of pyroclastic density currents. Δ is the filter width, which is equal to $(dx \cdot dy \cdot dz)^{1/3}$ (minimum and maximum values are indicated) in all simulations except A3, where it is constant. The time step is 0.01 s, corresponding to a CFL of about 0.1 for the finest mesh. Roughness length is equal to 1m in all simulations.

The propagation of a PDC (see Fig.1) is characterized by the formation of a current head (the PDC *nose*), the development of a Kelvin-Helmoltz (KH) instability (that generates transversal eddies at the upper interface between the current and the atmosphere) and the Lobe-and-Cleft (LC) instability (which is associated to the engulfment of air by the flow front that generates positive bouyancy at the current head [8]). The highest resolution that was affordable for 3D simulation (run A1 in Tab. 1) qualitatively reproduce the phenomenology of the PDC propagation, as shown in Fig.1.

Increasing the minimum vertical grid size to 4 m (B1 run, Fig. 2a) significantly reduces the intensity of the LC instability, although the overall PDC structure is captured. A dramatic change in the PDC large-scale behaviour is observed (Fig. 2b) when the vertical grid size is too coarse to describe the boundary layer and the PDC head structure (C1 run). In this case, LC insta-

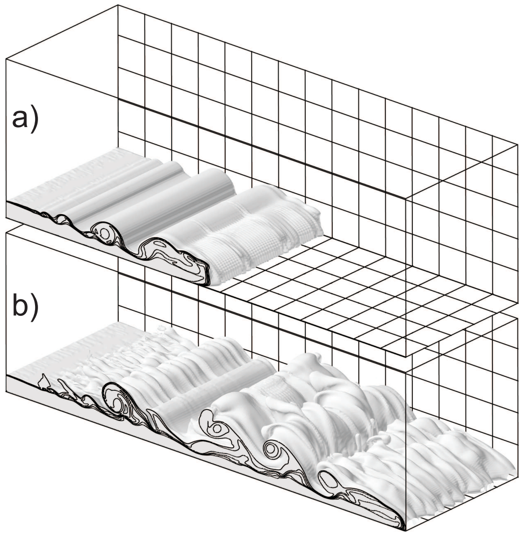


Fig. 1. Structure of the pyroclastic density current represented by the isosurface of the gas temperature (T=323 K) at 50 s (a) and 100 s (b) from the flow injection, for simulation A1. The isolines of the gas temperature, every 50 K, are also plotted on the front (y=0) plane. Gridding every 200 m.

bility is damped out, the flow is considerably faster and the number of KH rolls is largely reduced.

Concerning the effect of the SGS model parameters, model parameters, fixing the filter length scale to 10 m (A3 run, Fig. 2c) does not significantly influence the large-scale structure of the PDC, whereas removing the model by imposing the Smagorinsky constant $C_s = 0.0$ (A2 run, Fig. 2d) completely changes the PDC dynamics. In the latter case, the lower viscosity in the model produces a much thinner boundary layer profile, so that the horizontal momentum transferred to the basal layer by the effect of the sedimentation is not dissipated. As a result, the flow head develops a wedgelike shape that causes a suppression of the LC instability mechanism, since it inhibits the entrainment of atmospheric air from the bottom.

The vertical profile of a PDC results from the concurrent effect of the wall shear stress (that generates a boundary layer), sedimentation (that decreases the mixture density at the current top while concentrating particles at the base) and air entrainment. In Fig.3 we present the profiles of dynamic pressure of the mixture $P_d = 1/2\rho_m v_m^2$, averaged in time, at 1.5 km from the inlet and along the central axis (the uniform value at the inlet is also displayed for reference). Simulations A1 and B1 give comparable results, whereas run C1 significantly underresolves the flow boundary layer and underestimates the concentration gradient near the wall. Interestingly, a similar net effect is observed when the SGS model is removed at higher resolution (A2 run). In

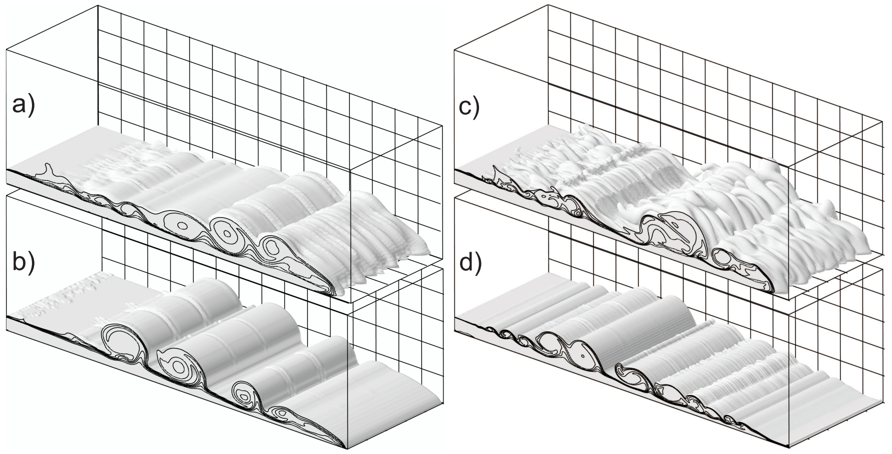
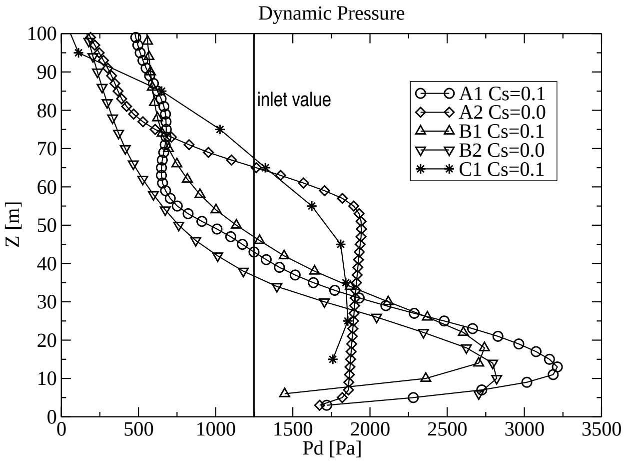


Fig. 2. Effect of the grid size and SGS filter size on the numerical results. Isosurface of the gas temperature for B1 at 100 s (a), C1 at 88 s (b), A3 at 100 s (c) and A2 at 75 s (d). See Table 1 and Figure 1 for parameters and comparisons.

this latter case (A2), the finer vertical grid size is responsible for the steeper concentration gradient and the reduced shear stress near the wall, which prevent the formation of the PDC nose, air entrainment from the head and the subsequent growth of the LC instability. As a result, the concentration profile is controlled by the sedimentation rate only and the current maintains a "constant settling zone" (with *top-hat* profile) for longer (see also Fig. 2d). Simulations with a coarser mesh (B1-B2) seem less sensitive to the SGS model, probably because of the larger numerical diffusion associated to the grid.
The value of dynamic pressure in the first cell above the ground (reported in the legend of Fig. 3) increases on finer grids, reflecting the strong sensitivity of the concentration to the cell size (also observed in 2D simulations [9]). This value should then be considered carefully, also because the multiphase flow formulation at high concentration do not account for particle-particle friction. Although direct measurements of PDC profiles are presently out of our technical possibilities, future studies should try to make the present results more quantitative, by comparing numerical to laboratory experiments (e.g. [6]).

4 Flow-building interaction

We finally present here the application of the 3D multiphase flow model to the analysis of the impact of a PDC on a building. Such study is mainly motivated by the need of estimating the action of the flow on a structure engulfed by a PDC and to design appropriate mitigation actions [19]. The damage on the infrastructures is also often utilized as an indirect measure of the maximum flow dynamic pressure [17]. However, the interaction between a PDC and a



Run	P_d-av	P_d-base
A1	1570	5160
A2	1470	6550
B1	1390	2610
B2	1530	11500
C1	1450	2460

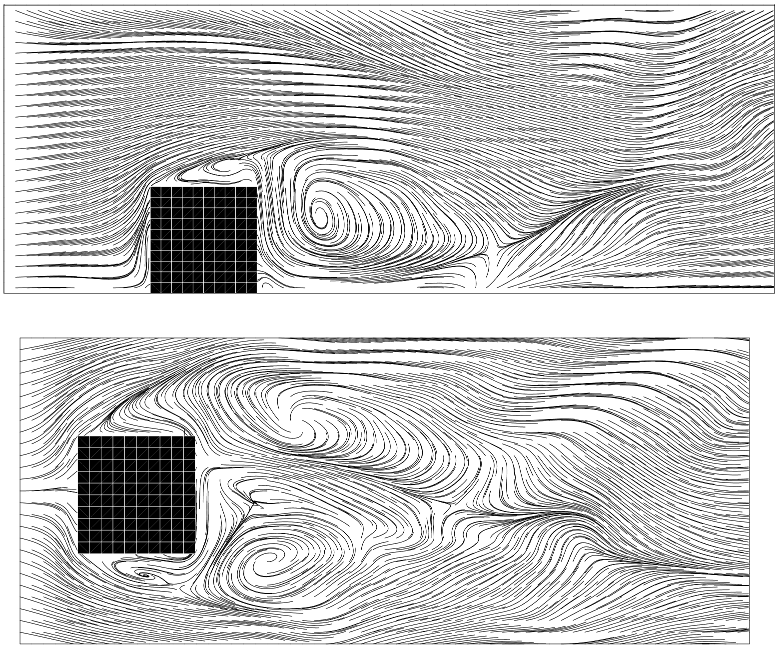
Fig. 3. Time-averaged vertical profile of the flow dynamic pressure at 1.5 km from the inlet. Time averaging is performed from the time of passage of the front up to 100 s. The value in the first computational cell above ground (P_d-base), omitted for the sake of plot clarity, is reported in the legend on the right, together with the vertically averaged value (P_d-av) over a flow thickness of 100 m.

building is considerably complicated by 1) the presence of solid particles in a wide range of sizes and densities, 2) the stratified nature of PDCs and 3) the transient nature of the PDC emplacement. Therefore, the relationship between the (average) flow dynamic pressure and the action on the structure needs further investigation.

Numerical simulation have been performed by adding an obstacle of $20 \times 20 \times 20$ m^3 at 1.5 km from the inlet, in the same simulation conditions described above. Numerical results describe the flow separation on the building edge, the reattachment of the current downstream and the formation of a complex and unsteady eddy structure (Fig.4).

The time-dependent action on the obstacle has been computed by integrating the pressure field along the building envelope. The PDC action on the building fluctuates around 2 kPa (consistent with the estimate of the average dynamic pressure, around 1.5 kPa) but it is significantly underestimated in the lowest resolution run C1.

The effect of a change of the particle diameter has been also estimated for comparison and plotted (in grey) in Fig. 5, since the grain-size distribution represents one of the eruptive parameters most subject to uncertainty. The associated uncertainty in the computed drag force is of the same order of magnitude of the error associated to the grid size, thus making it difficult to estimate a unique relationship between the flow action and the dynamic pressure for PDCs.



(a)

(b)

Fig. 4. Vortex structure around a cubic obstacle engulfed by a PDC, within the A1 run. The streamlines represent gas velocity on the (a) longitudinal (xz) and (b) horizontal (xy) planes at half width and heigth, respectively and at 50 s. The grid size of 2 m is also represented within the obstacle.

5 Conclusions

Numerical results suggest that, despite the significant numerical diffusion associated to the upwind discretization, the LES subgrid model is needed to reproduce the qualitative behaviour of PDC (particularly the formation of a turbulent flow head with a *nose* structure and the development of KH and LC instabilities). In the adopted simulation conditions, the medium-resolution (4-40 m) mesh is able to resolve the flow boundary layer and to catch the qualitative behaviour of a PDC, giving a comparably good estimate of the flow action on a cubic obstacle. For the purpose of large-scale impact analysis (where the grid resolution cannot fully resolve the flow at an urban scale [5]) the averaged flow dynamic pressure results to be an acceptable proxy for the force per unit surface acting on the building envelope, although simulation C1 (the lowest resolution investigated with 10 m grid size) significantly underestimate it of a factor of 2-3. Present results also show that the effect of a change in the grain-size distribution may be comparable to that associated to the numerical grid and SGS filter size.

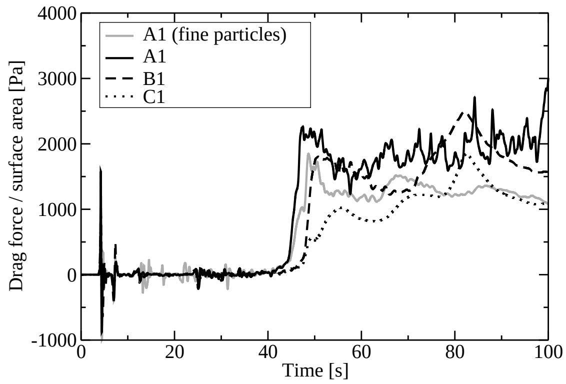


Fig. 5. Drag force per unit surface as a function of time. Black lines refer to A1 (solid), B1 (dashed) and C1 (dotted) runs. The grey, solid line refer to the A1 run with only one particle class of 30 μm and the same mixture density.

Physical and numerical models in volcanology are indeed subject to a variety of uncertainties. The multiphase formulation of the eruptive mixture dynamics is not univocal and intial and boundary conditions are subject to a large *epistemic* and aleatory uncertainty [18]. This implies that the absolute verification and validation of a model is inherently impossibile [14, 11]. Moreover, in the study of explosive eruptions it is difficult to test the congruence of numerical models to observational data, given the rarity of the events and their catastrophic nature.

However, numerical models can be used for sensitivity analyses, to elucidate the relative importance of model variables, and to compare single realizations in order to identify the most important eruptive parameters that define an eruptive scenario. Within this context, the assessment of quality and reliability of model results appears as an extraordinary challenge in which numerical benchmarking should be accompanied by an effort in combining modelling with uncertainty analysis, through statistical techniques leading to the construction of response surfaces relative to the variation of the different simulation parameters and possibly to their optimization. To this aim, however, the improvement of remote measurement techniques is also needed, to better characterize a natural phenomenon to which we have incomplete access.

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