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PERSPECTIVES

A framework for validation and benchmarking of pyroclastic current models

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Abstract
Numerical models of pyroclastic currents are widely used for fundamental research and for hazard and risk modeling that supports decision-making and crisis management. Because of their potential high impact, the credibility and adequacy of models and simulations needs to be assessed by means of an established, consensual validation process. To define a general validation framework for pyroclastic current models, we propose to follow a similar terminology and the same methodology that was put forward by Oberkampf and Trucano (Prog Aerosp Sci, 38, 2002) for the validation of computational fluid dynamics (CFD) codes designed to simulate complex engineering systems. In this framework, the term *validation* is distinguished from *verification* (i.e., the assessment of numerical solution quality), and it is used to indicate a continuous process, in which the credibility of a model with respect to its intended use(s) is progressively improved by comparisons with a suite of ad hoc experiments. The methodology is based on a hierarchical process of comparing computational solutions with experimental datasets at different levels of complexity, from unit problems (well-known, simple CFD problems), through benchmark cases (complex setups having well constrained initial and boundary conditions) and subsystems (decoupled processes at the full scale), up to the fully coupled natural system. Among validation tests, we also further distinguish between *confirmation* (comparison of model results with a single, well-constrained dataset) and *benchmarking* (inter-comparison among different models of complex experimental cases). The latter is of particular interest in volcanology, where different modeling approaches and approximations can be adopted to deal with the large epistemic uncertainty of the natural system.

Keywords Pyroclastic currents · Numerical models · Validation · Verification · Benchmarking

Introduction and motivation

The main objectives of physical, mathematical, and numerical models of volcanic processes are interpretation of the available geological and geophysical data in order to reconstruct and understand fundamental eruption processes, and prediction of the occurrence and impact of future eruptions. The latter is required for hazard and risk assessment and for the design of risk mitigation measures. Among the variety of volcanic processes, pyroclastic currents (also called pyroclastic density currents, pyroclastic flows, and pyroclastic surges) are particularly challenging to model (Neri et al. 2014; Dufek et al. 2015; Dufek 2016). Despite significant and continuous progress, our predictive capability of pyroclastic currents is indeed still limited by (1) incomplete knowledge of the multiphase and multiscale processes controlling gas-particle flow dynamics across a wide range of dynamical regimes (Dufek et al. 2015; Dufek 2016); (2) constrains on numerical model resolution and capability of modeling a broad range of spatial/

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temporal scales and turbulent regimes (Esposti Ongaro et al. 2011; Cerminara et al. 2016a); and (3) by aleatory uncertainty in initial and boundary conditions that are related to incomplete data and the inherent randomness of the natural eruptive phenomena (Sparks and Aspinall 2015; Neri et al. 2014; Neri et al. 2015).

Based upon detailed field observation, sedimentological studies of pyroclastic deposits, controlled laboratory experiments, and physical laws, a conceptual model of pyroclastic currents can be built upon the following elements:

- Continuum approximation. Pyroclastic current transport can be described by the laws of continuum fluid mechanics, with the flow regime strongly controlled by particle concentration (Druitt 1998; Freundt and Bursik 1998; Valentine and Fisher 1986, 2000; Freundt et al. 2000; Branney and Kokelaar 2002; Sulpizio et al. 2014). Pyroclastic currents encompass a spectrum of multiphase flow types and flow regimes ranging from high-particle-concentration (volume fraction of particles > 0.1) flows in which particle-particle interactions and pore-gas pressure dominate clast transport (also referred to as pyroclastic flows) to dilute (volume fraction < 0.001) flows (also referred to as pyroclastic surges) within which clast transport is governed by a combination of turbulent suspension and bed-load processes. The granular rheological behavior and turbulent gas-particle interactions are deeply dependent on volumetric particle concentrations, with transition between dense and dilute flows occurring between solid volume fractions $\epsilon_s \approx 0.01$ and $\epsilon_s \approx 0.1$ (Balachandar and Eaton 2010; Weit et al. 2019). Despite the lack of a strong scale separation (i.e., the separation between the microscopic and macroscopic length and time scales; Goldhirsh 2008), continuum granular flow models are able represent the dynamics of such multiphase granular mixtures down to the scale of flow deposit (Fig. 1). In the lower portion of a flow, where particle-particle interactions become important, transitions between processes captured by the continuum framework and discrete particle regimes need consideration (Staron and Phillips 2014).
- Compressibility. Compressible flow phenomena can be relevant in many processes occurring before and during flow, when and where the local flow velocity approaches or exceeds the speed of sound. The speed of sound of gas-particle mixture is significantly lower than that of the carrier gas (Wohletz et al. 1984; Fink and Kieffer 1993; Esposti Ongaro et al. 2011).
- Buoyancy. Pyroclastic currents are mostly gravity-driven flows. Negative buoyancy is relevant on steep slopes as a longitudinal driving force (avalanche dynamics; McEwen and Malin 1989; Pudasaini and Hutter 2007) but also on gentle slopes and flat topographies as an effect of the horizontal gradient of hydrostatic pressure (gravity current dynamics; Huppert et al. 1986; Dade and Huppert 1996). On the other hand, entrainment of air and deposition of particles reduces the average density of the current, which eventually can reverse its buoyancy to positive, lift off, and stop its horizontal propagation (Sparks et al. 1993).
- Sedimentation/deposition. Gravity also acts as a driver for particle settling and deposition. Variable gas-particle and particle-particle coupling regimes lead to density stratification of the current and eventually to the deposition of particles (Branney and Kokelaar 2002). This is one of the main mechanisms for momentum loss in the currents (Bursik and Woods 1996).
- Polydispersity. It is well known that pyroclastic currents transport and deposit particles over a wide range of grain sizes (Walker 1971; Sparks 1976). The interactions among grains of different sizes is still not completely understood, and modeling approaches are still under validation (Benyahia 2008). However, recent experiments have highlighted the key role of grain size distribution, and in particular of fine particles, in the runout distance of gravity currents (Gladstone et al. 1998), recently recognized as an effect of modified pore-pressure transport and diffusion (Roche et al. 2011).
- Granular flows. In the basal, concentrated flow region, deposition of particles and momentum dissipation are controlled by granular flow phenomena and particle-particle friction, which in turn can be modulated by pore-gas pressure. Of primary importance in modeling pyroclastic current dynamics is the involvement of the granular flow theory (Campbell 1990; Iverson and Vallance 2001; Dufek 2016) in description of the lower part of the currents, which is dominated by particle-particle interactions. Dynamic transitions between granular, gas-fluidized, collisional, and kinetic regimes is one of the key aspects of pyroclastic current dynamics (Fisher 1983).
- Turbulence. In the upper flow region, at the interface with ambient atmosphere, fluid turbulence controls the entrainment and heating of atmospheric air. Entrainment contributes to dilution of the current, and gas-particle heat exchange is one of the controlling processes of pyroclastic current thermodynamics (Bursik and Woods 1996; Neri et al. 2003a, b; Benage et al. 2016).
- Topography. Interaction with topography can control the dynamics of pyroclastic currents in different ways, including hydraulic effects (associated to changes in slope, current height and width), stratified flow effects (blocking and modification of the vertical flow profile; Valentine 1987), flow diversion and decoupling (Fisher 1990; Woods et al. 1998; Bursik and Woods 2000; Branney and Kokelaar 2002), and basal friction through roughness (Stinton et al. 2004).

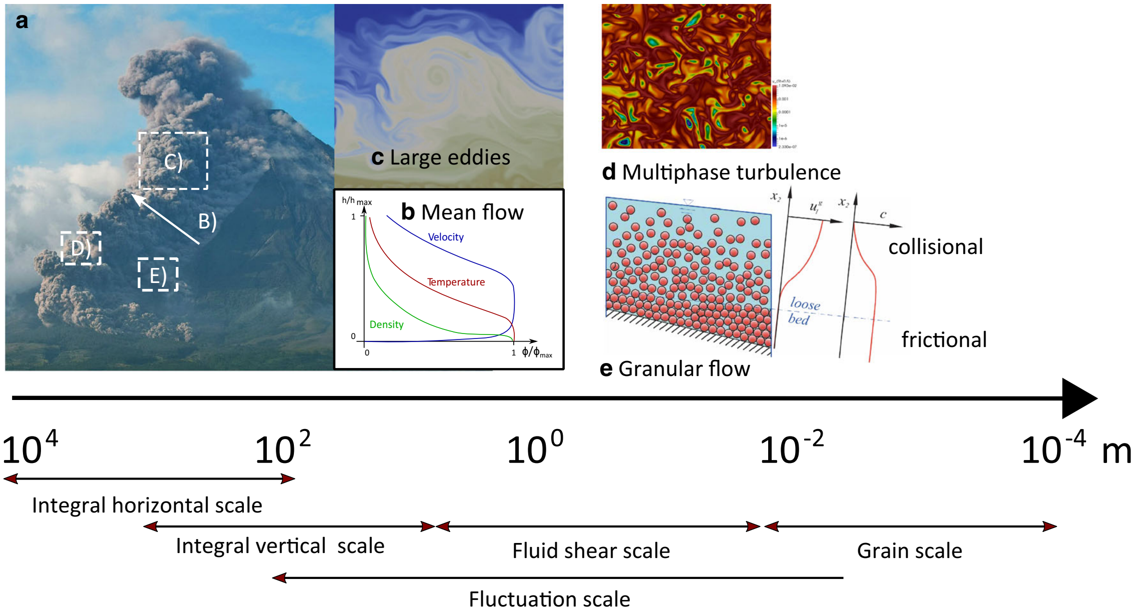

Fig. 1 Dynamic scales in pyroclastic current dynamics. (A) Integral scale (observations): pyroclastic current at Mayon (photo by J Esmeria CC BY-SA 4.0). (B) Fluid scale: time-averaged mean flow profile. (C) Fluid scale: large eddy fluctuations. (D) Fluctuations scale: preferential concentration of particles by fluid turbulence in the dilute ash cloud (Cerminara et al. 2016a). (E) Fluctuations scale: granular temperature in the concentrated basal granular flow (sketch by Armanini 2013)

Other processes, usually considered as having second order relevance, include substrate erosion, water phase transitions, particle aggregation and secondary fragmentation, chemical reactions, radiative heat transfer, meteorological conditions (including wind), and electrostatic phenomena. In principle, the above phenomenological factors can be incorporated into mathematical language expressing the conservation of mass, momentum, and energy in a system of coupled partial differential equations. This can have varying degrees of complexity depending upon simplifications that are made for a given application or intended use. In practice, however, some of the processes mentioned above are still poorly understood and the definition of the appropriate model, and of the initial and boundary conditions (in particular, current stratification and flow rate), can be challenging.

In addition to the difficulties related to model formulation, numerical methods are necessary to solve the systems of equations. The numerical solution procedure involves discretization of the equations, usually by means of the subdivision of the spatial and temporal domain into discrete spatial elements. Fluid dynamics equations are intrinsically nonlinear, and eruptive processes usually involve coupling of variables over a broad range of spatial and temporal scales. Since it is presently not possible to simultaneously solve the equations at all relevant scales, so-called sub-grid scale (SGS) models (Mason 1994; Esposti Ongaro et al. 2011; Cerminara et al. 2016a, b) are usually adopted. SGS models, similar to constitutive models describing continuum behaviors, are semi-empirical models developed from a combination of experimental and theoretical information. Their formulation and validation are key steps of the modeling process.

Finally, modeling of pyroclastic currents carries with it both epistemic and aleatoric uncertainties (Sparks and Aspinall 2015). Epistemic uncertainty arises from a lack of perfect knowledge of the physical system, the possibility of alternative models, and limitations in our ability to pragmatically describe the system. Aleatoric uncertainty is associated with the difficulty of measurements of the natural phenomenon, the scarcity of data, the limited repeatability of observations, and irreducible randomness of volcano behavior. While we can work to reduce both epistemic and aleatoric uncertainty, they can never be eliminated; thus, it is important to quantify them when conducting pyroclastic current modeling.

The above considerations, together with the global importance of model predictions to support decisions in the context of hazard and risk assessment, heighten the need to establish the limits and constraints on the use of models and to establish a consensus on the methodology to determine their accuracy and assess their credibility in different situations. All geoscientific models are in principle impossible to "verify" in the sense that their "truth" is impossible to establish (Oreskes et al. 1994). This is due to the non-repeatability of the observations, unsteadiness of the system, incomplete knowledge of data, and the consequent possible non-uniqueness of the solutions (i.e., different models can potentially explain the same observations). Strict validation, in the sense of testing whether a model adequately represents a physical system of interest for the purpose at hand, is a necessarily incomplete process, since a proper metric cannot be accurately defined; validation should be considered to be never complete and always evolving.

This paper aims to establish a framework for validation of pyroclastic currents model by (1) proposing a common terminology on verification, validation, and benchmarking; (2) describing different approaches to pyroclastic currents models, and their strengths and weaknesses, to facilitate designing of appropriate benchmark cases; and (3) proposing a path towards satisfactory pyroclastic model validation. A community-driven effort will be needed to consensually evaluate the accuracy of numerical models in representing pyroclastic currents-related phenomena, to establish best practices to estimate the error and uncertainty associated with numerical predictions, and to drive future interdisciplinary research while increasing awareness of the strengths and limitations of various modeling tools.

Terminology

Before describing the verification, validation, and benchmarking procedure, we briefly review the related terminology and we report some examples from the scientific literature on pyroclastic currents.

Verification

Oberkampf and Trucano (2002) define verification as "The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model." A key phrase in this definition is *description of the model*, which in this case is a particular form of the governing equations, the form of which is determined by the simplifications and assumptions made. This definition largely overlaps with Oreskes et al. (1994) definition of model benchmarking: "The practice of comparing numerical and analytical solutions." A simple way to put it is that verification checks that a discrete numerical approximation accurately represents the system of continuous functions and differential equations. It is needed as a preliminary step of any validation procedure in order to quantify the error related to the numerical solution method. This is different from checking whether the system of equations adequately represents a physical system of interest (validation).

Verification of multiphase models for pyroclastic currents can be challenging. Most previous efforts to do so in volcanology have focused on the comparison with one-dimensional discontinuous solutions (see Table 1). Although this is a good test for numerical fluid solvers, it is limited by the availability of analytical solutions. A viable alternative that complex volcanological models might benefit of is to use so-called manufactured solutions. This method allows testing of numerical implementations by imposing a source term to the model (generally, in simplified configurations) in such a way as to obtain a prescribed analytical solution (Roache 2002). The method also gives an empirical estimate of the numerical scheme accuracy (Jacobs et al. 2012).

Validation

In general terms, we define *validation* as the process of demonstrating that a system of equations and their numerical approximation reasonably represents the researcher's physical conceptual model for a process. In other words, does the system of equations adequately represent the physics at hand (where *adequately* depends upon the intended use of the model and upon the desired level of accuracy)? Validation assumes some level of prior verification (previous section). Validation normally involves comparison of a model with a suite of experiments that are meant to represent, as much as possible, the physical processes described in the conceptual model. Our usage of the term is consistent with Oberkampf and Trucano (2002) terminology that defines validation as "The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model." Validation of pyroclastic models is, in this framework, a continuous process, in which empirical datasets are systematically compared with model results. The greater the number and diversity of confirming observations, the *more probable* will be that the conceptualization embodied in the model is not flawed (Oreskes et al. 1994).

In practice, though, it is difficult, if not impossible, to devise experiments that capture the full range of processes that can occur in pyroclastic currents, even in large-scale experiments (Dellino et al. 2007; Lube et al. 2015). In rare cases, an example of a natural pyroclastic current might have adequate constraints and observational data to also be used for validation.

As explained in the next section, when comparing a model with a specific experimental or field dataset we thus suggest avoiding statements such as "model *A* has been validated," and instead propose using the term *confirmation* or *confirmed* for a specific problem. The level of accuracy at which the model has been confirmed should be also specified, by reporting the confidence interval obtained for key observables.

Confirmation

Confirmation, according to Oreskes et al. (1994), is the matching of "the distribution of the dependent data in a numerical model with observational data." Confirmations only "support the probability of the veracity of a model,"

Table 1 Some examples of model *verification* in volcanology

Verification case	References
Analytical 1D shock tube	Carcano et al. (2014); Esposti Ongaro et al. (2007); Dartevelle (2007, 2011); Cerminara et al. (2016a, 2016b)
Dam-break analytical solution	Galas (2008); Shimizu et al. (2017)
1D Riemann problem	de' Michieli Vitturi et al. (2019)
Manufactured solution	Jacobs et al. (2012)

but "… no matter how much data we have there will always be the possibility that more than one theory can explain the available observations." In this sense, confirmation can be seen as the constituent part of a more structured validation process. As stated above, we propose therefore to use the term confirmation instead of validation for single, successful comparisons between model results and experimental/observational data.

For example, Valentine and Sweeney (2018) compared their model results on a type of impinging jet to a specific experimental dataset on impinging jets, which confirmed the applicability of MFIX (a multiphase flow numerical code) for the problem they were addressing. Breard et al. (2019a, b) confirmed the same code's ability to reasonably reproduce results of experiments with concentrated, fluidized flows (Roche et al. 2010). Similar confirmation efforts have been carried out using depth-averaged models and inverse modeling on well-constrained natural case studies of past pyroclastic current events at Merapi and Soufriere Hills (Charbonnier and Gertisser 2012; Ogburn and Calder 2017; Gueugneau et al. 2019). These studies include the different processing steps required to reduce uncertainties in objectively defining the different input parameters and to correctly evaluate the output variables of such models (Sheridan et al., 2005). Confirmation of results has been based on a rigorously defined metrics based on the comparison of the areas inundated (Charbonnier et al. 2018). A more complete list of confirmation examples for pyroclastic current models is reported in Tables 2 and 3.

Calibration

Calibration, quoting Oreskes et al. (1994), is the process of "manipulating the independent variables (and parameters) to obtain a match between the observed and simulated distribution of dependent variables." Calibration establishes some "empirical model adequacy." However, "even if a model result is consistent with present and past observational data, there is no guarantee that the model will perform at an equal level when used to predict the future" (and in different conditions) (Oreskes et al. 1994).

Calibration of scaling parameters, empirical constants, transport coefficients, and other constitutive equations is usually implicit in many fluid dynamics models used in volcanology. Calibration plays a key role especially for reduced order or low-dimensionality models, usually involving a priori undetermined empirical coefficients. For example, the determination of the air entrainment coefficient in one-dimensional models of turbulent pyroclastic currents (Bursik and Woods 1996) or the front Froude number (Esposti Ongaro et al. 2016) are examples of model calibration studies (see also Table 4). Another significant case is that of granular friction parameter for depth-averaged flows: for a Coulomb rheology, calibration studies indicate a range of bed friction angles between 2° and 15° and internal friction angle of 30° (Kelfoun 2011). If a model is not capable of predicting an outcome within this calibration range, it is failing at interpolation, which is a serious issue (Charbonnier and Gertisser 2012). This calls for extending the calibration range or assume that the model is flawed.

Table 2 Some examples of pyroclastic current model *confirmation* (subsystems)

Subsystem	
Blast unit (Soufrière Hills, 1997)	Esposti Ongaro et al. (2008)
Blast unit (Mount St. Helens, May 18, 1980)	Esposti Ongaro et al. (2012)
Individual pyroclastic current unit (Vulcano, Breccia di Commenda)	Rosi et al. (2018)
Plinian column collapse unit (Vesuvius, AD79)	Neri et al. (2003a)
Sub-Plinian column collapse unit (Tungurahua, 2006)	Bernard et al. (2014); Benage et al. (2016)
Individual dome collapse (Merapi, June 2006)	Charbonnier and Gertisser (2012)
Individual dome collapse (Soufrière Hills, 25 June 1997)	Widiwijayanti et al. (2004); Gueugneau et al. (2019)
Individual dome collapse (Merapi, November 2010)	Kelfoun et al. (2017)
Individual dome collapse (Unzen, 1991)	Ishimine (2004)

Table 3 Some examples of pyroclastic current model *confirmation* (unit problems)

Unit problem	References
Compressible flows	Dartevelle (2007), Carcano et al. (2014)
Turbulent forced plumes	Dartevelle (2007); Cerminara et al. (2016a, 2016b)
Kinematics of a homogeneous gravity current over a flat surface	Dufek and Bergantz (2007a, 2007b); Esposti Ongaro et al. (2016)
Particle settling in still water	Jacobs et al. (2012)
Homogeneous/isotropic and multiphase/isotropic turbulence	Cerminara et al. (2016a, 2016b)
Heat transfer	Cerminara et al. (2016a, 2016b)
Granular lock-exchange flow	Roche et al. (2011); Meruane et al. (2010)
Supersonic impinging jets	Valentine and Sweeney (2018)
Dam-break granular flows	Breard et al. (2019a, 2019b); Webb and Bursik (2016)
Fluidization experiments	Neri and Gidaspow (2000), Breard et al. (2019a, 2019b)

Benchmarking

We use the term benchmarking specifically for comparison of computational models with each other. Such comparisons normally use a defined problem that is either based upon an experimental (Table 5) or natural dataset. Model approximations, asymptotic regimes, numerical resolution effects, and error propagation are often difficult to evaluate for benchmarking purposes. Therefore, a key goal is to integrate well-constrained experimental data in such process to correctly assess the "empirical adequacy" of the different numerical models (Oreskes et al. 1994). Although this overlaps in some ways with confirmation, the aim is different. Rather than testing the ability of a specific model to represent physical processes of interest, benchmarking is intended to elucidate the relative strengths and weaknesses of models with respect to each other, and the different degrees of approximations and related uncertainties. These strengths and weaknesses depend upon the desired application. Thus, benchmarking is not intended to pick "winners" and "losers."

For example, a complex, multiphase, three-dimensional model might provide a better match to a benchmarking dataset related to a volcano that is experiencing unrest than does a simplified depth-averaged model. However, the former model might take days or even weeks to set up and run individual scenarios, whereas the simpler model can be quickly run over a wide range of scenarios and produce a probabilistic forecast that is useful on an urgent time scale. In this case, the latter model might be selected for the application of obtaining quicker forecasts, but the benchmarking exercise would provide a basis for quantifying its uncertainties and limits. On the other hand, the multiphase model might be selected for a study of fundamental pyroclastic current processes that is not time constrained and will only involve subject matter experts; similarly, though, the benchmarking exercise would have provided insight into the limitations and uncertainties in the complex model, and sensitivity to empirical input parameters. An emerging added value of benchmarking studies is also the possibility of calibrating such empirical laws of low-dimensional models via three-dimensional numerical simulations (e.g., Costa et al. 2016). Therefore, to design a benchmark for pyroclastic currents, the variety of available models, existing approaches, and their main applications should be considered.

Benchmarking of pyroclastic current fluid dynamic models

In this section, we summarize the features and major approaches to pyroclastic current modeling, and recall the main mathematical operations that allow the inter-comparison of results in a benchmark study. The development of

Table 4 Some examples of pyroclastic current model *calibration*

Calibration parameter	References
Air entrainment coefficient (depth-averaged models)	Bursik and Woods (1996)
Non-dimensional parameters (integral box model)	Neri et al. (2015); Esposti Ongaro et al. (2016)
Granular friction parameters (depth-averaged models)	Ogburn and Calder (2017); de' Michieli Vitturi et al. (2019); Kelfoun (2011)
Kinematic front conditions	Takahashi and Tsujimoto (2000); Widiwijayanti et al. (2009); Wadge et al. (1998)
Sedimentation rate	Druitt et al. (2007); Girolami et al. (2010)

Table 5 Some examples of experimental configurations suited for pyroclastic current model *benchmarking*

Experimental benchmark cases	References
Large-scale, dilute, turbulent, polydisperse gravity current over an incline	Breard et al. (2016); Breard and Lube (2017)
Large-scale axisymmetric polydisperse gravity current from jet collapse	Dellino et al. (2010)
Concentrated, fluidized/non-fluidized granular current over an incline	Lube et al. (2011); Chédeville and Roche (2015); Rodriguez-Sedano et al. (2016); Chedeville and Roche (2018)
Turbulent gas-particles flows with buoyancy reversal	Andrews and Manga (2011)
Interaction of stratified gas-particle gravity currents with obstacles; sedimentation rate.	Andrews and Manga (2012); Woods et al. (1998)

computational fluid dynamic (CFD) models for pyroclastic currents has traditionally followed two main approaches. The first one has aimed at developing transient three-dimensional, multiphase flow models, built upon a physical description of the microphysics of gas-pyroclast mixtures (referred to here as the multiphase flow approach). The second approach has focused on the development and application of low-dimensional models, typically depth-averaged homogeneous models, either transient or steady-state (referred to here as the depth-averaged approach). Note that in our discussion about different pyroclastic current CFD approaches (and their validation), we do not include models based on empirical or statistical correlations such as H/L (e.g., Calder et al. 1999; Widiwijayanti et al. 2009), energy-line models (Sheridan and Malin 1983; Tierz et al. 2016; Ogburn and Calder 2017), or kinematic models for the pyroclastic flow front (McEwen and Malin 1989; Wadge et al. 1998; Rossano et al. 2004; Saucedo et al. 2005), as well as more sophisticated mechanical models (Takahashi and Tsujimoto 2000). Such models cannot be derived from mass, momentum, and energy conservation laws by some formalized mathematical operation, or filter (such as averaging or integration). They are essentially data fits, and they can only be calibrated, not rigorously validated.

It is not the purpose of this section to review or criticize either of the two main approaches, since there are very good reasons to adopt each of them for different purposes and in different contexts and applications (see Table 6). Instead, we aim to demonstrate that the use and comparison of the different modeling approaches in the framework of a rigorous benchmarking process enhances them as complementary tools for improving our understanding of pyroclastic current dynamics and for improving our capabilities in hazard assessment. Because it is extremely difficult to evaluate a priori the advantages of the use of different approximations, assessing the sensitivity of model results to uncertain initial conditions should be one of the steps of the validation process.

Here, we present the different pyroclastic current modeling approaches in a hierarchical scheme, highlighting the formal mathematical assumptions and the hypotheses at the base of their different approximations (Fig. 2). Benchmark cases proposed in this validation framework should be applicable to models at any level of approximation.

Eulerian and Lagrangian approaches

Most models of pyroclastic currents are based on continuum approximations (Eulerian approach) that describe solid particles as fluid fields (Gidaspow 1994; Armanini 2013, Goldhirsh 2008). This approach involves some general assumptions that are worth recalling here:

- At the microscopic scale, particle-particle collisions are uncorrelated, isotropic, and homogeneous.
- The mean free path λ is much larger than the particle size, $\lambda \gg d_s$.

The mean free path is much smaller than the macroscopic scale of interest, $\lambda \ll L$ (in particular, of the scale L of variation of an average quantity ψ, $L \sim \frac{\psi}{d\psi/dx}$).

Eulerian multiphase flow models have been used for the study of pyroclastic current dynamics for at least 30 years (e.g., Dobran et al. 1993; Neri et al. 2003; Dartevelle and Valentine 2007; Dufek and Bergantz 2007a, b; Esposti Ongaro et al. 2008, 2012; Carcano et al. 2013; Sweeney and Valentine 2017; Valentine and Sweeney 2018) and their applicability to the transport regime of pyroclastic currents is generally accepted (Dufek 2016). Opposite to Eulerian ones, Lagrangian methods (such as the Discrete Elements Method; Guo and Curtis 2015) solve the Newton's equations for a number of interacting particles. While attractive for describing granular flows, especially in the depositional regimes, where particle concentration increases and the mean free path decreases (Staron and Phillips 2014), Lagrangian methods are still computationally unmanageable to represent the actual number of particles at the geophysical scale and are therefore not widely used in volcanology. Mesh-free discrete numerical solution methods for continuous models, such as smoothed particle hydrodynamics (SPH; Monaghan 2012) or multiphase-particle-in-cell (MP-PIC; Andrews and O'Rourke 1996), can also possibly be considered, although

Table 6 Physical processes and key phenomena in pyroclastic current dynamics and minimum dimensionality required to model them (asterisk indicates parameters directly relevant for pyroclastic current hazard assessment)

Key phenomena	Minimum dimensionality
Energy/mass balance, front kinematics, runout*	0D + time (integral or kinematic models)
Effect of slopes, radial distribution of flow variables*, distance of buoyancy reversal*	1D (steady-state depth-averaged models)
Waves and perturbations, front dynamics, unsteady boundary conditions	1D + time (transient, depth-averaged models)
Sedimentation, stratification, erosion, flow decoupling*, interaction with obstacles*	1D multilayer + time (transient, depth-averaged multilayer models)
	2D + time (2D transient models with Cartesian or cylindrical symmetry)
Turbulence, 3D topographic effects*, acoustic emission, generation mechanism	3D + time

their use is presently very limited in volcanology (Cao et al. 2018).

An effective approach is to couple Eulerian and Lagrangian models to describe different particle classes in the same solver (Dufek and Bergantz 2007b; Breard et al. 2018). In such cases, inter-comparison between numerical results from Eulerian and Eulerian-Lagrangian models can always be performed in the framework of benchmark studies by using the method for particle averaging over fixed control volumes (Goldschmidt et al. 2002). In the following, we will consider only Eulerian models.

Dimensionality: symmetry and depth-averaging

Eulerian fluid models are in general formulated in three dimensions, with appropriate boundary conditions representing the interaction with the topography, the volcanic source, and the atmosphere. Because of the higher computational cost of 3D models, reduction of model dimensionality can be done by assuming Cartesian or radial symmetry, or invariance. Inter-comparison between 3D and symmetric models can be done by averaging 3D models along the direction(s) where invariance is assumed.

Here, we put more emphasis on the depth-averaged approach, in which reduction of model dimensionality is obtained by formally integrating the fluid dynamics equations along the vertical dimension: the resulting equations are solved for the depth-averaged physical variables. For example, for a three-dimensional model where the vertical axis is oriented along z, the volume concentration of a given particle class $\epsilon_s(x, y, z, t)$ will be replaced by its depth-averaged value $\langle\epsilon_s\rangle(x, y, t)$, thus reducing the problem to a transient, two-dimensional one. Analogously, for a two-dimensional model (for example, in cylindrical coordinates), the depth-averaging procedure leads to a one-dimensional transient problem. At the same time, the vertical component of the velocity is set to zero, significantly reducing the computational complexity. The depth-averaged equations are valid under the assumption that the horizontal length scale of the flow is much greater than the vertical length scale, i.e., the fluid flow develops as a thin layer spreading horizontally over distances that are

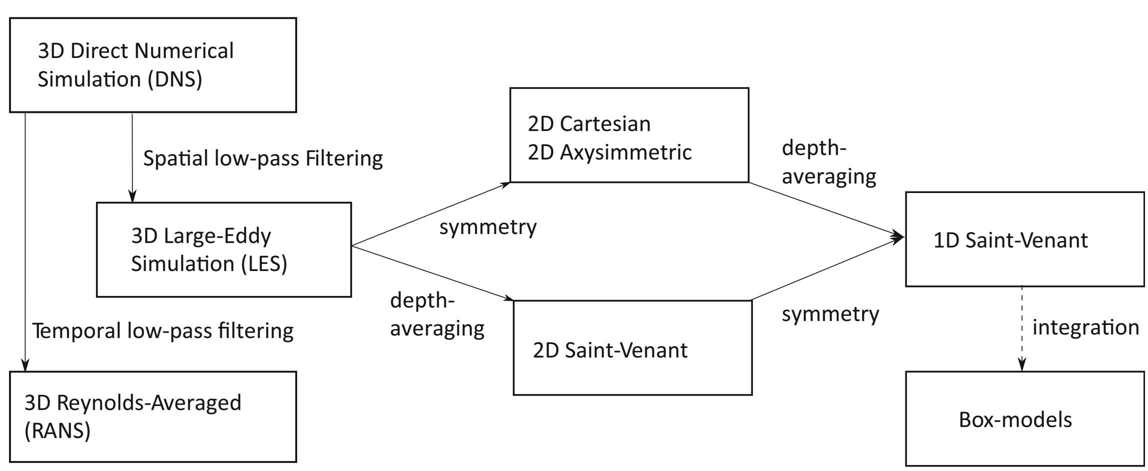

Fig. 2 Schematic representation of the different pyroclastic current modeling approaches, with the mathematical operations leading to simplification of the governing equations or reduction of model dimensionality. Benchmarking of different models should be done by applying the same operations to inter-compare model results. Notice that low-pass spatial or temporal filtering, leading to LES or RANS models, introduces SGS models, requiring validation (see "Constitutive models" section)

one or more orders of magnitude greater than its depth and that heterogeneities along the vertical direction are much smaller than those along the horizontal one. For this reason, this approach is widely used to simulate pyroclastic currents.

The depth-averaging procedure also often assumes an incompressible fluid, uniform horizontal and negligible vertical velocities, and a hydrostatic pressure distribution (Saint-Venant or shallow-water model: Benqué et al. 1982; Peakall et al. 2001). Bursik and Woods (1996) have posed the basis for the depth-averaged modeling of pyroclastic currents with an accurate description of the mixture thermodynamics, in steady-state conditions. Models used for the simulation of unsteady pyroclastic currents in concentrated regime include Titan2D (e.g., Patra et al. 2005), VolcFlow (e.g., Kelfoun and Druitt 2005), Shimizu et al. (2017) model, and IMEX_Sflow2D (de' Michieli Vitturi et al. 2019).

Inter-comparison between 3D and depth-averaged fields can be done by defining the flow thickness h by some appropriate criterion (defining the free, upper interface between the pyroclastic current and the atmosphere), and using the following relationships:

$$P(x,y,z) = \rho_m g\,(h(x,y) - z) + P_{atm}$$

$$\langle\psi(x,y)\rangle = \frac{1}{h}\int_0^{h(x,y)}\psi(x,y,z)dz$$

where (x,y,z) are the Cartesian coordinates, P is the flow pressure, g the gravity acceleration, P_{atm} is the atmospheric pressure, h is the flow thickness, and ψ can represent any flow field. However, because depth-averaging is not commutative with product, i.e., $\langle\psi\varsigma\rangle \neq \langle\psi\rangle\langle\varsigma\rangle$, it is recommended that when comparing 3D and depth-averaged models, integrals of conserved quantities (density, momentum, energy) are calculated instead of individual flow field (density, velocity, temperature). For instance, adopting a mixture formulation where ρ_{m}, U_{m}, e_{m} are the mixture density velocity and internal energy density:

$$\langle\rho_m(x,y)\rangle = \frac{1}{h}\int_0^{h(x,y)}\rho_m(x,y,z)dz$$

$$\langle U_m(x,y)\rangle = \frac{1}{h\langle\rho_m\rangle}\int_0^{h(x,y)}\rho_m U_m(x,y,z)dz$$

$$\langle e_m(x,y)\rangle = \frac{1}{h\langle\rho_m\rangle}\int_0^{h(x,y)}\rho_m e_m(x,y,z)dz$$

A key issue for depth-averaged models is the formulation of the stress tensor. Rather than applying a formal mathematical integration of the granular stress tensor expressed in tensorial form, the abovementioned depth-averaged models for pyroclastic currents adopt empirical rheological laws to express it. For concentrated pyroclastic currents (e.g., Iverson and Denlinger 2001; Patra et al. 2005; Kelfoun et al. 2009), the retarding stress is usually either based on frictional (Mohr-Coulomb) behavior or other rheological laws including some plastic, viscous, and velocity-dependent terms (Kelfoun 2011). For dilute currents (with solid concentration $\epsilon_s <$ 0.001), internal friction is generally neglected (e.g., Sparks et al. 1993; Bursik and Woods 1996; Engwell et al. 2016). In any case, it is becoming apparent that finding the "right" rheological model for depth-averaged simulation in all pyroclastic current regimes is a challenging aim, not only because of the complex behavior of dense granular flows (Kelfoun 2011) but also because of the stratified nature of pyroclastic currents.

To partially overcome this problem, two-layer, depth-averaged models have more recently allowed to describe the two-way interaction between a lower, concentrated basal layer and the upper, dilute turbulent ash cloud (Doyle et al. 2010; Kelfoun 2017), finally including the complex thermodynamics and thermal expansion of the dilute ash cloud and its mixing with the atmosphere (Shimizu et al. 2019). Such two-layer models appear to be an optimal compromise to represent stratified pyroclastic currents, but involve an increasing number of empirical relationships to describe the current dynamics. These include, in addition to the rheological laws, the mass/momentum exchange rates between the upper and the lower layer, the air entrainment coefficient, and the deposition/erosion rates, that often need specific calibration studies.

Box models

As the lowest dimensional approach, we recall here the formulation of integral (box) models (Table 6), since their use is relevant in volcanology especially in the context of probabilistic studies (Neri et al. 2015). They basically reduce to a mass conservation equation (volume conservation for an incompressible flow) and a kinematic condition for the front advancement, the so-called Von Karman's law:

$$U_f = \mathrm{Fr}\sqrt{g'h}$$

where the non-dimensional constant Fr is the Froude number, g' is the reduced gravity (as a function of the particle concentration), and h is the current thickness. A box model can be formally obtained by horizontal integration of the depth-averaged equations by imposing appropriate boundary conditions at the flow front (Benjamin 1968; Hallworth et al. 1998; Hogg et al. 2000). They are extremely sensitive to a few empirical free parameters (in particular to the Froude number), that need to be calibrated by means of appropriate benchmarks and calibration studies (Dade and Huppert 1996; Dade 2003; Neri et al. 2015; Esposti Ongaro et al. 2016; Fauria et al. 2016).

Multiphase VS mixture approaches

When adopting Eulerian models, regardless of dimensionality of the equations, there are several ways to describe gas-particle flows. The most common approach is the discretization of the grain size distribution into a finite number of *bins*, representing particle classes defined by the particle sizes and densities. In volcanology, it is a common practice to adopt a uniform discretization in the ϕ scale, where $\phi = -\log_2\left(\frac{d}{d_0}\right)$, where d is the particle diameter in millimeters, and $d_0 = 1$ mm. The Eulerian fluid transport equations for mass, momentum, and energy can be written for the interstitial gas and for every particle classes, treated as interpenetrating continua (Harlow and Amsden 1975; Valentine and Wohletz 1989; Dobran et al. 1993 and following works), interacting with each other by means of interphase momentum (drag) exchange and heat transfer. An alternative to discretization of particle sizes into bins can be based on the formulation of the transport equations for the moments of the particle distribution (method of moments; Fox 2008), but only early applications exist so far in volcanology (de' Michieli Vitturi et al. 2015).

The Eulerian multiphase flow approach can be extremely computationally expensive when the number of particle bins increases (as for the broad grain size distribution of pyroclastic currents). More efficient multiphase flow approaches can therefore be adopted in case of equilibrium or quasi-equilibrium regimes where particles are very well coupled in terms velocity and temperature with the carrier gas phase (implying very small particles). These approaches assume, based on the expected flow regime, some kind of approximation of the velocity and temperature difference between the phases. In particular, for particles characterized by low Stokes number (i.e., the ratio between the characteristic equilibrium time and the typical flow time; Burgisser and Bergantz 2002; Balachandar 2009; Cerminara et al. 2016a), the equilibrium (dusty-gas; Marble 1970) or quasi-equilibrium (equilibrium-Eulerian; Maxey 1987; Balachandar 2009; Cerminara et al. 2016b) assumptions can provide satisfactory and efficient approximations of the multiphase flow system (for a discussion, see e.g., Burgisser and Bergantz 2002; Ishimine 2005; Dufek and Bergantz 2007a, b; Carcano et al. 2014; Cerminara et al. 2016a). For some applications, a hybrid approach can be useful. For example, by adopting a dusty-gas or equilibrium-Eulerian approach for the continuous gas phase and the finest (low Stokes number) particles, while more poorly coupled particle size classes are modeled with the full Eulerian conservation equations (Carcano et al. 2014), or by a Lagrangian approach (Dufek and Bergantz 2007b; Doronzo et al. 2010).

Benchmarking of different multiphase flow models (dusty-gas, equilibrium-Eulerian, Eulerian-Eulerian) in the framework of validation studies is always feasible by comparing results for the average properties of the mixture (Marble 1970; Cerminara et al. 2016a).

$$\rho_m = \epsilon_g \rho_g + \sum_{k=1}^{M} \epsilon_{sk} \rho_{sk}$$

$$\boldsymbol{U_m} = \frac{1}{\rho_m}\left(\epsilon_g \rho_g \boldsymbol{U}_g + \sum_{k=1}^{M} \epsilon_{sk} \rho_{sk} \boldsymbol{U}_{sk}\right)$$

$$e_m = \frac{1}{\rho_m}\left(\epsilon_g \rho_g e_g + \sum_{k=1}^{M} \epsilon_{sk} \rho_{sk} e_{sk}\right)$$

In these equations, ϵ is the volume fraction, ρ is the density, $\boldsymbol{U}$ is the velocity, and e is the energy density. The subscripts g and s indicate the gas and solid phases, the subscript m indicates the gas-solid mixture, and M is the number of bins into which the grain size distribution has been discretized.

Constitutive models

Differently from classical fluid mechanics, there is not an established general consensus on constitutive equations in multiphase gas-particle flows. Particularly critical are the constitutive models of the stress tensor of the granular phase and of the interphase mass (including chemical reactions and phase transitions), momentum (including drag), and heat coupling (see e.g., Neri et al. 2003; Sweeney and Valentine 2017; and Dufek 2016 for a review). In general, constitutive models pertain to the microphysics of the gas-particle mixture and their accuracy can be constrained by ad-hoc numerical experiments at the lower levels of the validation hierarchy (e.g., unit problems, see above Table 3 and Breard et al. 2019a, b for examples), generally aimed at the calibration of free parameters.

Among constitutive models, turbulence models are needed to describe the nonlinear effects of the so-called sub-grid scales (SGS) of fluctuations on the resolved fluid motion. The need of SGS models derives from the application of spatial (large eddy simulation—LES models) or temporal (Reynold's averaged Navier-Stokes—RANS models) low-pass filters and from the non-linearity of Eulerian transport equations (Mason 1994). For pyroclastic currents, two aspects of turbulence modeling are important: (1) the turbulent mixing and entrainment of atmospheric air (Bursik and Woods 1996) and (2) the turbulent regime in the basal layer, including effects on friction (Valentine 1987), deposition, and erosion (Bernard et al. 2014). Turbulence SGS models differ from constitutive models because their formulation is not independent from the large-scale flow features, and it is strictly linked to the numerical discretization scheme (e.g., Özgökmen et al., 2007). For these reasons, SGS models are subject to the same verification, validation, and benchmarking procedure as the governing equations of mass, momentum, and energy transport, from unit problems up to the full system scale (Tao 2015).

A general validation hierarchy

To define a general validation framework for pyroclastic current models, we propose here to follow the same methodology that was put forward by Oberkampf and Trucano (2002) for the validation of CFD codes designed to simulate complex industrial and technological systems. The approach is based on a hierarchical process of comparing numerical models with experiments and observations (Fig. 3). However, there are differences between the use of CFD models in volcanology and in industrial processes, especially in the way of dealing with large epistemic uncertainty. Thus, we additionally emphasize the need to compare models with each other (benchmarking) in order to provide guidance on the applicability of a given model for a specific intended use and situation.

The process of validating models involves, in general, simulation and comparison at the four tiers. Confirmation of numerical results on the natural cases (at the system and subsystem level) is fundamental for assessing the quality of the hypotheses, physical models, and numerical implementation, but this requires a rigorous and quantitative confirmation of the models at the lower tiers (unit problems and benchmark cases). Benchmark cases, in particular, should be specifically conceived to systematically challenge different models at various levels of complexity, rigorously defining initial and boundary conditions and providing a common theoretical framework for comparing their outputs.

Tier 0. Complete system

The complete system is the full representation of the problem under investigation. It is characterized by the coexistence, possibly at different temporal and spatial scales, of different interacting subsystems, possibly related to different spatial domains. Some of the subsystems might be unknown or not

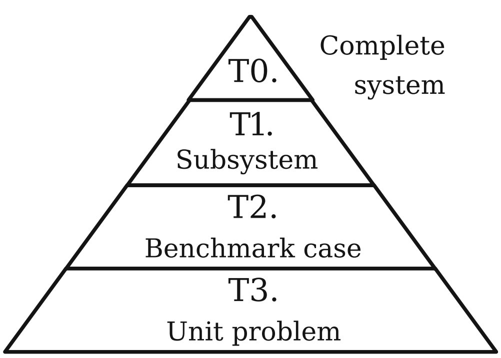

Fig. 3 Pyroclastic model validation hierarchy (adapted from Oberkampf and Trucano 2002)

directly observable. The combination of such processes makes the phenomenon extremely complex and requires validation steps at a highest level.

For engineering applications, the complete system can be, for example, a hypersonic missile (Oberkampf and Trucano 2002), with its propulsion system, airframe, and control elements. Because this is a built system, its geometry, and initial and boundary conditions are very well constrained compared to volcanic problems. For pyroclastic currents, the complete system is represented by the whole explosive eruption scenario (Fig. 4A). There is no doubt indeed that pyroclastic current dynamics are in general coupled to atmospheric dynamics, depend on eruption column (e.g., for Plinian eruptions) or on dome geometry and volume (for dome-collapsing eruptions), and are ultimately related to magma fragmentation and volcanic conduit, down to the magma chamber. An example of numerical modeling of the complete system is given by Clarke et al.'s (2002) simulation of one of the August 1997 Vulcanian episodes at Soufrière Hills volcano (Montserrat, West Indies). In that case, conduit, volcanic plume, and pyroclastic current dynamics are so tightly linked that they cannot be modeled independently.

Tier 1. Subsystem

Subsystems can be defined as parts of the system that, under certain conditions and hypotheses, and in rare cases of exceptional documentation, can be analyzed individually. Subsystems exhibit complex physics and multiscale (up to the full system scale) properties. Their dynamics are usually coupled to other subsystems, but the degree of coupling is limited so that it can be described as a boundary condition.

Oberkampf and Trucano (2002) exemplify it for the hypersonic missile as the aero/thermal protection subsystem (requiring modeling of laminar/turbulent/boundary layer airflow) or the structural subsystem (requiring to model, e.g., the heat transfer to the metal structure). For subsystems in nature, there are usually limited but some observational datasets. Indirect measurements include geophysical signals, imaging, and the sedimentological record. The definition of validation metrics and quantification/representation of uncertainty are usually problematic at this Tier. For pyroclastic currents, a subsystem (Fig. 4B) can be represented by individual stratified pyroclastic current units in a composite sequence (e.g., at Merapi volcano, Indonesia, in 2006 and 2010; Charbonnier and Gertisser 2012; Kelfoun et al. 2017), or by episodes of flow transformation in response to the interaction with the topography (e.g., at Unzen volcano, Japan, in 1991; Yamamoto et al. 1993; Fujii and Nakada 1999), where the interaction with the dynamics in the other subsystems (e.g., the magma ascent in the conduit) can be neglected or described in a simplified way through an appropriate boundary condition (e.g., a constant mass flow rate or initial collapse). In their numerical

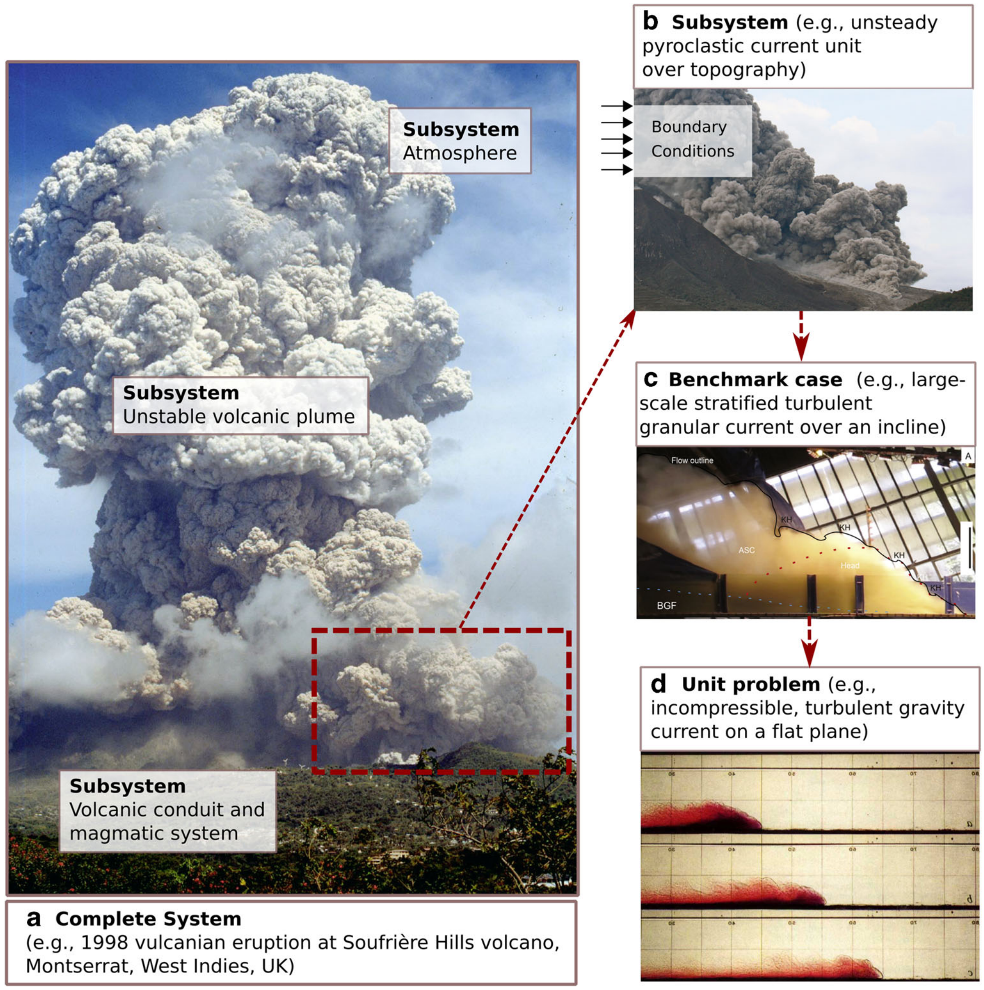

Fig. 4 Example of a hierarchy of validation tiers for pyroclastic currents. (A) Complete system (public domain photo courtesy of B. Voight, Penn State University). (B) Subsystem (public domain photo courtesy of Jonathan Stone). (C) Benchmark case (photo courtesy of G. Lube, Massey University, NZ). (D) Unit problem (picture modified after Hallworth et al. 1993)

model of the May 18 blast phase of the Mount St. Helens 1980 eruption, Esposti Ongaro et al. (2012) did not model the landslide preceding the pyroclastic current, but just considered its effect as a modified topographic boundary condition. Some further examples are reported in Table 2.

Tier 2. Benchmark cases

In Oberkampf and Trucano (2002), a benchmark case is the further level of decomposition of a subsystem. It is a somehow standard problem having some degree of complexity, mainly concerning geometrical and scaling complications. In general, validation at this level should be based upon comparison to appropriate, standardized laboratory experiments. In benchmark cases, a measure of accuracy, or error, is expected to be available and should be explicitly reported, both for the dataset and for the model outputs.

In the case of the hypersonic missile CFD problem (Oberkampf and Trucano 2002), benchmark cases can be represented by laminar, hypersonic flows with ablation, or heat transfer to metal substructure. For pyroclastic currents, because of the extreme conditions and wide range of physical scales involved, benchmark experiments might require special hardware and sensors, and large-scale experimental setups (Fig. 4C) that incorporate as many of the scales as possible are especially important (Dellino et al. 2007; Lube et al. 2015). In cases where experimental data are not available, synthetic benchmarks (they have also been called *inter-comparison* studies, for example Costa et al. 2016) can be conceived to define the differences/similarities of the numerical models, possibly providing the metrics for a quantitative comparison. Table 5 reports some recent experimental investigations that can be seen as benchmark case for pyroclastic current models. They are potentially suited for inter-comparison of different modeling approaches. While most of them focus on either dilute (Breard et al. 2016; Breard and Lube 2017; Andrews and Manga 2011) or concentrated (e.g., Lube et al. 2011, Chédeville and Roche 2015) end-member regimes, their simulation is still a challenge for numerical models. One key issue for benchmark studies concerns the standardization of data formats and the availability of datasets and metadata, either from laboratory experiments or numerical simulations.

Tier 3. Unit problems

Unit problems are well-understood processes, well-constrained by accurate experimental data and supported by a theoretical framework. Unit problems may be in some cases difficult to solve numerically, but the quality of the results can always be rigorously assessed. These problems should be a first tier in the overall validation procedure because they can pose some unexpected difficulties to the modeler, such as those related to the accuracy and stability of the solutions (for instance, in the description of discontinuous solutions and nonlinear instabilities), the dimensionality (the assumed invariances under symmetry or the steady-state regime), and sub-grid scale (SGS) models (e.g., for the microphysics, constitutive equations, and turbulence). Calibration of some semi-empirical parameters (e.g., coefficients of turbulence SGS models) could be needed at this Tier, and should always be explicitly specified.

For the hypersonic missile, unit problems can be constituted by laminar hypersonic flow over a simple body, boundary layer interaction, or heat conduction (Oberkampf and Trucano 2002). For pyroclastic currents, unit problems of interest include the settling of a polydisperse particulate mixture (Jacobs et al. 2012), a gravity current inertial flow over a flat surface (Fig. 4D; Dufek and Bergantz 2007a, b), collapse of a granular pile (Meruane et al. 2010; Breard et al. 2019a, b), thermal convective instabilities (Cerminara et al. 2016a, b), and supersonic phenomena in multiphase mixtures (Dartevelle 2007; Carcano et al. 2014; Valentine and Sweeney 2018). Other examples from the recent volcanological literature are reported in Table 3.

Conclusions and future directions

We have proposed a terminology for verification, confirmation, and benchmarking, and a general framework suited for validation of pyroclastic current models. We have also described the main types and the different levels of approximations of pyroclastic current models. From the analysis of the existing literature and the variety of the existing models, it is apparent that there is a need for systematic model benchmarking initiatives able to elucidate the potential and weaknesses of different approaches, especially in the context of hazard studies. Most pyroclastic currents propagate as strongly stratified currents, simultaneously displaying the features of dilute and concentrated granular flows, and potentially undergoing (rapid) transitions from one prevailing regime to the other. Nonetheless, we suggest that a pyroclastic current benchmarking initiative should initially focus on experimental datasets that relate specifically to the two end-members (dilute turbulent and concentrated frictional regimes) separately, in simplified but challenging conditions. They should provide initial and boundary conditions for the different models and the recipe for a coherent inter-comparison of numerical model results. It is also important for the volcanological community to develop some well-documented natural events to be taken as subsystem cases. Or, ideally, to start designing *in-natura* experiments at some active volcano to provide, in the near future, well constrained initial and boundary conditions to challenge numerical models at the full, natural scale.

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