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Large Eddy Simulation of gas–particle kinematic decoupling and turbulent entrainment in volcanic plumes

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ABSTRACT

In the framework of the IAVCEI (International Association of Volcanology and Chemistry of the Earth Interior) intercomparison study on volcanic plume models, we present three-dimensional (3D) numerical simulations carried out with the ASHEE (ASH Equilibrium Eulerian) model. The ASHEE model solves the compressible balance equations of mass, momentum, and enthalpy of a gas-particle mixture and is able to describe the kinematic decoupling for particles characterized by Stokes number (i.e., the ratio between the particle equilibrium time and the flow characteristic time) lower than 0.2 (or particles smaller than about 1 mm). The computational fluid dynamic model is designed to accurately simulate a turbulent flow field using a Large Eddy Simulation approach, and is thus suited to analyze the role of particle non-equilibrium in the dynamics of turbulent volcanic plumes. The two reference scenarios analyzed correspond to a weak (mass eruption rate $= 1.5 * 10^6$ kg/s) and a strong volcanic plume (mass eruption rate $= 1.5 * 10^9$ kg/s) in absence of wind. For each scenario, we compare the 3D results, averaged in space and time, with theoretical results obtained from integral plume models. Such an approach enables quantitative evaluation of the effects of grid resolution and the subgrid-scale turbulence model, and the influence of gas-particle non-equilibrium processes on the large-scale plume dynamics. We thus demonstrate that the uncertainty on the numerical solution associated with such effects can be significant (of the order of 20%), but still lower than that typically associated with input data and integral model approximations. In the Weak Plume case, 3D results are consistent with the predictions of integral models in the jet and plume regions, with an entrainment coefficient around 0.10 in the plume region. In the Strong Plume case, the self-similarity assumption is less appropriate and the entrainment coefficient in the plume region is more unstable, with an average value of 0.24. For both cases, integral model predictions diverge from the 3D plume behavior in the umbrella region. The presented analysis of 3D numerical simulations thus enables identification of the critical hypotheses that underlie integral models used in operational studies. In addition, high-resolution 3D runs allow reproduction of observable quantities (such as infrasound signals) which can be useful for constraining eruption dynamics during real events.

1. Introduction

Volcanic plumes are characterized by the injection of a high-velocity, high-temperature mixture of gases and pyroclasts of different densities and sizes, mostly in the range from a few tens of microns to several millimeters, into the atmosphere. The dynamics of volcanic columns are largely governed by turbulence, which controls air entrainment, heating and expansion, and the consequent transition from a momentum-driven jet to a positively buoyant plume or collapsing fountain (Sparks et al., 1997). Despite the advances in computational capability and the improvement of the measurement techniques in the laboratory, turbulence is still one of the least understood scientific problems. One major difficulty is that the governing equations of fluid dynamics are nonlinear and little is known about their solutions at high Reynolds number, even in simple geometries and for an ideal fluid. This picture is even more complicated when a dispersed solid phase is added to the turbulent flows, as occurring in volcanic plumes.

Nonetheless, the need for models to interpret volcanic observations and inform hazard forecast tools makes it urgent to develop and assess the quality and reliability of volcanic plume models. To this end, IAVCEI (the International Association of Volcanology and Chemistry of the Earth Interior) has promoted the volcanic plume model inter-

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comparison study, a systematic effort to compare different models performing a set of simulations using the same input parameters (Costa et al., 2016; Suzuki et al., 2016). These represent a weak (mass eruption rate $= 1.5 * 10^6$ kg/s) and strong (m.e.r. $= 1.5 * 10^9$ kg/s) volcanic plume in a stratified atmosphere. Input data were set assuming source conditions and representative atmospheric profiles, respectively, of the 26 January 2011 Shinmoe-dake eruption (Suzuki and Koyaguchi, 2013) and the 15 June 1991 Pinatubo eruption (see, e.g. Holasek et al., 1996). In this framework we have developed the present study, by considering plume development in windless conditions.

One-dimensional (1D) models based on various developments of the Morton et al. (1956) buoyant plume theory (we refer to them as *integral* or *1D* models) have been extremely useful in volcanology mainly because they have allowed the correlation of observed (or reconstructed) column height with the mass eruption rate, which is usually extremely difficult to measure directly (Wilson et al., 1980; Sparks, 1986). Integral models are also routinely used in hazard assessment studies, specifically when there is the need for computationally efficient tools to forecast volcanic plume heights, e.g. for atmospheric ash dispersal models (most of such 1D tools are reviewed by Costa et al., 2016). Unfortunately, such models are extremely sensitive to the choice of their main empirical parameter, the entrainment coefficient. The entrainment coefficient expresses empirically a proportionality between the rate of air entrainment at a given height and the average plume vertical velocity. It is usually calibrated from controlled experiments at the laboratory scale. The dominant control of the entrainment coefficient on integral model results is demonstrated, inter alia, by the analysis presented by de' Michieli Vitturi et al. (2015) in the framework of the same intercomparison study. A significant portion of the early and even more recent literature on volcanic plume models has thus been devoted to identifying, by means of experimental or theoretical studies, more accurate values of the entrainment coefficient, sometimes expressed as a function of height, density contrast or Richardson number (Kaminski et al., 2005; Carazzo et al., 2008; Woods, 2010).

To overcome this difficulty, computational fluid dynamics bypasses the shortcomings of analytical methods and integral numerical models by offering Direct Numerical Simulations (DNS), i.e., the simulation of the whole range of spatial and temporal scales in the turbulent flow. With respect to other investigation methods, DNS is more akin to an experiment, and no less valuable due to the immense quantity of data produced. Unfortunately, as demonstrated in Section 2, the DNS of volcanic plumes is presently computationally unaffordable, because it would require an extremely fine numerical grid. The main idea behind the Large Eddy Simulation (LES) approach adopted in this work is to reduce this computational cost by reducing the range of time- and length-scales that are being solved, using a low-pass filtering of the equations. Such a low-pass filtering effectively removes small-scale information from the numerical solution. However, nonlinearity causes the coupling between large and small scale processes, introducing subgrid-scale (SGS) terms that cannot in general be disregarded (Vreman et al., 1995). To mimic the SGS effect on the large scale, reproducing correctly the resolved turbulent spectrum, SGS models take advantage of the universal character of turbulence at the smallest scales.

In turbulent plumes, experimental and numerical studies (see e.g., da Silva et al., 2014, for a review) support the idea that the *rate* of air entrainment is controlled by the dynamics of the large eddies, at the so-called Taylor microscale (see Section 2). It is therefore necessary to understand the extent to which LES is suited to describe turbulent plumes and how the unresolved SGS part of the turbulent spectrum (which must be modeled) can be of practical volcanological interest. The first objective of this work is therefore to quantify the sensitivity of the three-dimensional (3D) LES of a volcanic plume to grid resolution and to provide an empirical quantitative estimate of the minimum grid size required to minimize the effect of the modeled subgrid turbulence.

In the past ten years, only a limited number of studies (Suzuki et al., 2005; Esposti Ongaro et al., 2008; Herzog and Graf, 2010; Cerminara et al., 2016; Suzuki et al., 2016), have utilized 3D LES for modeling volcanic columns. These studies have allowed exploration of the influence of realistic vent conditions on eruption dynamics and to put further constraints on semi-empirical parameters needed by integral models, in particular, the entrainment coefficient (Suzuki and Koyaguchi, 2010), accounting for wind and in some cases water microphysics (Suzuki and Koyaguchi, 2015; Van Eaton et al., 2015). The ASHEE (Ash Equilibrium Eulerian) model adopted in this work and described in Section 3 has been recently developed (Cerminara et al., 2016) to accurately simulate the spectral properties of dispersed multiphase turbulence for particles smaller than about 1 mm.

ASHEE is implemented to describe mean (e.g. plume shape and height) and fluctuation (e.g. turbulent infrasound) properties of volcanic plumes, and the effects of kinematic decoupling on the dynamics of turbulent gas–particle mixtures. It is indeed widely accepted that the structure of turbulent flows can be largely affected by the presence of solid particles (e.g., Elghobashi, 1991, 1994; Toschi and Bodenschatz, 2009). Because of their inertia, particles tend to preferentially concentrate in the regions of low shear (Balachandar and Eaton, 2010), thus creating large clusters which can eventually modify the eddy structure. How this phenomenon affects the turbulent mixing at the interface with the ambient fluid is still an open question. In this work, we address the problem by comparing LES of turbulent volcanic plumes carried out with and without including the effects of particle decoupling.

The buoyant plume theory provides a valuable tool to give insight into 3D simulation results, and it is therefore complementary to LES. In Appendix C, we introduce two integral models: a new formulation (ASH1D) of the 1D plume model proposed by Woods (1988), and its zero-dimensional asymptotic approximation for dilute regimes (ASH0D). A methodology to coherently compare time- and space-averaged 3D simulations and integral model outcomes is introduced in Section 3.4. Comparison between ASHEE, ASH1D and ASH0D results in Sections 4 and 5 enables the hypotheses underlying 1D models to be critically revised and, in particular, to discuss the entrainment hypothesis and the value of the entrainment coefficient which can be derived from 3D numerical models.

2. Time and length scales of volcanic plumes

Turbulence is a multiscale physical phenomenon involving many different scales, from the integral scale of the flow to the scale of the smallest eddy of the turbulent field. The turbulent entrainment process at the interface between two regions of different turbulent intensity (such as the boundary between the plume and the atmosphere) is carried out through two different mechanisms: large-scale eddies are responsible for the engulfment of parcels of air (Townsend, 1966), whereas small-scale turbulence controls the so-called nibbling process (Mathew and Basu, 2002; Bisset et al., 2002). Although experimental studies (Westerweel et al., 2005) suggest that the nibbling process controls the development of the turbulent/non-turbulent interface, it is still believed that the global rate of entrainment is imposed by the large-scale engulfment (e.g., Taveira et al., 2011; da Silva et al., 2014).

The smallest scale in a volcanic plume is given by the Kolmogorov scale (Pope, 2000)

$$\eta = A_\eta D \mathrm{Re}^{-\frac{3}{4}}. \tag{1}$$

Here, D is the vent diameter, A_η is a constant depending on the geometry of the problem and $\mathrm{Re} = DU/\nu$ is the Reynolds number based on the flow properties at the vent (U is the vent velocity and ν is the kinematic viscosity). Plourde et al. (2008) estimated $A_\eta \simeq 5.6$ for a pure plume. The Kolmogorov characteristic time scale of the smallest eddies is $\tau_\eta = \eta^2/\nu$. In volcanic eruptions, the order of magnitude of the Kolmogorov microscales typically is $\eta \approx 10$ μm and $\tau_\eta \approx 10$ μs.