The VOL-CALPUFF Model for Atmospheric Ash Dispersal: I. Approach and Physical Formulation

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Abstract. We present a new modeling tool, named VOL-CALPUFF able to simulate the transient and three-dimensional transport and deposition of volcanic ash under the action of realistic meteorological and volcanological conditions throughout eruption duration. The new model derives from the CALPUFF System, a software program widely-used in environmental applications of pollutant dispersion, that describes the dispersal process both in the proximal and distal regions and also in presence of complex orography. The main novel feature of the model is its capability of coupling a Eulerian description of plume rise with a Lagrangian representation of ash dispersal described as a series of diffusing packets of particles or puffs. The model is also able to describe the multiparticle nature of the mixture as well as the tilting effects of the plume due to wind action. The dispersal dynamics and ash deposition are described by using refined orography-corrected meteorological data with a spatial resolution up to 1 km or less and a temporal step of 1 hour. The modeling approach also keeps the execution time to a few minutes on common PCs, thus making VOL-CALPUFF a possible tool for the production of ash dispersal forecasts for hazard assessment. Besides the model formulation, the paper presents the type of outcomes produced by VOL-CALPUFF, shows the effect of main model parameters on results, and also anticipates the fundamental control of atmospheric conditions on the ash dispersal processes. In the companion paper (*Barsotti and Neri* [2007], this issue) a first thorough application of VOL-CALPUFF to the simulation of a weak plume at

Mount Etna (Italy) is presented with the specific aim of comparing model predictions with independent observations.

1. Introduction and Background

Amongst the processes associated with an explosive eruption, ash dispersal is probably the phenomenon occurring on the widest range of spatial and temporal scales. Ash particles can have mostly local and regional effects lasting for a few days, if the volcanic column is contained within the troposphere. On the other hand, larger plumes reaching the stratosphere can have a global impact and drive climatic changes for several years. Ash dispersal and fallout can also represent a major hazard for populations near volcanic centers, producing a serious risk for human and animal health and causing damage to crops, ground infrastructures, and aviation traffic (*Sparks et al.* [1997]; *Sigurdsson et al.* [2000]; *Martì and Ernst* [2005]). Due to such a frequent and wide impact of ash fallout the scientific community has produced, for many years, numerical models aimed at describing the rising phase and movements of volcanic particles in the atmosphere. Modeling volcanic ash dispersal is indeed a complex task. It needs detailed information on the system initial and boundary conditions as the volcanic source and temporal and spatial meteorological variations, as well as on the physics that govern the entire phenomenon. Historically, physical models can be roughly divided into two categories: 1) those aimed at describing the dynamics of the volcanic column, and 2) those focused on the description of pyroclast dispersal in the atmosphere and at the ground. In the following paragraphs the main physical models, developed to date, will be briefly recalled together with their main features.

Volcanic column Regarding this first category, early models adopted a pseudofluid approach in which solid particles and gases are assumed to be in thermal and mechanical equilibrium thus forming a mixture characterized by a bulk density (*Wilson* [1976]; *Wilson and Walker* [1987]; *Sparks et al.* [1997]). The main features of the rising plume phase were described by solving the conservation equations of mass and momentum for the homogeneous mixture and assuming a steady time-averaged 1-D axisymmetric column. Later on, the equation sets of these so-called "plume-theory" models were integrated by adding the energy conservation equation in different forms (*Woods* [1988]; *Glaze and Baloga* [1996]). Further developments concerned the modeling of thermal disequilibrium (*Woods and Bursik* [1991]), particle fallout from the column (*Woods and Bursik* [1991]; *Ernst et al.* [1996]), and umbrella cloud (*Bursik et al.* [1992b]; *Bonadonna et al.* [1998]) and particle recycling into the eruption column (*Ernst et al.* [1996]; *Veitch and Woods* [2002]; *Veitch and Woods* [2004]; *Textor et al.* [2004]). Crosswind influence on plume tilting has also been addressed based on experimental and theoretical work on turbulent buoyant plumes in cross flow (*Hoult and Weil* [1972]; *Wright* [1984]; *Ernst et al.* [1994]; *Bursik* [2001]). These types of models were also used to obtain simple correlations to estimate column height (*Carey and Sparks* [1986]; *Bursik et al.* [1992a]; *Bonadonna et al.* [1998]). The evaluation of column height is indeed crucial for quantifying the area affected by ash fallout. These correlations link column height with the excess thermal energy associated with the column (*Morton et al.* [1956]; *Morton* [1959]) or directly with the mass flow rate (*Sparks* [1986]; *Sparks et al.* [1997]). Similar dimensional arguments are used to estimate column height in a windy environment (*Wright* [1984]). The dynamics of buoyant volcanic columns have also been recently investigated by adopting transient, multidimensional, and multiphase flow models able to describe new features of the phenomenon. For instance, the ATHAM code (*Oberhuber et al.* [1998]; *Herzog et al.* [1998]; *Graf et al.* [1999]; *Textor et al.* [2004];

Textor et al. [2006a]; *Textor et al.* [2006b]) is a fully 3D non-hydrostatic limited area circulation model able to describe the eruption column behavior, including accurate cloud physics and microphysical processes, on spatial scales of a few hundred kilometers and up to few hours of eruption time. Similarly, *Dartevelle et al.* [2004] recently analyzed the 2D transient behavior of buoyant volcanic clouds of different scales by using a two-phase mixture description. The influence of the third dimension and turbulence closure has been discussed by *Suzuki et al.* [2005] by using a pseudogas approximation of the multiphase mixture.

Pyroclastic dispersal and deposition With respect to this second category of models, first attempts were by *Suzuki* [1983], *Armienti et al.* [1988], *Macedonio et al.* [1988], *Macedonio et al.* [1990] and, more recently, by *Macedonio et al.* [2005] and *Costa et al.* [2006], who adopted advection-diffusion equations and solved them in 2D and 3D domains. Other studies based on this approach discuss the effect of various parameterizations of the source and the production of probabilistic hazard maps (*Bonadonna et al.* [2002]; *Bonadonna et al.* [2005]; *Pfeiffer et al.* [2005]). In these models the volcanic column is parameterized by an empirical source function and particles diffuse under the action of constant winds. An alternative approach, mostly used to reproduce the deposit features, assumes the wind-advected volcanic material to be spreading radially as an intrusive gravity current above the level of neutral buoyancy (*Sparks et al.* [1991]; *Bursik et al.* [1992b]; *Bonadonna et al.* [1998]). Models based on alternative approaches have also been developed by different groups. The PUFF model (*Searcy et al.* [1998]) describes the movements of a collection of discrete ash particles representing a sample of the eruption cloud by using a Lagrangian scheme and treating the source as a virtual pre-assigned vertical distribution of mass.

Similarly, the HYSPLIT code (*Draxler and Taylor* [1982]; *Draxler and Hess* [1998]) describes, by means of a Lagrangian approach, the evolution of puffs (containing material particles with diameters up to 30 μm) without taking account of buoyancy effects. Other codes are in use at the Volcanic Ash Advisory Centers (VAACs). CANERM (*Simpson et al.* [2002]) (operative at the Canadian Meteorological Center), is a 3D Eulerian model used for medium- and long-range transport which assumes a virtual source described by a vertical mass distribution. Similarly, MEDIA (*Piedelievre et al.* [1990]) (operative at Toulouse Meteo France), is a Eulerian atmospheric transport/diffusion model focused on long-range dispersal of particles ejected from a source at a given altitude. NAME (*Watkin et al.* [2004]) (operative at the UK Met Office), is a Lagrangian particle model that can be applied on either regional or global scales and is able to consider areal as well as point-like sources. Finally, VAFTAD (*Heffter and Stunder* [1993]) (developed by NOAA ARL and in use at the Washington and Anchorage VAACs), is a 3D time-dependent Eulerian model which needs the maximum height reached by the volcanic column to model the input source. Currently all the above models are of limited value for volcanic ash dispersal forecasting, despite being used at VAACs, in that they all lack a source-term matrix derived from an understanding of basic eruption physics (GGJ. Ernst, pers. communication). This realization is one of the key motivations for developing the present work.

2. Aim of the Work

From the above summary it is clear that the dynamics of the rising volcanic plume and of the dispersal and depositional processes have been mostly treated separately despite their being part of the same phenomenon and being strictly inter-related. Moreover, volcanic plume models typically cannot be applied under realistic meteorological conditions and, similarly, dispersal models do not account for realistic source conditions as they adopt what may appear as subjective parameterization of the source. Finally, most of the dispersal models in use at research and operative centers are relevant only to medium- and long-distance areas, whereas the importance of forecasting the ash dispersal also in proximal regions is crucial for nearby inhabited areas and aviation routes. In this case a treatment of meteorological datasets able to include effects on wind fields due to the presence of complex orography is also necessary. The aim of this work is to present a new modeling system, named VOL-CALPUFF, able to simulate the transient and three-dimensional injection, transport and deposition of volcanic ash under the action of realistic and unperturbed meteorological and volcanological conditions. The main novel feature of the model is its capability of coupling a Eulerian plume rise model with a Lagrangian representation of ash dispersal described as a series of diffusing packets of particles or "puffs". Like several other codes used in volcanological applications, VOL-CALPUFF has its origin in an air quality modeling code named CALPUFF designed for the transport of pollutants at local and long-distance scales (*Nguyen et al.* [1997]; *Scire et al.* [2000]). The VOL-CALPUFF code differs from the original CALPUFF code in several aspects fully described in this paper, which makes it suitable for volcanological applications. The main differences include the implementation of a multiparticle plume model, the possibility of treating particles larger than a few microns, the consideration of puff dispersal well above the atmospheric boundary layer, and the consideration of various settling velocity laws as a function of particle size and shape. It is also worth noting that the VOL-CALPUFF code can describe the whole dispersal dynamics and deposition by using very refined orography-corrected meteorological data - with a final resolution up to 1 km or less - while keeping the execution time in the order of minutes on common PCs. All these features also make VOL-CALPUFF a promising tool for the production of ash dispersal forecasts for hazard assessment. In the following sections an overview of the CALPUFF System, the main features of the new VOL-CALPUFF code, and some sensitivity tests for weak plumes, will be presented. The companion paper (*Barsotti and Neri* [2007], this issue) will present a first complete application of the new code to a weak plume of Mt. Etna.

3. An Overview of the CALPUFF System

With the term "CALPUFF System" we mean the whole numerical procedure that from meteorological and geophysical input data computes hourly the concentration of released material, gaseous or particulate, in the atmosphere and at the ground. The CALPUFF system was developed by Earth Tech Inc. (now TRC Companies, Inc.) in the 1990s and it is freely available on line at the website http://www.src.com/calpuff/calpuff1.htm. CALPUFF is a quite complex model composed of a great number of sub-processors linked to each other by an input-output data flow. It has a modular structure, so that, depending on the available input data and type of information required, the model elaboration can follow different patterns. Fig. 1 shows a simplified basic configuration of the system such as the one we have used in our study. The procedure starts with the elaboration of the geophysical information, such as terrain elevation and land-use data, once the choice of the computational domain under investigation is made. In parallel with the elaboration of the geophysical information, processing of the meteorological data occurs to provide CALMET (see hereafter) with the necessary input data. The meteorological processor CALMET is a diagnostic code; this means that it computes the values of meteorological variables on a finer grid without solving the time-dependent equation of motion. CALMET works in two steps that refine and correct an initial guess field typically provided by a prognostic code (e.g. MM5, ETA). In the first step the initial data are interpolated on a grid usually much finer than that used in mesoscale models, and the local orography effects are accounted for (*Scire et al.* [1990]; *Scire and Robe* [1997]). In the second step, surface or upper air data, when available, are considered to correct the computed wind field through an objective analysis that assigns appropriate weight to each data. The output provided by CALMET contains the 3D fields (such as wind and temperature) and the 2D field of micro-meteorological variables (like friction velocity, Obukhov length, atmospheric boundary layer height and Pasquill-Gifford-Turner stability classes). All these variables are computed with the temporal resolution required by the dispersal model and on a grid in a terrain-following coordinate system with a vertical and horizontal user-defined resolution. This file, together with that containing the data related to the volcanic source, is fed as input to the system's core, i.e. the CALPUFF dispersal model.

The CALPUFF code describes atmospheric ascent and dispersion of a gaseous mixture under the action of advective, turbulent wind fields. The rising plume phase is computed in a Eulerian way by solving the plume theory equation, whereas dispersal is described in a Lagrangian framework. In particular, assuming a hot gaseous mixture, CALPUFF reproduces the plume up to its maximum height, corresponding to a null vertical velocity. At this altitude continuous material emission is discretized in several packets (the *puffs*), so that at each time-step a finite number of puffs are released. The mass flow rate associated with the puffs matches the mass flow rate computed at the top of the rising plume. Each puff is associated with a given particle size and release time. The number of puffs is mainly determined by the wind speed at the source and is computed to adequately represent a continuous release. The wind present at the altitude at which the puffs are injected causes the puff center to move in the horizontal direction, whereas the settling velocity, also acting on the puff center, brings the puffs towards the ground. During the displacement the material inside the puff is affected by vertical and horizontal diffusion, which causes the puff to spread. Under the assumption of Gaussian packets, their diffusion is described by lateral and vertical standard deviations. Finally, it is worth noting that the CALPUFF System has been validated through extensive comparison of model predictions with experimental data such as the Cross-Appalachian Tracer Experiment (CAPTEX). The CAPTEX experiment involved the release of a unique series of tracers for the purpose of providing data to evaluate and improve computer models of pollutant dispersion and to provide insight into the mechanisms of long-range transport and dispersion. To compare CALPUFF to other widely used codes, further studies (Kincaid and Lovett data set) were conducted; these studies suggest that the CALPUFF dispersion model allows appropriate characterization of both local-scale and long-range transport and dispersion (*EPA U.S.* [1998d]; *Earth Tech, Inc.* [2002]). Due to the model performance, the U.S. Environmental Protection Agency (*EPA U.S.* [1998a]; *EPA U.S.* [1998b]; *EPA U.S.* [1998c]; *Irwin* [1998]; *Scire et al.* [2000]) proposed CALPUFF as a guideline model for regulatory applications involving long-range transport and near-field applications where non-steady-state effects may be important.

4. The VOL-CALPUFF Code

Fig. 2 illustrates the main features of the VOL-CALPUFF code we developed in the present work. In the following sub-sections, the main equations and features of the new model will be described by highlighting the main developments carried out with respect to the original CALPUFF code.

4.1. Meteorological Pre-processors

The need to describe dispersal under the forcing of realistic meteorological conditions makes the treatment of the original weather forecasting data a crucial step. The flow-chart reported in Fig. 1 shows the presence of two different meteorological pre-processors needed to provide VOL-CALPUFF with the required meteorological information. The first, CALITA, is aimed at decoding and rewriting, in a format readable by CALMET, the data produced in grib (GRIdded Binary, see *Stackpole* [1994]) format by the mesoscale prognostic code. CALITA is optimized for working on meteorological data coming from different sources as those produced by the Italian Lokal Modell (COSMO's web-site [2004]). CALITA can also use meteorological data coming from the Reanalysis Archive of the European Center for Medium-Range Weather Forecast (ECMWF) and National Centers for Environmental Prediction (NCEP-NOAA) in such a way that they can be read by CALMET. Using CALITA it is possible to define the subdomain being investigated and the number of atmospheric levels the user is interested in. It provides CALMET with 3D fields of pressure (and related geopotential height), temperature, wind direction, wind speed, pressure vertical velocity and relative humidity, together with 2D field of pressure at sea level, total rainfall accumulation and snow cover indicator. The second pre-processor, CALMET, is a diagnostic model able to produce a quite simplified analysis of the atmosphere by describing either mesoscale dynamics or micrometeorological processes. The latter includes an energy budget model for the computation of appropriate boundary layer scaling parameters such as surface heat flux, surface momentum flux and boundary layer height, which are used to derive the friction velocity, the convective velocity scale and the Monin-Obukhov length (*Scire et al.* [1990]). In this study, we run CALMET in a "non-observational" mode, i.e. without including assimilation of meteorological data coming from weather stations, using mesoscale output files as an initial guess field. The spatial resolution adopted is 1 km and applies to the entire computational domain.

4.2. Rising Plume Phase

This part of the VOL-CALPUFF code is new since the built-in plume rise model already implemented in CALPUFF was able to treat only gaseous emissions with a density lower than atmospheric. Therefore a more general plume rise model was implemented in VOL-CALPUFF to take into account the presence of a number of solid particulate phases. The equation set was solved in a 2D Cartesian coordinate system (s, φ) by considering the bulk properties of the eruptive mixture (see Fig. 2). The plume is assumed with a circular section along the curvilinear coordinate s and an inclination on the ground defined by an angle φ between the axial direction and the horizon. This last feature is needed to describe the evolution of weak explosive eruptions which are strongly affected by atmospheric conditions.

As in the plume theory, the entrainment (due to both turbulence in the rising buoyant jet and to the crosswind field) is parameterized through the use of two entrainment coefficients, α and γ. The theory assumes that the efficiency of mixing with ambient air is proportional to the product of a reference velocity (the vertical plume velocity in one case and the wind field component along the plume centerline in the other), α and γ (*Morton* [1959]; *Briggs* [1975]; *Wright* [1984]; *Weil* [1988]). Although this simplified approach can be used to reproduce the first-order features of plume ascent (e.g. final plume height), it does not explicitly describe more complex observed dynamics such as the double-vortex structure (*Ernst et al.* [1994]). The equation set consists of the equations of conservation of mass, momentum and thermal energy for the bulk mixture with height, equations expressing the conservation of mass for pyroclasts of different sizes, and those describing the variation of specific heat and mixture gas constant. The equation system is completed by the perfect gas law for the gaseous phase by assuming equilibrium pressure conditions between the volcanic plume and surrounding atmosphere. The total mass conservation equation solved by the model is:

$$\begin{aligned}\frac{d(\beta U_{sc} r^2)}{ds} &= 2r\rho_a[\alpha|U_{sc} - U_a cos\varphi| + \gamma|U_a sin\varphi|] + \\ &-p\beta r(1-n)\sum_{i=1}^{N} w_s(i) y_i \qquad (1)\end{aligned}$$

The variation of mass flux (l.h.s. term) is due to air entrainment and loss of solid particles (first and second r.h.s. terms, respectively). In Eq. (1), U_{sc} represents the velocity of the plume cross-section along its centerline, r the plume radius, β the mixture bulk density and U_a is the horizontal wind speed. This equation is similar to that used by *Bursik* [2001], the only difference being the lack of the re-entrainment term, which we assume to be negligible for the low intensity bent-over plumes discussed below and in the companion paper (*Ernst et al.* [1996]; *Bursik* [2001]). The factor p reflects, from a geometrical point of view, the possibility of each particle falling out from the rising plume and, by assuming clasts are lost only from the sloping plume margins, it is a function of the radial entrainment coefficient only (*Bursik et al.* [1992a]):

$$p = \frac{2((1+\frac{6}{5}\alpha)^2 - 1)}{(1+\frac{6}{5}\alpha)^2 + 1} \qquad (2)$$

For our values of α, the p factor varies between 0.2 and 0.33 (α=0.09 and α=0.15, respectively). The influence of the two entrainment coefficients, α and γ, was investigated through sensitivity studies (see next section), but in most cases they were set to 0.09 and 0.6, respectively, as determined in experimental studies by *Morton et al.* [1956], *Briggs* [1975] and *Weil* [1988]. As shown in the companion paper (*Barsotti and Neri* [2007], this issue), these values for the two coefficients can provide quite consistent estimates of plume height and deposit accumulation for the 2001 Etna plume investigated. In Eq. (1), the quantities $w_s(i)$ and y_i are the settling velocity and mass fraction, respectively, of the i-th granulometric class. The term in which they appear is the contribution of particle sedimentation from the plume.

Defining n as the mass fraction of the gaseous phase, the term $\pi\beta U_{sc}r^2(1-n)y_i$ represents the mass flux in the plume of the i-th particulate class. To compute the variation of the mass flux of solids during ascent the model solves the N mass conservation equations for the N particulate phases; which result in:

$$\frac{d(\beta U_{sc}r^2(1-n)y_i)}{ds} = -pw_s(i)\beta r(1-n)y_i \qquad i = 1, ..., N. \tag{3}$$

The X- and Z-components of the momentum balance solved by the model are:

$$\frac{d(\beta U_{sc}r^2(u-U_a))}{ds} = -r^2\beta w\frac{dU_a}{dz} - up\beta r(1-n)\sum_{i=1}^{N} w_s(i)y_i \tag{4}$$

$$\frac{d(\beta U_{sc}r^2 w)}{ds} = gr^2(\rho_a - \beta) - wp\beta r(1-n)\sum_{i=1}^{N} w_s(i)y_i \tag{5}$$

where the two components of plume velocity along the X and Z axes are u and w, respectively, and are linked by the relation $U_{sc} = \sqrt{u^2+w^2}$. In the r.h.s. of Eq. (4) appear the terms related to the exchange of momentum due to the wind and to momentum loss from the fall of solid particles. Similar contributions are evident in the r.h.s. term of Eq.

(5) where the vertical momentum is changed by the gravitational acceleration term and the segregation of particles.

Finally, following the above adopted notation, the equation for conservation of thermal energy solved by VOL-CALPUFF is described as:

$$\frac{d(\beta U_{sc} r^2 C_{p_{mix}} T_p)}{ds} = 2r\rho_a C_a T_a(\alpha|U_{sc} - U_a cos\varphi + \gamma|U_a sin\varphi|) +$$
$$-r^2 w\rho_a g +$$
$$-T_p p\beta r(1-n) * \sum_{i=1}^{N} C_s(i) w_s(i) y_i \qquad (6)$$

The first term on r.h.s. describes the cooling of the plume due to ambient air entrainment, the second one takes into account atmospheric thermal stratification, and the third term allows for heat loss due to sedimentation of solid particles. A thermal equilibrium between solid and gaseous phases is assumed. This formulation is similar to that proposed by *Glaze and Baloga* [1996] adapted for a two-dimensional and multi-phase treatment.

Finally, two equations for the variation rate of mixture specific heat and for the mixture gas constant were derived. Both variables were defined as weighted averages on the mass fraction of the components. We report the expression for the gas constant only, obtained knowing that the variation of gaseous mass fraction with height is solely due to entrained air:

$$\frac{dR_g}{ds} = \frac{n_0 \beta_0 U_{sc_0} r_0^2 (R_{air} - R_{gv})}{n^2 \beta^2 U_{sc}^2 r^3} * 2\rho_a[\alpha|U_{sc} - U_a cos\varphi| + \gamma|U_a sin\varphi|] \qquad (7)$$

where R_{gv} is the gas constant for the specific volcanic gas component. This formulation reduces, for particular cases, to the expressions of *Woods* [1988] and *Glaze and Baloga* [1996]. The plume rise equations were solved with a predictor-corrector Heun's scheme that guarantees a second-order accuracy, keeping the execution time in the order of seconds. Vent boundary conditions include the initial plume radius (r_0), mixture velocity (U_{sc_0}) and temperature (T_0), gas mass fraction (n_0) and the physical properties of the granulometric population.

4.3. Puff Transport and Diffusion

The mass flow rate feeding the puffs corresponds to the particle flow rate feeding the plume at the vent corrected for the amount radially lost during ascent. VOL-CALPUFF then describes pyroclast transport and diffusion in the atmosphere by tracking the movements of a number of Gaussian puffs, calculating their position, their lateral and vertical diffusion, and their amount of mass. Puff center displacement is computed by the simple relation $\overline{S} = \overline{V} * t$. Horizontally, the puff center is subjected to vertically-averaged zonal and meridional winds ($\overline{V}_H = \sqrt{U_{ave}^2 + V_{ave}^2}$), whereas vertically it is subjected only to the fall velocity ($\overline{V}_V = V_{set}$). The vertical component of the wind field is indirectly accounted for through a vertical spreading of the puff obtained by varying the vertical dispersion coefficient as a function of the vertical velocity gradient (*Scire et al.* [2000]). During puff movement, the mass distribution of a given particle size within the puff changes due to turbulent phenomena. Puff concentration is described by a Gaussian distribution whose standard deviations, horizontal and vertical, are computed for each time step. For a circular puff, the mathematical expression of such a distribution, which also represents the puff contribution to the concentration computed at a given location (*receptor*), is the following:

$$C(s) = \frac{Q(s)}{2\pi\sigma_y^2} g_t e^{\frac{-R^2(s)}{(2\sigma_y^2)}} \tag{8}$$

$$g_t = \frac{1}{(2\pi)^{\frac{1}{2}}\sigma_z} \sum_{n=-\infty}^{\infty} [e^{\frac{-(z_r - H_e + 2nh)^2}{(2\sigma_z^2)}} + e^{\frac{-(z_r + H_e + 2nh)^2}{(2\sigma_z^2)}}] \tag{9}$$

where s is the distance traveled by the puff from the source, $R(s)$ is the horizontal distance between puff center and receptor, and g_t is the vertical term, also called the coupling term, which depends on the puff and receptor relative positions. In particular, in case of puffs below the atmospheric boundary layer the coupling term takes into account, through the infinite sum over the index n, the material entrapment between the ground and the mixing lid of thickness h. Puff mass is represented by the variable Q and it varies with time by material removal due to sedimentation. Finally, the sigmas represent the horizontal and vertical diffusions. Their formulation is expressed as follows:

$$\sigma_{y,n}^2 = \sigma_{yt}^2 + \sigma_{ys}^2 + \sigma_{yb}^2 \tag{10}$$

$$\sigma_{z,n}^2 = \sigma_{zt}^2 + \sigma_{zb}^2 \tag{11}$$

where the horizontal term (Eq. (10)) contains the contribution due to atmospheric turbulence (σ_{yt}), the contribution due to a lateral (cross-wind) scale of the vent area-source (σ_{ys}) and the contribution due to plume buoyancy at the time of release (σ_{yb}). A similar formulation is valid for the vertical term (Eq. (11)), where the contribution due to areal extension is missing. These expressions show how the model allows the puffs to spread not only in response to atmospheric turbulence (σ_{yt} and σ_{zt}), but also in relation to the dynamics of the plume and to its structure when reaching the maximum rise height. In particular, the puffs are characterized by lateral dispersal coefficients (σ_{yb} and σ_{zb}) which are a function of the plume top radius. Furthermore the sigmas ($\sigma_{y,n}$ and $\sigma_{z,n}$) are functions of travel time (from source to receptor) and are computed each time the puff has a non-null contribution to the receptor. Finally, it should be noted that, in contrast to CALPUFF, the VOL-CALPUFF code is able not only to track the transport of puffs well above the atmospheric boundary layer (which can vary from hundreds of meters to a few kilometers above the ground), but also to compute their concentrations at the receptor locations. This extension of the code is indeed necessary due both to the much greater heights reached by volcanic plumes with respect to emission from industrial stacks and to our interest in mapping ash concentration anywhere, i.e. not only on the ground. Additional features implemented in VOL-CALPUFF are related to the consideration of particles with different diameters (up to several millimeters) and to the effect of particle shape on their settling velocity. With respect to the first aspect, VOL-CALPUFF can represent the multisize nature of the eruptive mixture by considering, at each time step, different independent puffs, each one characterized by a specific particle diameter. This is possible due to the dilute nature of the dispersal system that makes the interaction between particles negligible (*Crowe et al.* [1998]). Regarding the second aspect, several past and recent studies have highlighted the importance of describing the effect of particle sizes (*Bonadonna et al.* [1998]) as well as non-sphericity on their falling velocities (*Walker* [1971]; *Wilson* [1972]; *Wilson and Huang* [1979]; *Riley et al.* [2003]; *Dellino et al.* [2005]). The original CALPUFF code restricts the computation of settling velocity to the atmospheric layer affected by default activities and, as default, uses Stokes's formulation for spherical particles. VOL-CALPUFF adopts a formulation of the settling velocity as function of the Reynolds number. In particular, it adopts Stoke's drag coefficient expression C_D=24/Rey for Reynolds numbers smaller than $Rey < 0.1$ and $C_D \sim 1$ for $Rey > 1000$ (*Walker* [1971]). For Reynolds numbers in the 0.1-100 range, the Wilson and Huang formulation is used (*Wilson and Huang* [1979]). The latter formulation appears to be a good trade-off between ease of formulation and accuracy of results. It defines the following relationship between the drag coefficient, C_D, and Reynolds number :

$$C_D = \frac{24}{Rey} F^{-0.28} + 2\sqrt{1.07 - F} \quad (12)$$

in which particle shape affects the factor F through the equation $F = \frac{b+c}{2a}$, where a, b, and c are the three principal axes of the particle. Lastly, for intermediate values $100 < Rey < 1000$ a linear interpolation between the above described correlations is assumed for C_D (as already suggested by *Pfeiffer et al.* [2005]). The settling velocity of non-spherical particles is also allowed to vary as a function of height above the ground due to major variations in air density and viscosity with altitude (*Wilson* [1972]). In contrast, particle aggregation processes are not described by the present model, although they can play a major role in some conditions (*Textor and Ernst* [2004]; *Veitch and Woods* [2004]).

5. Initial Analyzes and Model Outputs

In this section first applications of the VOL-CALPUFF will be presented to show some of its standard outputs and type of results it is able to provide. In particular, the plume model was applied to the investigation of some interactions between plume rise and dispersal processes and the atmospheric environment, in the case of weak explosive events. Meteorological data used were produced by the non-hydrostatic EURO-LM Model (COSMO's web-site [2004]).

Plume dynamics Several simulations were performed by varying the conditions of the eruptive mixture at the vent in a still vs. windy environment. The results obtained were plotted in terms of variations of column density, velocity, and temperature with height and also compared to previous models (*Woods* [1988]; *Bursik and Woods* [1991]; *Bursik* [2001]). As an example, keeping constant the meteorological data and the vent velocity, and increasing vent radius, the model reproduced the shift in eruptive style from buoyant to super-buoyant and then to collapsing plumes, already predicted for plumes rising in a still atmosphere (*Bursik and Woods* [1991]). But the novel feature of VOL-CALPUFF is its ability to describe the effect of horizontal wind field on column evolution. As illustrated in the companion paper (*Barsotti and Neri* [2007], this issue), this is an important new feature of the code that strongly affects dispersal and deposition processes. This effect is shown in Fig. 3 where the column height evolution with time is reported for a still (thin line) and windy environment (bold one), for two intensities and for two seasonal periods. Even for constant vent feeding, weather conditions can modify column height by up to 100% or more. The sensitivity of plume dynamics to wind action is shown for an intensity range typical of weak explosive eruptions. In the absence of wind, the influence of atmospheric stratification on column height can also be inferred by comparing the temporal column evolutions in different seasonal periods (summer vs. winter). During colder periods, for both intensities, the plume reaches slightly greater heights in the atmosphere (*Wilson and Walker* [1987]).

The effect of the wind field on plume tilting can be seen in Fig. 4. The figure reports two different wind speed profiles (bold lines) and the associated distances reached by the column axis along the vertical and downwind directions. In particular, Fig. 4a shows the plume response to the tilting effect of wind for two real meteorological conditions, in the early morning and at midday, for a mass flow rate of $6.6 * 10^3$ kg/s. Similarly, Fig. 4b shows the results for a higher plume intensity ($2.5 * 10^4$ kg/s). The investigated wind profiles produce quite different plume rise trajectories. From the figure it is evident how the plume, meeting the more intense wind, rises about 25 % less high than that affected by the weaker winds; whereas the downwind distance of the plume top is only slightly sensitive.

VOL-CALPUFF can also be used to assess the sensitivity of results to the model parameters, for instance to the entrainment coefficients. Fig. 5a and Fig. 5b show the variation of column height, calculated each hour during a 72-hour run with constant vent conditions, as a function of the two entrainment coefficients. The figure clearly shows the irregular trends which reflect the temporal variability of meteorological conditions met by the column during ascent. However, the role of the entrainment coefficients (Eq. 1) in the determination of column height is also evident. Keeping the wind-entrainment coefficient γ equal to 0.6, the radial-entrainment coefficient α was varied in the range 0.09-0.15 (Fig. 5a). The first value was proposed by *Morton et al.* [1956] and is typically assumed for buoyant volcanic plumes (*Sparks et al.* [1997]). The second value comes from laboratory experiments (*Hewett et al.* [1971]). In agreement with *Morton et al.* [1956] and *Wilson and Walker* [1987], increasing the radial coefficient, α, the column reaches decreasing altitudes. The VOL-CALPUFF results show that, in a windy environment, this variation is reflected in an approximately 30% change of column height.

A similar sensitivity study was performed for a variation of γ in the range 0.6-1.0 (derived by *Briggs* [1975] and *Hewett et al.* [1971], respectively), confirming the inverse relation between column height and entrainment coefficient. The two simulations, keeping α equal to 0.09, show a stronger dependence on wind-entrainment variation, which produces a difference of up to about 40% in column height (Fig. 5b).

Ash dispersal In addition to the analysis of plume evolution, VOL-CALPUFF provides consistent estimates of atmospheric ash concentrations and particle deposition at the ground. Each hour it computes the quantity of emitted material still airborne and the amount deposited. In our standard applications the domain is sliced into eight terrain-following levels at 800 m intervals with each one made up of 5625 points. Both the number of levels as well as the gridded points can be increased. Particle concentration is computed at each receptor. Fig. 6 shows a vertical section of the domain used in the application at Mt. Etna (discussed in the companion paper), in which levels have been remapped referring to sea level. The horizontal levels are parallel planes in which the color is graduated depending on the amount of computed ash. More intuitive is a planar view representation where the contouring of particle concentration (g/m^3), at a specific altitude above the ground, is superimposed on a 2D topography (Fig. 7). The code's Lagrangian nature and the algorithms's structure make it easy to quantify the presence of ash in specific locations and at any height of interest, for example in correspondence of airplane flight levels or corresponding to areas with anthropogenic activities. Ash concentration estimates at plume levels may prove valuable to fine tune remote-sensing instruments as regards particle diameter and density, as well as, detection thresholds. Finally, at the ground level, VOL-CALPUFF can compute the dry-fluxes of depositing material from which the ash load is estimated in kg/m^2. A 3D representation of this output is provided by Fig. 8, in which the computed deposit is *spread* on a 3D orographic profile.

6. Conclusive Remarks

The VOL-CALPUFF model is a new quantitative tool for simulating atmospheric dispersal and deposition of volcanic ashes. The main new feature of the model is its ability to combine plume rise and ash dispersal models to describe their dynamics under the action of realistic 3D and time-dependent meteorological conditions. The model, by adopting a mixed Eulerian-Lagrangian formulation, is able to describe effectively the rising column and regional ash dispersal throughout the eruption. The Lagrangian description of ash dispersal provides a reliable model both in the distal and proximal areas. Moreover, spatial and temporal resolution scales in the order of 1 km and 1 hour, respectively, can be provided by VOL-CALPUFF by keeping the computational time to a few minutes even for eruptive events lasting several days. This feature makes VOL-CALPUFF a promising tool also for the production of quasi real-time ash dispersal forecast simulations to be used for warning and hazard analysis (*Barsotti et al.* [2006]). Results from initial simulations clearly highlight the novel features of the model and the important implications that they allow regarding dispersal dynamics. With specific reference to the rising plume dynamics, the results presented show the extensive influence of meteorological conditions on plume height. The wind speed variations during the three-day period investigated result in the plume height variations of well above 100%. An increase in wind speed by a few meters per second at low altitude can significantly tilt the rising plume, shifting the plume top several hundreds of meters closer to the ground (see Fig. 4). In absence of wind, the column height also shows sensitivity to the variations of atmospheric thermal stratification.

In the companion paper (*Barsotti and Neri* [2007], this issue) VOL-CALPUFF is used to model a weak plume from Mt. Etna, and results are compared to independent observations to better describe VOL-CALPUFF capabilities and limitations. Model applications to larger plumes are being prepared and will be presented in future works.

Acknowledgments.

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Notation

a	major mean particle axes
b	median mean particle axes
c	minor mean particle axes
$C_{p_{mix}}$	heat capacity of mixture
C_a	heat capacity of ambient air
C_D	drag coefficient
C_s	heat capacity of solid phase
$C(s)$	concentration at receptor
F	particle shape factor
g_t	coupling vertical term
H_e	effective puff height
h	mixing layer height
n	gas mass fraction
n_0	initial gas mass fraction
p	probability of fallout
$Q(s)$	amount of material in each puff
r	plume radius
r_0	initial plume radius
R_{gv}	gas constant for volcanic gas component
R_g	gas constant for mixture gas phase
R_{air}	gas constant of ambient air
Rey	Reynolds's number
s	downstream coordinate or source-puff distance
$\overline{S}$	generic puff displacement
t	time
T_a	ambient temperature
T_p	plume temperature
T_0	initial mixture temperature
U_{ave}	zonal wind averaged over lateral puff extension
U_{sc}	centerline plume velocity
U_{sc_0}	initial centerline plume velocity
U_a	wind speed
V_{ave}	meridional wind averaged over lateral puff extension
V_{set}	settling velocity
$\overline{V}$	generic velocity (both horizontal and vertical) driving puff displacement
$\overline{V}_H$	horizontal puff velocity
$\overline{V}_V$	vertical puff velocity
$w_s(i)$	settling velocity of i-th granulometric class
y_i	mass fraction of i-th granulometric class
z_r	receptor height

Notation

α	radial entrainment coefficient
β	mixture bulk density
β_0	initial mixture bulk density
γ	wind-entrainment coefficient
φ	angle between plume axis and horizon
ρ_a	air ambient density
$\sigma_{y,n}$	lateral dispersion coefficient at n time step
σ_{yb}	lateral dispersion coefficient due to plume buoyancy
σ_{ys}	lateral dispersion coefficient due to lateral scale of an area-source
σ_{yt}	lateral dispersion coefficient due to atmospheric turbulence
$\sigma_{z,n}$	vertical dispersion coefficient at n time step
σ_{zb}	vertical dispersion coefficient due to plume buoyancy
σ_{zt}	vertical dispersion coefficient due to atmospheric turbulence

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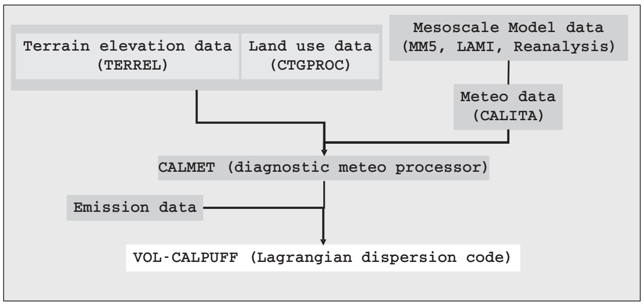

Figure 1. The simplified flowchart of CALPUFF as used in our application. It represents the minimal structure for running the system. It contains the meteorological and geophysical preprocessors (TERREL, CTGPROC, CALITA), the diagnostic meteorological model (CALMET), and the dispersal code (VOL-CALPUFF).

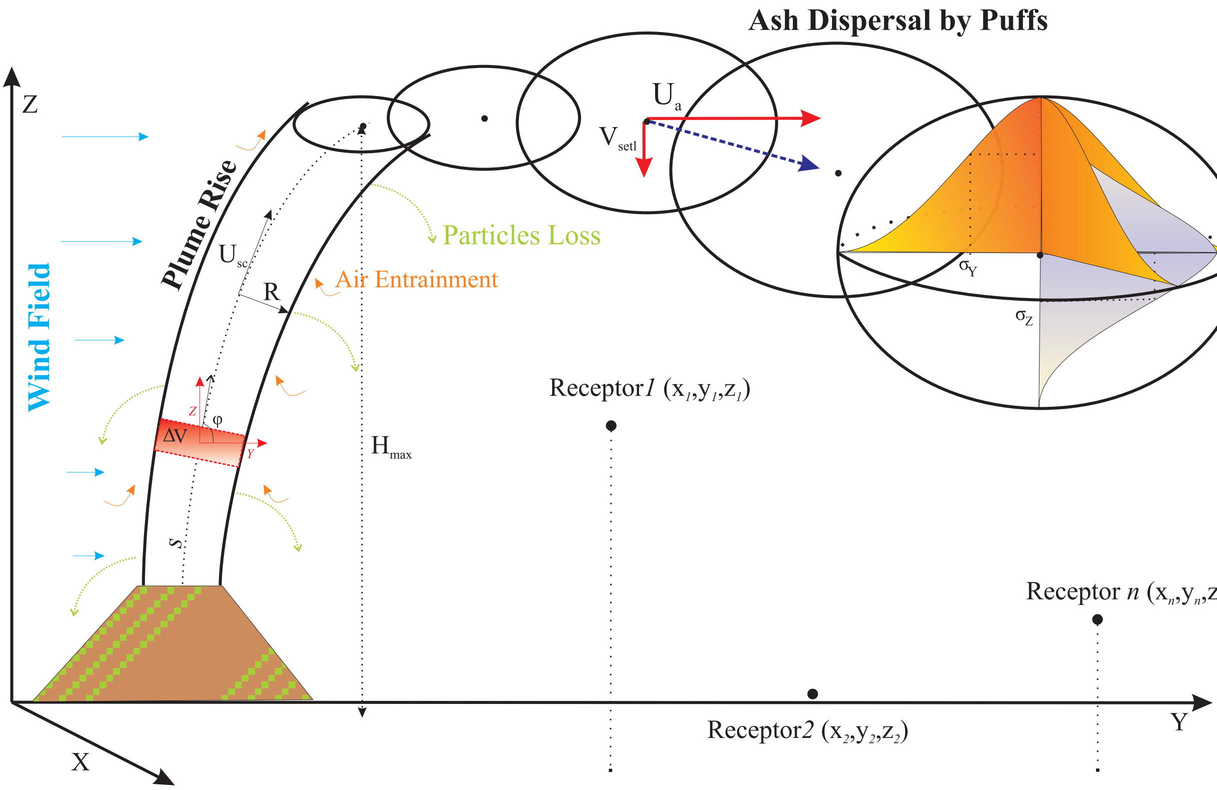

Figure 2. Schematic representation of the VOL-CALPUFF approach. Plume ascent is described by adopting a Eulerian formulation whereas dispersal is represented by a Lagrangian approach, i.e. following the movement and diffusion of a discrete number of puffs.

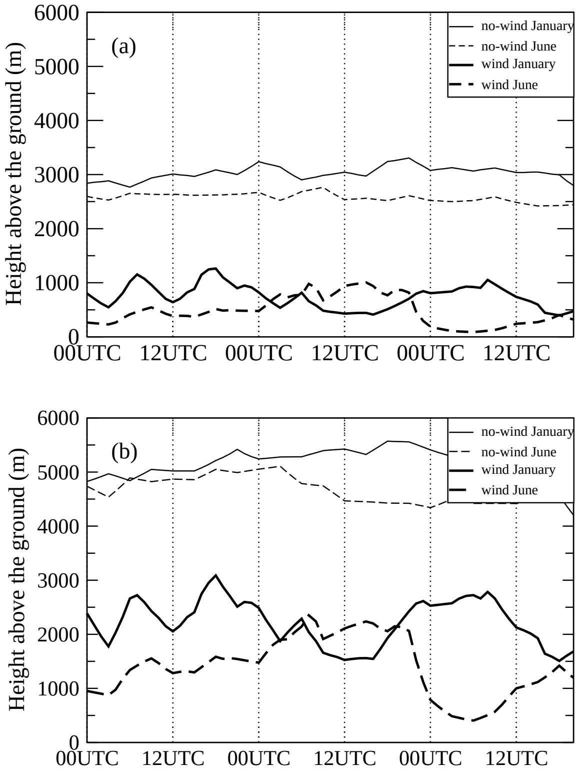

Figure 3. Variation of column height for two plume intensities, (a) $6.6 * 10^3$ kg/s (T_0=1300 K, U_{sc_0}=20 m/s, r_0=4.8 m, n_0=3%) and (b) $2.5*10^4$ kg/s (T_0=1300 K, U_{sc_0}=25 m/s, r_0=8.7 m, n_0=3%). Curves refer to a still (thin line) and windy (bold line) atmosphere, and to two different seasonal periods. In detail dashed lines refer to three days of June 2005 whereas the continuous ones indicate three days of January 2006.

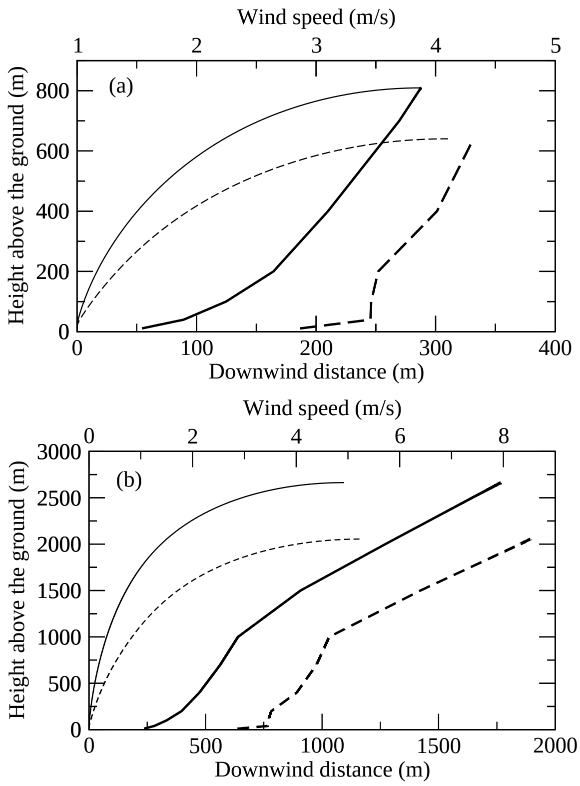

Figure 4. Effect of wind field on plume height and tilting for two different plume intensities and meteorological conditions. The intensities correspond to (a) $6.6 * 10^3$ kg/s and (b) $2.5 * 10^4$ kg/s and vent conditions are the same as Fig. 3. Wind profiles refer to 0600UTC and 1300UTC on 4 January 2006. From the figure it is clear how more intense speeds (dashed line) tilt the columns more than in the weaker cases (continuous line), reaching lower heights.

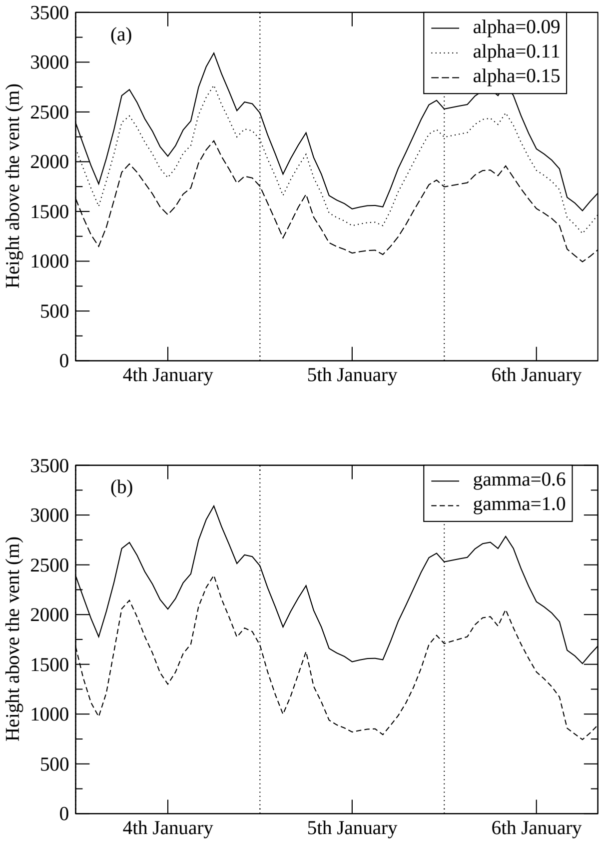

Figure 5. Temporal variations of column height for a mass-flow rate equal to $2.5 * 10^4$ kg/s (the vent conditions are the same as Fig.3). The figures report the height trend over about three days (4-6 January 2006) under the forcing of realistic 3D meteorological conditions. The curves were obtained using different entrainment coefficient values. Keeping γ=0.6 three values of α are investigated (a): $\alpha = 0.11$ (dotted line), $\alpha = 0.15$ (dashed line) and α= 0.09 (continuous line). And, keeping α=0.09, two values of γ (b): $\gamma = 0.6$ (continuous line) and γ=1.0 (dashed line).

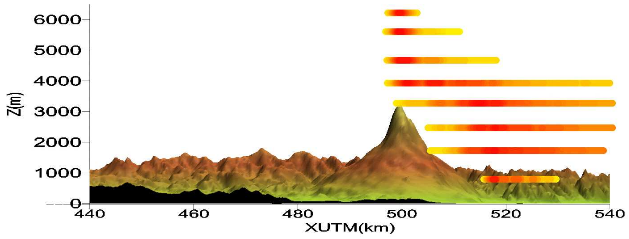

Figure 6. Vertical section of the 3D physical domain in which the horizontally extended levels, remapped from the standard terrain-following ones, are visible. In this case, VOL-CALPUFF adopted eight levels each one made up of 5625 nodes.

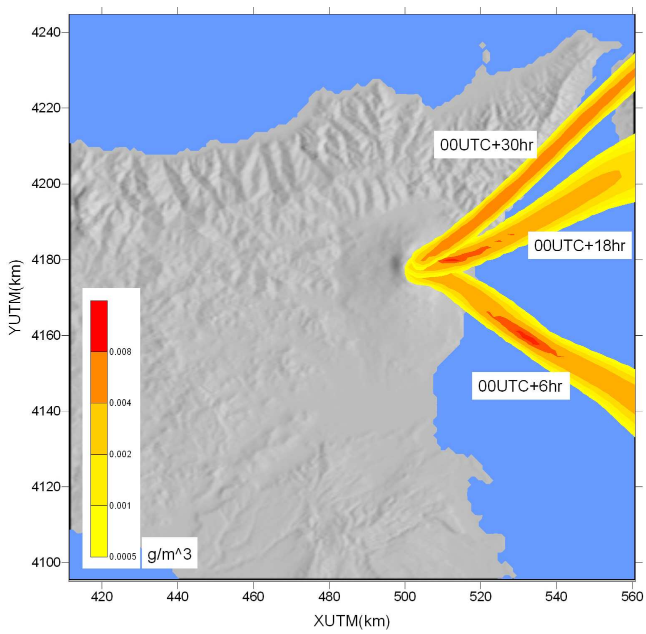

Figure 7. Contouring of 64μm particles concentration at 2400 m a.g.l. in a 2D representation of the VOL-CALPUFF outputs. The three snapshots correspond to three temporal instants at 12hr intervals. Variations in wind direction deflect the plume from SE to a NE dispersal.

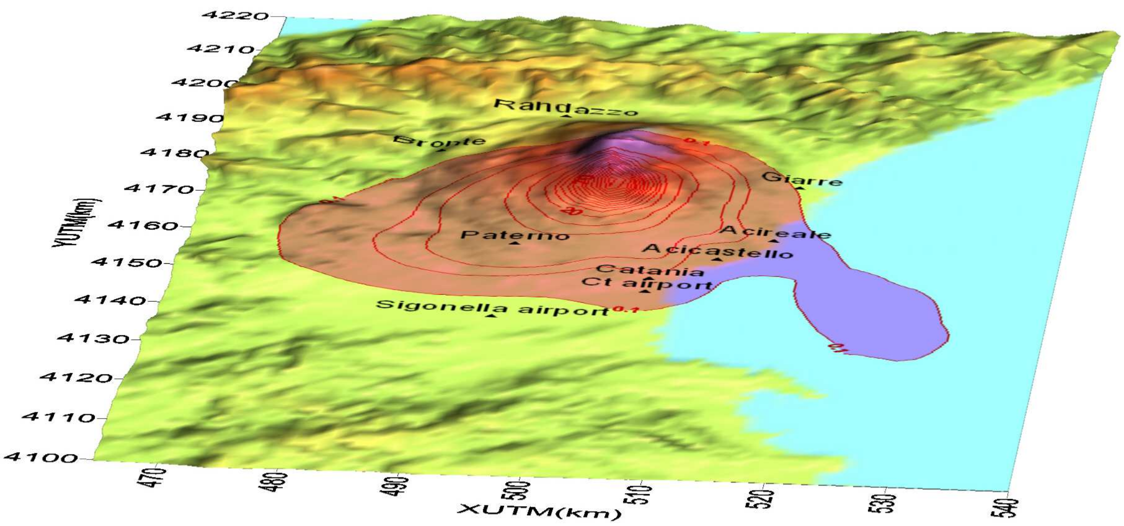

Figure 8. A given example of deposit on the ground at Mt.Etna. VOL-CALPUFF computes the deposited ash amount in kg/m^2; the lower reported value is equal to 0.1.