PYFLOW User's Manual

A computer code for the calculation of the impact parameters of Dilute Pyroclastic Density Currents

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31/12/2013

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1. Introduction

PYFLOW is a multi-block code for the calculation of the flow field variables of dilute pyroclastic density currents (hereafter DPDCs) starting from the deposits characteristics. The code, written in Fortran 90, solves an improved version of the model of Dellino et al. (2008): it calculates the vertical profiles of particle volumetric concentration, flow density, velocity and dynamic pressure, and builds probability functions for each one of the flow field variables. This new probability function tool allows to perform a probabilistic analysis of the results and, subsequently, to calculate the flow field variable at a desired exceedance probability. Thanks to these new features, PYFLOW can be used for the assessment of the hazard related to DPDCs, provided that an extensive field study and a precise laboratory analysis of the deposits' sample is carried out.

The code is available for Unix/Linux/Mac OS X/Windows Operating Systems. The input data come from DPDC deposits analysis (e.g. particles diameter, density, layer thickness, substrate roughness, etc.).

2. Model

In this section the model is described. The user should also refer to Dellino et al. (2005, 2008, 2010; Mele et al., 2011) for further details.

2.1. Turbulent Boundary Layer Shear Flows (TBLSF) as an approximation of DPDCs

A TBLSF forms when a fluid moves over a solid surface (Furbish, 1997; Schlichting and Gersten, 2000). The analogy between TBLSFs and geophysical surface flows has been proposed for many decades, in particular for the sediment mechanics of particle-laden turbulent flows (Middleton and Southard, 1984). The TBLSF approximation has been already used to calculate average velocity and density of DPDCs of some explosive eruptions at Vulcano, Aeolian Islands (Dellino and La Volpe, 2000, Palizzi eruption) and Campi Flegrei (Dellino et al., 2004, Astroni and Agnano-Monte Spina eruptions). A complete sedimentological model was presented in Dellino et al. (2008) and experimentally validated in Dellino et al. (2010).

In a DPDC pyroclastic particles are held in suspension by the effect of gas turbulence, as the fluctuating part of velocity directed upward contrasts with the downward particles' settling velocity (Dellino et al., 2008). Indeed, as it follows from Prandtl's assumption (Furbish, 1997; Schlichting and Gersten, 2000) the shear stress at the base of the current is $\tau_0 = \rho_f u_*^2 \approx -\rho_f \overline{u'w'}$, where ρ_f is the flow density, u_* is the shear velocity and $\overline{u'w'}$ is the covariance of the fluctuating velocities in the stream (x) and upward (z) directions.

A peculiar characteristic of DPDCs is the particle concentration stratification caused by the diffusive effect of the gas turbulence over the particles transported in turbulent suspension. The concentration profile can be calculated by the Rouse equation (Rouse, 1939):

$$C(z) = C_0 \left(\frac{z_0}{z_{tot} - z_0} \frac{z_{tot} - z}{z} \right)^{P_n} \quad (1)$$

where C is the particle volumetric concentration, C_0 is the particle concentration at the reference level z_0, z_{tot} is the total flow thickness (fig. 1a).). z_0 is the base level at which the particles are being settled from suspension, i.e. where $C(z)$ approaches the maximum packing limit typical of the very thin bedload at the base of a sediment current (that can be assumed to be equal to 0.75, as in Dellino et al. (2008)). P_n is the Rouse number, a dimensionless quantity defined as:

$$P_n = \frac{w}{ku_*} \quad (2)$$

where w is the particle settling velocity and k is Von Karman's constant (equal to 0.4). As can be easily inferred, P_n describes the tendency of particles to be transported by a turbulent flow. When $P_n > 2.5$ a particle settles down, whereas when $P_n < 2.5$ it can be held in suspension (Middleton and Southard, 1984). Actually in the DPDC the solid phase is represented by a population of particles, each one characterized by different size, density, drag, i.e. different settling velocity w. For this reason P_n represents an average value of the population.
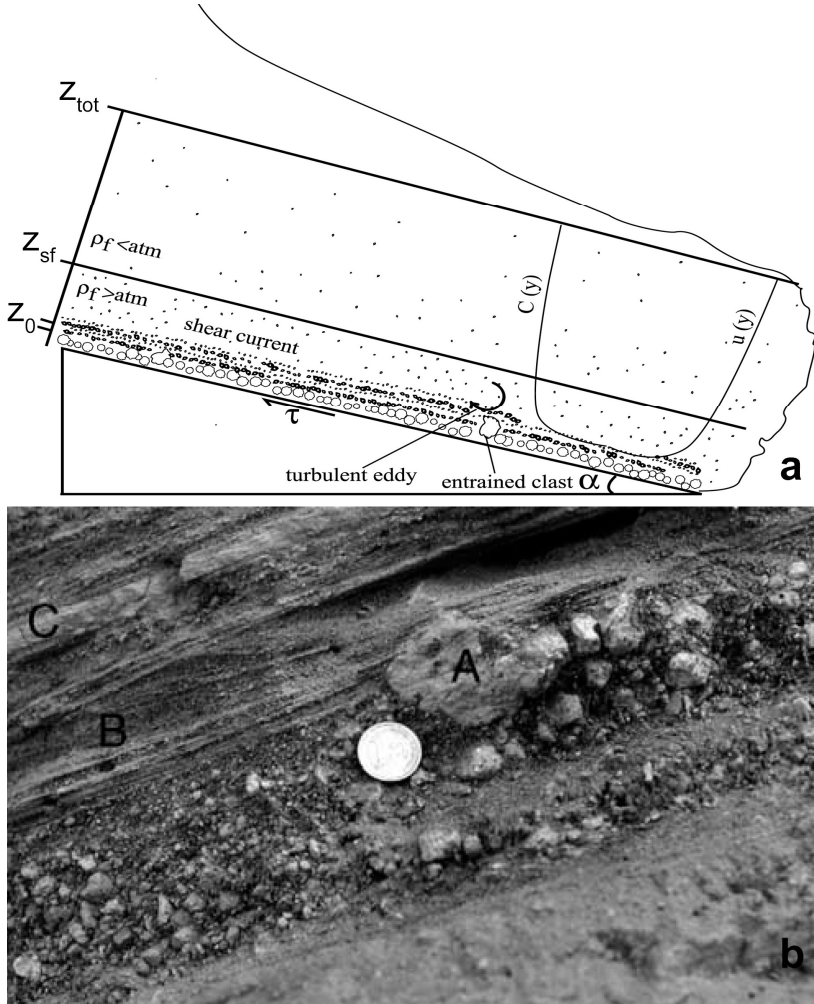

Fig. 1. a: scheme of a DPDC moving on an inclined slope. The reference level z_0, the shear flow thickness z_{sf} and the total flow thickness z_{tot} are shown, together with the concentration profile $C(z)$ and average velocity profile $u(z)$. **b:** picture of a complete DPDC deposit, with the layer of coarse lapilli and bombs (A), the laminated layer (B) and the massive thin ash layer (C).

The particle concentration profile determines the flow density profile:
$$\rho_f(z) = (1 - C(z))\rho_g + C(z)\rho_s \quad (3)$$
where ρ_g and ρ_s are the gas and solid particle density, respectively. As the hot gas is lighter than the atmosphere, and since the current is density stratified, a DPDC can be divided into a basal portion denser than atmosphere (that induces a shear stress on the ground) and an upper portion that is less dense than the atmosphere (fig. 1a). The basal portion is the shear current, which is the part of major interest for the calculation of the DPDCs impact parameters and hazard assessment. Furthermore, this shear current can be described according to the TBLSF theory (Dellino et al. 2008) and is characterized by the "law of the wall", which defines the time-averaged velocity profile of the current:

$$\frac{\overline{u}(z)}{u_*} = \frac{1}{k}\ln\frac{z}{k_s} + 8.5 \quad (4)$$

where k_s is the roughness parameter of the substrate.

In the dense part of the DPDC (i.e. the shear flow), particles settle down from suspension and form the bed load, which represents a minor thickness (less than 1%) compared to the total flow height. The combination of the stress exerted from the overlying shear flow on the bed load, and the continuous sedimentation of particles from suspension, determines a progressive aggradation of sediment to form thin tractional laminae (Branney and Kokelaar, 1992; Sulpizio and Dellino, 2008) that sum up and lead to the formation of wavy beds, which are the distinguishing features of DPDCs deposits (Dellino et al., 2008). The complete facies architecture characterizing the stratigraphic sequence of a DPDC deposit is composed of three layers (fig. 1b): (A) a bed of coarse lapilli and bombs representing particle entrained at the base of the current (this layer can be lacking, especially far away from the volcanic vent); (B) a finely laminated layer originated by the lamina by lamina aggradation process described above; (C) a thin massive fine-ash layer representing the fine ash deposited during the waning stage of the flow (Dellino et al., 2004, 2008).

If such a sequence is observed in the field and the beds composing it are described in detail and sampled for successive laboratory investigations, it is possible to use PYFLOW to invert deposit data and define the fluid dynamic characteristics of the parent current. It is to note that the values calculated by PYFLOW represent the current characteristics at the particular location where deposits have been recognized in the field. In the case that multiple outcrops of deposits of a DPDC are found, by applying PYFLOW to each of them, it would be possible to define the variation of pyroclastic density current behavior over the dispersal area. It is to recall that the model is based on the TBLSF approximation of DPDCs, thus it is expected to give reliable results only in the case of dilute currents. In fact, Dellino et al. (2008) carried out a stress test in which it was shown that, upon applying the model to a thick massive deposit related to a highly concentrated flow of the Pollena eruption at Vesuvius, the t-Student test (which will be presented below) fails, thus indicating that the model is not applicable if samples come from deposits that are not formed from dilute density currents. The t-Student test is therefore a check of both the applicability of the PYFLOW model and of the reliability of results.

2.2. Shield and suspension-sedimentation criterions

In a DPDC there are particles that are never transported in suspension but can be moved over the substrate by the current shear stress (e.g. particles with P_n much higher than 2.5 or particles already lying on the ground before the DPDC passage). This phenomenon can be described by the Shield or entrainment criterion (Miller et al., 1977)), which compares the DPDC shear stress to the buoyancy force of the coarse particle in the flow:

$$\theta = \frac{\rho_f u_*^2}{(\rho_{s1} - \rho_f)gd_1} \quad (5)$$

where g is gravity acceleration, ρ_{s1} and d_1 the density and diameter of the entrained particle, respectively; θ is a constant depending on the particle Reynolds number, which is equal to 0.015 for a particle Re number larger than 1000 (Miller et al., 1977). This is generally the case of coarse particles moved at the base of DPDCs able to move coarse particle. since, if one considers a clast of 2 cm diameter (generally clasts moved at the base of pyroclastic density currents are much larger) and a shear current with a shear velocity of 1 m s^{-1} and a kinematic viscosity of $1.6*10^{-5}$ Pa s^{-1} (reasonable values even for quite small DPDCs with a fluid phase represented by gases at 300 °C), Re is higher than 1000.

On the other hand, at the limit of transportation by turbulent suspension when $P_n = 2.5$ and, from eq. (2), since $k = 0.4$, it follows that:

$w = u_*$ (6)

This is the suspension-sedimentation criterion (Middleton and Southard, 1984), which means that particles stay suspended until their settling velocity is less than flow shear velocity. In other terms, deposit particles that are settled from suspension (the laminae-forming bed load) give an indication of the current shear velocity, once their terminal velocity is defined. Particle settling velocity w can be calculated by the so-called Newton impact law (Dellino et al., 2005):

$$w = \sqrt{\frac{4gd(\rho_s - \rho_f)}{3C_d\rho_f}}$$ (7)

where d is the particle equivalent diameter (i.e. the diameter of the sphere having the same volume of the settling particle), C_d is the drag coefficient. Upon combining (6) and (7), it follows that:

$$u_*^2 = \frac{4gd(\rho_s - \rho_f)}{3C_d\rho_f}$$ (8)

The shear velocity is actually the shear stress at the base of the current normalized by the flow density:

$$\tau_0 = \rho_f u_*^2$$ (9)

When the stratigraphic sequence described in the previous section is recognized in the field (fig. 1b: 1) the coarse layer of lapili and bombs moved by shear at the base of the current; 2) the laminated layer of ash formed by particles settled from turbulent suspension) it is possible to apply both the Shield and the suspension-sedimentation criteria for calculating the flow parameters. However, the layer of entrained coarse lapilli or bombs, which is is typical of proximal locations around the eruptive vent, is often missing in distal outcrops, thus preventing to use the Shield criterion far away from the volcanic vent. In that case, an alternative method based on the hydraulic equivalence of particles can be used. The system of equation to be applied in the two cases will be discussed in the next sections 2.4 and 2.5.

2.3. Particle analysis for providing input data

In order to use eqs. (5) to (9) and solve for current shear velocity and density, it is necessary to measure ρ_{s1} and d_1 of the clasts from the basal coarse layer; ρ_s and d for the particle deposited in the laminated layer. In particular, juvenile glassy particles are considered here (which are usually the most abundant component of eruptive mixtures), with d representing the equivalent diameter of the median size of the juvenile particles grain-size distribution. ρ_s and d of other components (e.g. crystals, lithics) are also needed, as it will be discussed in Section 2.5. Furthermore, shape parameters of particles coming from the laminated layer are needed in order to compute the drag coefficient C_d.

For the entrained clast at the base of the current, d_1 can be measured by means of a caliper by taking the geometric mean between the three axes. Alternatively d_1 is calculated as the diameter of the equivalent sphere d_{sph} by measuring the weight m and the density ρ_{s1} of the clast.

$$d_1 = d_{sph} = \sqrt[3]{\frac{6m}{\pi\rho_{s1}}}$$ (10)

The clast's density ρ_{s1} is obtained via a standard picnometer.

For samples of the laminated layer, a grain-size analysis is performed by hand-sieving in the fraction between -6 ϕ and 3 ϕ, and using a Coulter Multisizer for the fraction between 3.5 ϕ and 6.5 ϕ ($\phi = -\log_2 d_{mesh}$, where d_{mesh} is the mesh size in mm). The grain-size distributions of each component are obtained by component analysis: for each grain-size class of the whole sample, the different particles are picked by hand for the classes between -6 ϕ and 0 ϕ, while for finer classes a counting procedure with the stereomicroscope is employed. By knowing the proportion between the single class and the whole sample weight and the number of the particles of each component, the

component grain-size distribution is readily obtained (Mele et al., 2011). The median size Md_ϕ and sorting σ_ϕ are then computed with the `grainsize` program (which can be requested separately). The mass m and the density ρ_s of particles are also measured by picnometric measurements, in order to obtain the diameter of the equivalent sphere d_{sph} (eq. 10)

Since pyroclastic particles are not well approximated by spheres (Dellino et al., 2005), d_{sph} is adjusted by means of the following relationship in order to obtain the equivalent diameter of the median size (Dellino et al., 2008):

$$d = \frac{\overline{d}_{\phi(\phi_i-\phi_j)}}{\overline{d}_{sph(\phi_i-\phi_j)}} Md_\phi \quad (11)$$

where $\overline{d}_{\phi(\phi_i-\phi_j)}$ is the average diameter of the sieve mesh between the ith and j^{th} size classes and

$\overline{d}_{sph(\phi_i-\phi_j)}$ is the average diameter of the equivalent sphere between the ith and j^{th} size classes. The equivalent diameter of the median size is the most representative value of the size of the particles that settle from the suspension (Dellino et al., 2008), as long as the grain-size distribution is unimodal, approximating a Gaussian curve. The program `grainsize` checks for this condition to be satisfied via a Chi-squared test.

The particle shape factor ψ is calculated by applying the procedure explained in Dellino et al. (2005). This is a time-consuming procedure, thus in figure 2 particles of different shapes with the relative values of ψ are displayed. As a first very crude approximation the user can compare the particles with this figure to get an idea of the shape factor. Anyway it's recommended to measure the shape factor whenever possible. Recently Alfano et al. (2011) provided a list of approaches that can be used for calculating the particle shape factor: BET, 2D or 3D image analysis are used for obtaining shape parameters, and different empirical relationships are applied for calculating terminal velocities. Modern devices, like Pharmavision 830® (Malvern Instruments) or Camsizer® (Retsch Technology), also provide fast particle size and shape analysis. In a future version of PYFLOW, further relationships for particle shape factor and/or terminal velocity (Alfano et al., 2011) will be likely implemented.
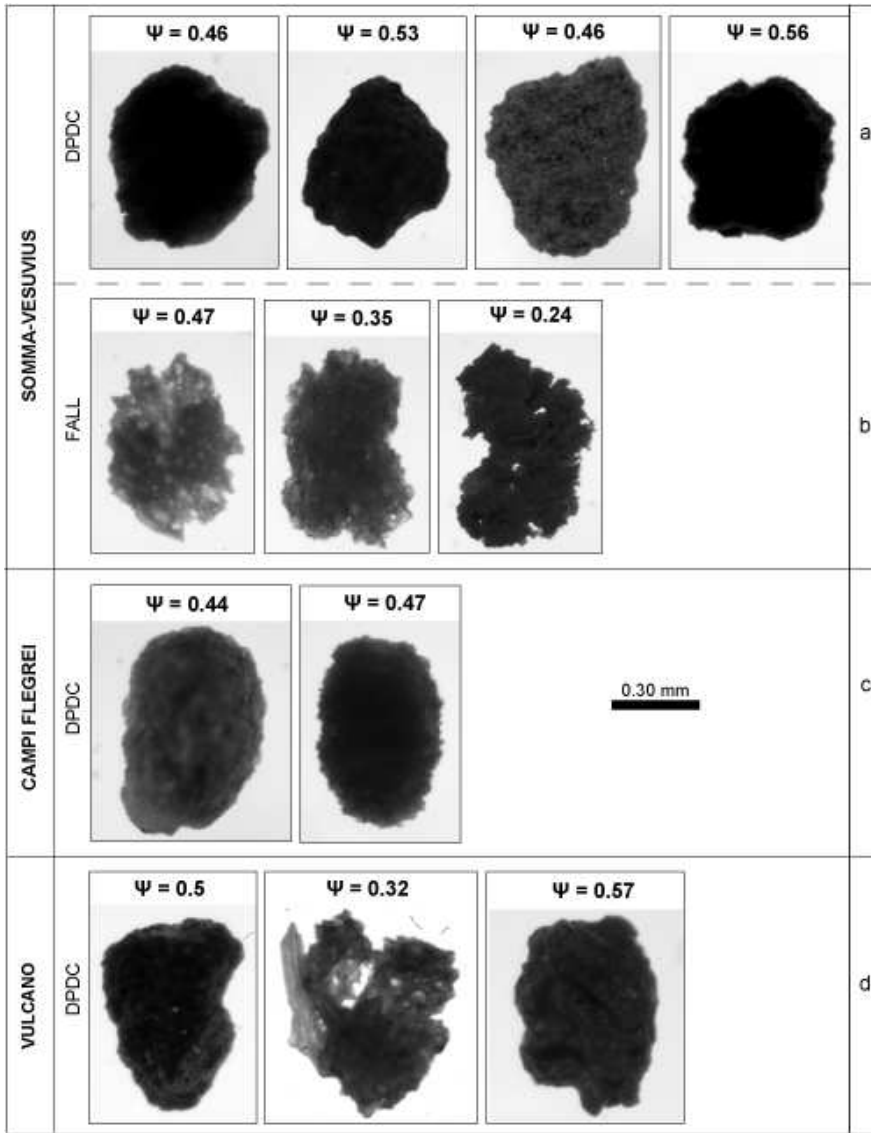
Fig. 2: typical pyroclastic particles from different eruptions. For each one the shape factor ψ is reported. Redrawn after Mele et al. (2011).

The shape factor has a strong influence on terminal velocity w, as it influences particles drag coefficient C_d. Here, the model proposed by Dellino et al. (2005) is used:

$$C_d = \frac{0.69 g d^3 \rho_f \left(1.33\rho_s - 1.33\rho_f\right)}{\eta^2 \left(\frac{g \psi^{1.6} d^3 \rho_f \left(\rho_s - \rho_f\right)}{\eta^2}\right)^{1.0412}} \quad (12)$$

where η is gas viscosity. The gas can be represented by steam at 300 °C, with a viscosity of $2*10^{-5}$ Pa s^{-1}.

2.4. Two-layers model

When the complete fining upward sequence (fig. 1b) is observed in the deposit, it can be inferred that during the depositional history of the DPDC, at the interface between the basal and laminated layers the coarse particles lying on the substrate (or in the forming deposit) were just moved by the shear stress at the base of the current (Dellino et al., 2008). The overlying laminae are formed by particle settling from turbulent suspension. The interface between the two layers represent the zone of maximum shear stress in the current. The value of shear velocity and density resulting from the

solution of the system of equations 5, 8 and 9 thus represent the characteristics of the shear current at the considered location where the sample has been collected.

It is to remark that the parameters on the right side of eq. 8 refer to a population of particles rather than single particles, and therefore represent average values over the entire population. The average value is the equivalent diameter of the median size d; the range of variation is represented by the sorting σ_ϕ of the grain-size distribution. Consequently also the drag coefficient C_d, which is a function of d (eq. 12) varies accordingly. In order to better evaluate the range of solutions (shear velocity and flow density) of the system of equations 5 and 8, it is convenient to group the parameters having a range of variation (d and C_d) in a ratio C_d/d. Upon rearranging the equations:

$$\frac{C_d}{d} = \frac{4(\rho_s - \rho_f)}{d_1 \theta 3(\rho_{s1} - \rho_f)} \quad (13)$$

A range of values is calculated as a function of a realistic range of flow density ρ_f. As stated in Section 1, the shear current is denser than atmosphere; furthermore, the particle volumetric concentration is expected to be limited to a few percent, in order to conform with the dilute current assumption. Thus, a reasonable range of flow density is between 2 and 100 kg m^{-3}. The validity of this assumption has been discussed in detail in Dellino et al. (2008).

The values of C_d/d corresponding to realistic flow density values are named $C_d/d(2 \ kg \ m^{-3})$ and $C_d/d(100 \ kg \ m^{-3})$. By isolating ρ_f in eq. 5 and substituting it into (13), the ratio C_d/d as a function of the squared shear velocity is obtained:

$$\frac{C_d}{d} = \frac{4g\left(\rho_s - \dfrac{\theta g d_1 \rho_{s1}}{u_*^2 + \theta g d_1}\right)}{3u_*^2 \left(\dfrac{\theta g d_1 \rho_{s1}}{u_*^2 + \theta g d_1}\right)} \quad (14)$$

Substituting the values of $C_d/d(2 \ kg \ m^{-3})$ and $C_d/d(100 \ kg \ m^{-3})$ into (14), the corresponding values of the squared shear velocity $u_*^2 \ (2 \ kg \ m^{-3})$ and $u_*^2 \ (100 \ kg \ m^{-3})$ are calculated. By using the theorem of the average value of a function, the average model ratio of C_d/d is found:

$$\frac{C_d}{d} avg = \frac{1}{u_*^2(2kg/m^3) - u_*^2(100kg/m^3)} \int_{u_*^2(100kg/m^3)}^{u_*^2(2kg/m^3)} \frac{4g\left(\rho_s - \dfrac{\theta g d_1 \rho_{s1}}{u_*^2 + \theta g d_1}\right)}{3u_*^2 \left(\dfrac{\theta g d_1 \rho_{s1}}{u_*^2 + \theta g d_1}\right)} du_*^2 \quad (15)$$

With the same approach the average particle drag coefficient C_d (eq. 12) can be calculated in the 2-100 kg m^{-3} flow density range:

$$C_d avg = \frac{1}{100kg/m^3 - 2kg/m^3} \int_{2kg/m^3}^{100kg/m^3} \frac{0.69 g d^3 \rho_f (1.33\rho_s - 1.33\rho_f)}{\mu^2 \left(\dfrac{g \psi^{1.6} d^3 \rho_f (\rho_s - \rho_f)}{\mu^2}\right)^{1.0412}} d\rho_f \quad (16)$$

$C_d avg$ can be considered to be a good estimate of the population of particles settling from turbulent suspension if the grain-size distribution approximates a Gaussian curve, which is usually the case of this kind of samples and is verified in the auxiliary program `grainsize` (see Section 4.2.1-a). A model value for the particles diameter can be obtained by the following relationship:

$$d_{mod} = \frac{C_d avg}{\dfrac{C_d}{d} avg} \quad (17)$$

This value can be compared with that measured from the sample d by means of a statistical Student t-test, by defining the t variable as:

$$t = \frac{d - d_{\mathrm{mod}}}{\sigma\sqrt{\dfrac{1}{n}}} \quad (18)$$

where the model value d_{mod} represents the population mean of the test and the value of the experimental data d represents the sample mean. The standard deviation σ is the sorting of the grain-size distribution σ_ϕ. One should note that all the size values in (18) are expressed in ϕ units in order to be compatible with σ_ϕ. The degrees of freedom n are equal to $n_{classes}$ - 1, where $n_{classes}$ is the number of size classes in the grain-size distribution. At this point PYFLOW performs a two-tails test; by default the significance level of the statistical test is set to 0.05, but the user can set a different value. If the t-test succeeds, d_{mod} is an appropriate model of the experimental data, meaning that the initial assumption that $2\ kg\ m^{-3} < \rho_f < 100\ kg\ m^{-3}$ is reasonable and the model results are a significative solution of actual deposit data. The t value at the significant level of 0.05 is known and tabulated but, as PYFLOW allows one to change the significance level, the code searches for the t value from the cumulative t distribution:

$$p(t) = \frac{B\left(\dfrac{t + \sqrt{t^2 + n}}{2\sqrt{t^2 + n}}, \dfrac{n}{2}, \dfrac{n}{2}\right)}{B\left(\dfrac{n}{2}, \dfrac{n}{2}\right)} \quad (19)$$

where B is the Beta function. Eq. 19 is solved with Brent's method of bisection (Press et al., 1996). After the t-test, model results are normalized to experimental data. By substituting $C_d/davg$ into eq. 13 an average model density $\rho_{f,mod}$ is obtained. Next, the settling velocity of the particles calculated with d_{mod} and the experimental d are equated:

$$\frac{4gd\left(\rho_s - \rho_{f,norm}\right)}{3C_d\rho_{f,norm}} = \frac{4gd_{\mathrm{mod}}\left(\rho_s - \rho_{f,\mathrm{mod}}\right)}{3C_d\rho_{f,\mathrm{mod}}} \quad (20)$$

In (20) the only unknown is $\rho_{f,norm}$, which is the flow density normalized to the experimental data. This density is substituted in eq. (13) to get the normalized ratio $C_d/dnorm$ that is in turn used in eq. 14 to get the normalized squared shear velocity $u_{*\,norm}^2$. The shear stress associated to $u_{*\,norm}^2$ and $\rho_{f,norm}$ are then used in (9) to calculate the average value of the shear stress τ_{avg}.

Once the average values of shear velocity, flow density and shear stress are known, PYFLOW defines an interval of variation equal to ±1 unit of standard deviation around the average, corresponding to the maximum and minimum acceptable model solutions, respectively. In a Gaussian distribution the range enclosed in this interval corresponds to a probability of 68%, 34% on the left and 34% on the right of the average. This range is considered as covering a significant spectrum of model solutions for the obtainment of a statistic range of impact parameters to be used for hazard assessment. By using this standard, PYFLOW calculates the interval by subdividing the total area subtended by the function of C_d/d vs. u_*^2 into two parts, one on the left and one on the right side of the average value. If one assigns to each part 100% of probability and calculates the total area on that part with the following equation

$$\frac{C_d}{d} = \int\limits_{u_*^2(100kg/m^3)}^{u_*^2avg} \frac{4g\left(\rho_s - \dfrac{\theta g d_1 \rho_{s1}}{u_*^2 + \theta g d_1}\right)}{3u_*^2\left(\dfrac{\theta g d_1 \rho_{s1}}{u_*^2 + \theta g d_1}\right)} du_*^2 \quad (21)$$

it turns out that 68% of this quantity represents the C_d/d value corresponding to 34% of the probability to the left of the average, C_d/d_{left}. With the same approach the right value C_d/d_{right} is calculated. Upon substituting C_d/d_{left} and C_d/d_{right} in eq. 14 the corresponding squared shear

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velocities, i.e. $u_{*\,min}^2$ and $u_{*\,max}^2$ respectively, are obtained. Again Brent's method of bisection is used for solving this non-linear equation. Using these values together with the corresponding C_d/d values, the associated minimum and maximum densities ($\rho_{f,min}$ and $\rho_{f,max}$) and the minimum and maximum shear stresses (τ_{min} and τ_{max}).

2.5. Two-components model

As previously stated, the complete sequence of layers involving both the coarse particles moved at the base (which are generally found in proximal locations, Dellino et al. (2008)), and the overlying laminated layer can be not found in the deposit stratigraphy. Frequently, the coarse layer (A in fig. 1b) is lacking from the bed-set (especially in distal localities), thus preventing the application of the Shield criterion (eq. 5). Anyway it is still possible to apply the model even if only the laminated layer is present (B in fig. 1b). The laminated layer is composed of different types of particles (components) having different densities, grain sizes and shapes. Since all the components in a lamina are deposited at the same flow conditions and the same settling velocity, one may assume that aerodynamic equivalence exists between the different components. By considering, for example, juvenile particles and loose crystals, the following equations hold:

$w = w_{xx}$ (22)

leading to:

$$u_*^2 = \frac{4gd(\rho_s - \rho_f)}{3C_d\rho_f} = \frac{4gd_{xx}(\rho_{s,xx} - \rho_f)}{3C_{d,xx}\rho_f} \quad (23)$$

where the subscript xx refer to crystals while no subscript is used for the juvenile parameters, in agreement to the previous section.

By simplifying eq. 23, the ratio C_d/d can be obtained for this method:

$$\frac{C_d}{d} = \frac{C_{d,xx}(\rho_s - \rho_f)}{d_{xx}(\rho_{s,xx} - \rho_f)} \quad (24)$$

and an equation of C_d/d as a function of u_*^2 is obtained:

$$\frac{C_d}{d} = \frac{g\left(\dfrac{3C_{d,xx}\rho_s}{gd_{xx}} + \dfrac{4(\rho_s - \rho_{xx})}{u_*^2}\right)}{3\rho_{xx}} \quad (25)$$

Eq. 24 and 25 play the same role as eq. 13 and 14 of the two layer method of Section 2.4. The procedure then follows the same steps. It is to note that also lithic components can be used for solving the system of equations, assuming that a careful estimation of their physical characteristics is made, which sometimes is more difficult than for ashy glass grains or crystals, since lithics can show a wider variation of density and shape characteristics.

2.6. Flow stratification model

The density of the shear current obtained with any of the two model discussed so far is the average value of the density profile from the base of the current to the height at which flow density becomes equal to atmospheric density (top of the shear current). Actually, it is a function of particle concentration and gas density (eq. 3). From (3), upon assuming a gas density, the average particle concentration C in the shear current is readily obtained. If one assumes that the particle settling rate is constant during the formation of the whole laminated layer, the total height of the flow z_{tot} can be obtained by the ratio between C and the laminated layer total thickness z_{lam}. Is is worthily noting that the average concentration varies according to the flow density calculated previously, this in turn affects the range of variation of the flow thickness z_{tot}.

The shear current is composed of gas and a mixture of particles, in which those with $P_n = 2.5$ are at settling condition. Finer particles are held in suspension by turbulent stress and contribute to the concentration profile $C(z)$, but their average Rouse number $P_{n,susp}$, which is lower than 2.5, is still unknown. Also, the thickness of the shear flow z_{sf} is unknown. In order to get these two unknowns, a system of two equations can be written:

$$\rho_{atm} = \rho_g + \left((\rho_s - \rho_g)C_0 \left(\frac{z_0}{z_{tot} - z_0} \frac{z_{tot} - z_{sf}}{z_{sf}} \right)^{P_{n,susp}} \right) \quad (26)$$

$$\rho_f = \frac{1}{z_{sf} - z_0} \int_{z_0}^{z_{sf}} \rho_g + \left((\rho_s - \rho_g)C_0 \left(\frac{z_0}{z_{tot} - z_0} \frac{z_{tot} - z}{z} \right)^{P_{n,susp}} \right) dz \quad (27)$$

The first equation states that the atmospheric density is reached at the top of the shear flow z_{sf}; the second one defines the average flow density calculated between z_0 and z_{sf}. The solutions are seeked via the iterative Newton-Raphson method for non-linear systems of equations. This system of equation is solved in two different steps:

1) first, by setting $z_0 = z_{lam}$, and considering the average solutions of z_{tot} and ρ_f, the system is solved to find the average shear flow thickness $z_{sf,avg}$ and the average solution of the Rouse number $P_{n,susp,avg}$. After the average values of the Rouse number and of the shear flow thickness have been determined, by knowing the average shear stress and flow density found previously, the slope α of the substrate over which the DPDC was moving can be calculated by:

$$\tau = (\rho_f - \rho_{atm})g \sin \alpha z_{sf} \quad (28)$$

2) Once the average values of the shear flow thickness, the Rouse number and the slope are found, from the same system it is possible to calculate the maximum and the minimum solution of z_0 and $P_{n,susp}$. For the maximum solutions ($z_{0,max}$ and $P_{n,susp,max}$), the flow density is set equal to the previously calculated maximum solution $\rho_{f,max}$. Then, the corresponding shear flow thickness is calculated by (28). Since at the maximum density corresponds the minimum shear velocity (Dellino et al. 2008), $\tau = \tau_{min}$ when $\rho_f = \rho_{f,max}$. Thus, the shear flow thickness in this case is the minimum value, $z_{sf,min}$. Also the total flow thickness is set equal to its maximum solution. For the minimum solutions ($z_{0,min}$ and $P_{n,susp,min}$) the procedure is the same but the opposite values are used.

The atmospheric density is set equal to 1.22 kg m^{-3}, and for ρ_g the density of steam at 300 °C is used, as it is considered as a reasonable value for DPDCs (Dellino et al., 2008).

It is now possible to create the profiles of the DPDC parameters; for each variable, an average, maximum and minimum solution profile is created. Concentration, density, velocity and dynamic pressure profiles are calculated by using (1), (3) and (4), respectively. It is now possible to calculate the dynamic pressure profile:

$$P_{dyn}(z) = \frac{1}{2} \rho_f(z) u^2(z) \quad (29)$$

PYFLOW calculates and stores the profiles in separate output files. Furthermore it calculates specific dynamic pressures at different heights (10 m by default and at user requested heights), i.e. the dynamic pressure averaged over the height:

$$P_{dyn,sp} = \frac{1}{z_{sp} - z_0} \int_{z_0}^{z_{sp}} \frac{1}{2} \rho_f(z) u^2(z) dz \quad (30)$$

where z_{sp} is the chosen height. Also in this case the parameter is calculated for the average, maximum and minimum solutions. This is an important choice for hazard assessment: the default value of 10 m is typical of small-medium buildings; PYFLOW allows to select other heights, which can be more suitable for the hazard assessment of a specific area.

2.7. Probability functions of the impact parameters

For each fluid dynamic variable of the DPDC, PYFLOW calculates three solutions: average (corresponding to the 50th percentile), maximum (68th percentile) and minimum (34th percentile). From these values it builds probability functions with the aim to calculate, for each studied DPDC, the value of the variable (e.g. dynamic pressure, particle concentration at a specific height, etc.) at the percentile of interest.

As a reference probability distribution, PYFLOW employs the Gaussian distribution:

$$f(y) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(y-\mu)^2}{2\sigma^2}} \quad (31)$$

This choice is based both on the fact that the general model starts from a statistical test (see the Student-t test illustrated in section 2.4) on grain size data, which generally show a Gaussian tendency when expressed in phi units, and also that generally continuous (random) physical variables show a Gaussian tendency. In order to allow the variables solution distribution to conform to the standardized Gaussian distribution, first the 84th and 16th percentile values where rendered symmetrical around the mean. By indicating the average, maximum and minimum solutions with μ, max and min, respectively, the best value for the symmetrization parameter ms is searched for satisfying the following relationship:

$$max^{ms} - \mu^{ms} = \mu^{ms} - min^{ms} \quad (32)$$

Eq. 32 has two solutions, among which 0 (the trivial solution) is discarded. PYFLOW then searches for the other solution with Brent's method of bisection (Press et al., 1996). The new distribution parameters can be calculated by using ms:

$$\mu_{simm} = \mu^{ms} \quad (33)$$

$$\sigma_{simm} = max^{ms} - \mu^{ms} = \mu^{ms} - min^{ms} \quad (34)$$

where μ_{simm} and σ_{simm} are the median and the standard deviation of the symmetrized probability function, respectively. Using these parameters it is possible to calculate the variable value y linked to a desired probability $p(y)$ via the standardized normal distribution Z ($\mu = 0$, $\sigma = 1$). Indeed, given a probability, the corresponding standardized variable Z_{std} is readily obtained by the tabulated values. Actually PYFLOW uses the cumulative distribution function for the Z distribution:

$$p(Z_{std}) = \frac{1}{2}\left(1 + erf\frac{Z_{std}}{\sqrt{2}}\right) \quad (35)$$

where erf is the error function. Once Z_{std} is found (again by using the Brent's method), and given the standardization formula:

$$Z_{std} = \frac{y - \mu_{simm}}{\sigma_{simm}} \quad (36)$$

the value of the variable is readily obtained:

$$y = \sigma_{simm}Z_{std} + \mu_{simm} \quad (37)$$

The output of PYFLOW provides the symmetrization parameter ms, μ_{simm} and σ_{simm} for each variable. Then it gives out the variables values at the desired probabilities, which the user provides in the command line when requested. The detailed procedure will be discussed in Section 4.2.

3. Solution algorithm

PYFLOW is structured in different, separate, subroutines called by the main program `main`. The basic program structure is shown in fig. 3.
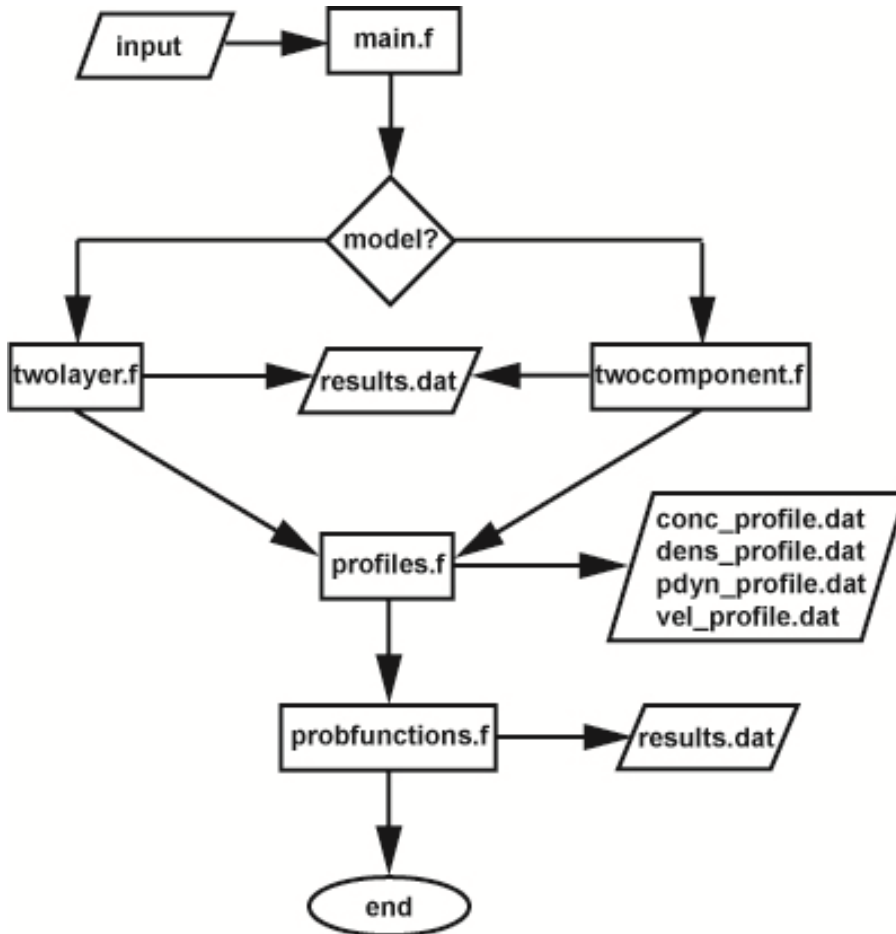
Fig. 3: simplified flowchart of PYFLOW.

The main routine defines the variables, open results and log files (`results.dat`, `con_profile.dat`, `dens_profile.dat`, `vel_profile.dat`, `log.dat`) and reads the input file `input`. Input data can be read alternatively from command lines or from an input file, that must be structured as explained in Section 4.2.1. Depending on the user's choice (i.e. available data) PYFLOW calls the routine `twolayer` or `twocomponent` (see Section 2.4 and 2.5, respectively). The transfer of input data and results between the main block and the subroutines is performed via common block statements. `main` writes the results in the `results.dat` file and then calls the routine `profiles` (Section 2.6), which calculates the vertical profile of the fluid-dynamic variables (dynamic pressure, velocity, etc.) and writes the results in the corresponding data files. Finally the routine `probfunctions` is invoked for defining the probability functions as explained in Section 2.7.

There are other external routines invoked several times from the program. The routine `testt` performs the t-Student test of the model solution (Section 2.4); `qtrap` calculates numerically the definite integral of a function with the trapezoidal rule (Press et al., 1996); `zbrent` is the function that solves the non-linear equations via the Brent's method (Press et al., 1996), invoked in `testt`, `twolayer`, `twocomponent` and `probfunctions` routines. `newt` is the routine that solves the

system of non-linear equations (26) - (27) with the Newton-Raphson iterative method (Press et al., 1996); this routine uses also the module `fminln`.

Other modules are necessary for compiling and running PYFLOW. `inputdata` stores the used constants (e.g. gravitational acceleration, gas viscosity, etc.) and defines the variables for the input data. The modules `nrtype`, `nrutil` and `nr` are available in the literature (Press et al., 1996) and invoked from the numerical recipes routines (e.g. `newt`); they define data types and stores libraries of functions (e.g. the Beta function used in (19)).

Typical computational times range between 5 to 10 minutes, the most time-consuming routine being newt, which solves iteratively the system of equations (26) and (27).

4. Program setup and execution

4.1. Installation

The package contains all the routines presented in the previous section, each one in a separate .f90 file. The user has to compile the Fortran files and build the executable. In order to simplify this operation, a script file (named `Makefile`) is also included in the package. The script has to be invoked with the freeware Gnu Make software. The user should only run the Make program in the folder in which all the source files and the script are stored by typing `make`. The command `make clean` deletes some files created during the compilation: `.mod` and `.o`.

4.1.1. Linux

In Linux operating systems Make should be installed by default, otherwise the user can download and install the program with the package manager specific of the OS or by typing the proper command on the command shell (e.g. `apt-get install` for Ubuntu, `yum` for Fedora, etc.). The command `which make` gives information on whether and where Make is installed.

The Makefile is written assuming that Gfortran compiler is used. If this is not the case, the user can edit the second line of the Makefile by replacing "gfortran" with the proper command invoking the desired compiler.

4.1.2. Windows and Mac OS

For Windows and Mac operating systems the user can find the make executable on Internet. For these OSs only the executable is available, which has to be placed in the same folder where the Makefile script and the source code are. The other possibility is to work with a Linux emulator (e.g. Cygwin for Windows).

4.2. Execution

The compilation produces the executable file `pyflow.exe`. The execution is launched by typing the proper command on the command prompt (`./pyflow.exe` for Linux or Linux emulators for Windows and Mac OS, `pyflow.exe` or simply `pyflow` in the Windows command prompt). Once launched, the program asks for the model (two layer or two components) to be used (fig. 4). The user should type 1 for two layer model, 2 for two component model. Any other type will cause an error message to be displayed, then the user can choose again.

Fig. 4. Screenshot of the command prompt during PYFLOW execution. Here the two components model is chosen.

After this choice, the programs asks for the method of data input (fig. 4). By typing 1 the program reads the input data file (see next section), while 2 lets the program to ask the data one by one with the keyboard. The first choice is recommended, as with the second possibility the chance to make mistakes is way higher. Anyway the program always displays a data summary that the user can check, and asks if the provided input data are correct (fig. 5).

Fig. 5. Screenshot of the command prompt during PYFLOW execution. Here the input data are listed for checking. The program asks if the data are correct before to proceed.

If the user confirms that data are correct (by typing 1), the calculations start. First temporary results are displayed, together with the residuals of the calculations performed via iterative methods (fig. 6):

Fig. 6. Screenshot of the command prompt during PYFLOW execution. Here the first results are displayed, together with the residuals of the calculation of the *t* value at a given level of significance (eq. 19).

The name of the chosen method is again reported; then the values of $C_d avg$ for the first component (here C_d1, using an equation analogous to eq. 16), the ratios C_d/d at the two different flow densities ($C_d/d(2 \ kg/m^3)$ and $C_d/d(2 \ kg/m^3)$, eq. 24), the values of the corresponding squared shear velocities ($ush^2(2 \ kg/m^3)$ and $ush^2(2 \ kg/m^3)$, eq. 25), the average C_d/d ratio ($C_d/d \ avg$, using an equation analogous to eq. 15), the average drag coefficient of the second component (C_d2), the model diameter (d_{mod}) of the second component in meters (by default the second component is the less dense one, *d2mod (m)*, eq. 17 converted in meters) and the model diameter of the second component in phi units (*d2mod (phi)*, eq. 17) are displayed. Afterwards the t-Student test is performed, for which the *t* value at the level of significance of 0.05 is calculated by eq. 19 with the Brent's method. The residuals are displayed, as the convergence criterion is based on two parameters (see Press et al. (1996) for details): one has to be equal to 0 (second column), or the other must be less than the selected tolerance value (first column). By default the tolerance is set to about 10^{-15} for the Brent's method; the user can change this value by editing the source code in `zbrent.f90` file. Once the *t tabulated* value is calculated, this is compared to the calculated value (eq. 18) (which is reported as *t calculated*) and, if this is less than the tabulated value, the test succeeds and the message *Test t OK* is displayed. If not, the user is asked for either reducing the level of significance and retry (thus reducing the significance of the results) or stop the calculations. After this fundamental step, the calculations continue and the model density $\rho_{f,mod}$ (*Denmod* in fig. 7), the flow density normalized to real data $\rho_{f,norm}$ (*Den norm*), $C_d/dnorm$, the normalized squared shear velocity (*ush^2 norm*) (see Section 2.4) are displayed.

Fig. 7. Screenshot of the command prompt during PYFLOW execution. Here data normalized to real data and first maximum and minimum solutions for shear velocity, density, concentration and total flow thickness are shown.

As previously explained, for the calculation of squared shear velocity Brent's method is used, thus again the residuals are shown. Once the maximum and minimum solutions for the squared shear velocity are found, the corresponding C_d/d values (*Cd/d(ush^2 min)*, *Cd/d(ush^2 max)*) and the associated minimum and maximum densities (*Den(Cd/d(ush^2 min))* and *Den(Cd/d(ush^2 max))*) are calculated and written. With the method explained in Section 2.6 the particle concentration (the solutions corresponding to different percentiles, *C 50th*, *C 84th*, *C 16th*) and the corresponding total flow height (*Htot 50th*, *Htot 84th*, *Htot 16th*) are computed. After these parameters are calculated, it is possible to solve the system of equations 26 and 27 with the Newton-Raphson iterative method. During the iterations the code displays the calculation residuals. The execution of the Newton-Raphson iterations stops when one of four residuals calculated in the `newt` subroutine is less than a fixed value (Press et al., 1996). These residuals are displayed continuously during the iterations; they are named `res1`, `res2`, `res3`, `res4`. The first two are actually identical, but calculated in different parts of the Newton-Raphson routine. The conditions to be satisfied at convergence are, sequentially:

1) `res1` < TOLF = 10^{-4}
2) `res2` < TOLF = 10^{-4}
3) `res3` < TOLMIN = 10^{-6}
4) `res4` < TOLX = machine dependent value

In fig. 8 a part of the residuals displayed during the calculation of the average $P_{n,susp}$ (*Pnsusp avg*), α (*Slope (°)*) and z_0 (*z0avg*) is shown:

Fig. 8. Screenshot of the command prompt during PYFLOW execution. Here the residuals of the calculations of the average values of Rouse number of the particle in turbulent suspension $P_{n,susp}$, reference height z_0 and slope α are shown. Results are then displayed when the solution converged.

The same output is displayed for the maximum and minimum solutions of $P_{n,susp}$ (*Pnsusp max*, *Pnsusp min*) and z_0 (*z0max*, *z0max*).

As already stated in Section 2.6 an average value of the dynamic pressure integrated over an height of 10 m for each solution (average, maximum and minimum) is calculated by default. The code asks the user to provide other heights if wanted (fig. 9). The program also calculates the particle volumetric concentration at $z = 2\ m$ and the user can choose another height if needed. The input of the additional heights can be stopped by typing "stop" on the keyboard; any other input will let the program to ask for another value.

Fig. 9. Screenshot of the command prompt during PYFLOW execution. Here the user is asked to provide other heights for the calculation of the average dynamic pressure and particle volumetric concentration, if wanted.

After these inputs, the program shows a summary of the results (fig. 10):

Fig. 10. Screenshot of the command prompt during PYFLOW execution. Here the summary of the results is reported.

Average, maximum and minimum solutions for flow density ρ_f, total flow thickness z_{tot}, shear flow thickness z_{sf}, shear velocity u_*, shear stress τ, average specific dynamic pressure (10 m) $P_{dyn,sp}$ and particle volumetric concentration at 2 m C are listed. Below the user requested outputs are displayed, with the chosen height (e.g. $z = 5\ m$) and the solutions (average, maximum and

minimum, together with the effective percentiles, as sometimes the 84th percentile solution is not the maximum solution due to the crossing of the profile curves, see Section 4.2.4). After these outputs, the program displays also a summary of the t-Student test results (fig. 11).
Once all the solutions have been found, PYFLOW starts to build the probability functions of the impact parameters (Section 2.7). Eq. 32 is solved for calculating the symmetrization parameter *ms* for the specific dynamic pressure at 10 m and the particle volumetric concentration at 2 m; furthermore, it is calculated also for the user-requested outputs. An example of the temporary results displayed on the screen is shown in fig. 11:

Fig. 11. Screenshot of the command prompt during PYFLOW execution. Here the summary of the t-Student test, the residuals of *m* calculation and the value of *ms*, μ_{simm} and σ_{simm} are listed.

The symmetrization exponent is searched on the right and on the left of the trivial solution 0; if the solution cannot be found on one side of 0, it searches it on the other side. In very rare cases there is no solution other than 0, thus preventing to calculating the probability functions. Once the symmetrization exponent is calculated, it is shown, together with the new median μ_{simm} and standard

deviation σ_{simm} of the symmetrized distribution. The output on fig.11 is the same also for the particle concentration at 2 m and for the user requested height.

Once the probability functions have been built, the user can calculate the value of the impact parameters at the desired percentile. Two examples are shown in fig. 12.

Fig. 12. Screenshot of the command prompt during PYFLOW execution. Here the function values at the desired percentile are calculated.

After the user chooses to calculate the function values, the probability function can be selected by typing the corresponding number. In fig. 12 the specific dynamic pressure at 10 m is chosen; then, the user should write the percentile and the program calculate the corresponding Z_{std} value (eq. 35) while it displays the residuals. Finally the function values is calculated by (37) and shown and, if the user doesn't want to calculate other function values, the program stops.

4.2.1. The input data file

The user can provide the input data via command lines or by editing the input data file, named `input`. The file must be structured as in the following example:

```
2570
0.08
3283
0.4
1.71
0.559
14
1750
1.286
1.54
0.47
18
0.05
0.2
0
0.75
0.04
```

The user can follow the instructions reported in the file `Input_instructions.txt`, in which the meaning of each line is explained. A further explanation follows here.

`Density of the entrained particle (kg/m^3):` ρ_{s1}. This value is ignored by the code if the two components method is used. Anyway, and hereafter, the user must write a number even if the value is ignored, in order to not alter the structure of the input file that PYFLOW can read in this version.

`Diameter of the entrained particle (mm):` d_1. Together with the previous value, this is used in the two layer method and it is ignored if the other method is chosen.

`First component density (kg/m^3):` put the density of the first component if the two components method is used, otherwise the code ignores this value. PYFLOW stores the first component as the denser one, thus the user should put the parameters of the denser component in the "first component" part of the input file. Anyway PYFLOW checks if this condition is satisfied, otherwise it exchanges the values.

`First component particle equivalent diameter of the median size (mm):` put the particle equivalent diameter of the median size of the grain-size distribution in mm (not in phi units!).

`First component sorting particle grainsize distribution (phi):` this value must be entered in phi units.

`First component particle shape factor (-):` particle shape factor of the first component calculated with the procedure explained in Dellino et al. (2005).

`First component classes number of the grainsize distribution (-):` number of the classes in the grain-size distribution of the first component.

`Second component density (kg/m^3):` the second component is the less dense component when the two components model is used; if the two layer model is used, it is the component for which the suspension-sedimentation criterion is applied.

`Second component particle equivalent diameter of the median size (mm):` as for the first component.

`Second component sorting particle grainsize distribution (phi):` as for the first component.

`Second component particle shape factor (-):` as for the first component.

`Second component classes number of the grainsize distribution (-):` as for the first component.

`Significance level t-test`: significance level for the t-Student test. A two-tailed test is performed, but the user must write the total significance level (i.e. of both the tails).

`Layer thickness (m)`: thickness of the laminated layer z_{lam} of the DPDC deposit.

`Sublayer thickness (m)`: thickness of the sublayer z_0; if it's not possible to evaluate it on the deposit, the user must write "0" and PYFLOW set z_0 equal to the diameter of the particles of the less dense component (e.g. juvenile).

`Particle concentration in the layer (-)`: usually C_0 is assumed to be 0.75, but it's possible to set different values.

`Substrate roughness (m)`: the substrate roughness k_s can be measured on the field; for example it can be taken as half of the diameter of the coarse particles lying on the substrate or that are at onset of entrainment.

4.2.1.a `grainsize` program

The `grainsize` program is an additional utility that can be requested separately. The program calculates the median Md_ϕ and sorting σ_ϕ of a given grain-size distribution. It also allows to carry out a Chi-squared test for checking the compatibility of the grain-size distribution with a normal Gaussian curve.

The input data must be entered via an input file, named `input_grainsize.dat` that has to be arranged as explained in the file `Input_instructions_grainsize.txt`, which is reported below:

`Phi interval`: the interval of the grain-size distribution in phi units (e.g. 0.5, 1, etc.).

`Phi min`: the minimum phi value for which the weight is larger than 0.

`Phi max`: the maximum phi value for which the weight is larger than 0.

`Hereafter write the weights for each class, in one column **********Caution! Use . not ,!!!*********************:grain-size` can read real numbers with the decimal point "."; "," is not permitted.

Below an example of an edited `input_grainsize.dat` file

```
0.5
-2.5
5
0.26
0.39
0.33
0.19
0.19
0.16
0.11
0.09
0.07
0.07
0.07
0.17
0.25
0.20
0.12
0.02
```

The distribution has a phi step (interval) equal to 0.5; it starts from -2.5 phi and ends at 5 phi. Then the weights are listed.
Once the program has been launched, it reads the input data and displays them as shown in fig. 13:

Fig. 13. Screenshot of the command prompt during `grainsize` execution. Here the input data are listed.

The input data are listed in four columns: weight in grams (*Wt. (g)*), weight fraction (*Wt.%*), fractional cumulative weight (*Fr.Cum.Wt*) and cumulative weight in % (*Cum.Wt.%*).
Then the program calculates the median Md_ϕ and sorting σ_ϕ; the median corresponds to the 50th percentile of the distribution (ϕ_{50}), while the sorting is defined as in Inman (1952):

$$\sigma_\phi = \frac{\phi_{84} - \phi_{16}}{2} \quad (38)$$

where ϕ_{84} and ϕ_{16} are the 84th and 16th percentile, respectively. As the reader can readily see in the last column of fig. 13, an interpolation procedure is necessary for finding the ϕ value corresponding to a definite percentile. This is possible by using a known probability distribution; in this case a standardized normal distribution is used (eq. 35), although it is assumed that the experimental distribution is not significantly different from a Gaussian distribution (see below). Let's consider the 50th percentile; the program searches the ϕ interval in which the 50th percentile lies (between ϕ_{inf} and ϕ_{sup}, to which the corresponding cumulative weight fractions are $wt(\phi_{inf})$ and $wt(\phi_{sup})$). By solving eq. 35, the Z_{std} values corresponding to $wt(\phi_{inf})$ and $wt(\phi_{sup})$ ($Z_{std,inf}$ and $Z_{std,sup}$) are defined; then the Z_{std} values corresponding to the percentile is found ($Z_{std,pct}$). In `grainsize` eq. 35 is solved with the numerical recipe `rtflsp`, which uses the false position method (Press et al., 1996). After these parameters have been calculated, it is possible to calculate ϕ_{50} by interpolating the extreme values with a straight line, whose slope is:

$$m_\phi = \frac{Z_{std,sup} - Z_{std,inf}}{\phi_{sup} - \phi_{inf}} \quad (39)$$

Then ϕ_{50} is readily obtained:

$$\phi_{50} = \phi_{inf} + m_\phi \left(Z_{std,50} - Z_{std,inf} \right) \quad (40)$$

where $Z_{std,50}$ is the Z_{std} value corresponding to the 50th percentile.
The residuals of the calculation of the various Z_{std} are continuously displayed on the command prompt (fig. 14).

Fig. 14. Screenshot of the command prompt during `grainsize` execution. Here the residuals of the Z_{std} values for the calculation of ϕ_{50} are displayed.

The program then asks to choose whether to perform the Chi-squared test or not and if yes the program asks for the significance level (fig. 15). It is recommended to perform the Chi-squared test χ^2, in order to validate or not the resulting median and sorting, which are based on the assumption that the measured grain-size distribution is not different from a Gaussian curve. If the test fails, the program provides anyway the median and sorting value, but the user should be aware that these value are not good estimate of the central tendency parameters. The χ value at a desired significance level is calculated with the probability density formula:

$$f_j(\chi) = \frac{1}{2^{j/2}\Gamma(j/2)} x^{j/2-1} e^{-x/2} \quad (41)$$

where k is the degrees of freedom and Γ is the Gamma function. For details of the Chi-squared test the user can refer to Davies (1986). Eq. (41) is solved with the false position method and residuals are displayed (fig. 15).

Fig. 15. Screenshot of the command prompt during `grainsize` execution. Here the Chi-squared choice is shown, together with the χ calculation residuals.

The program then displays the summarizing table of the test (*ztest*, *Oj*, *Ej*, *(Oj-Ej)^2/Ej*, see Davies (1986)) and writes the result of the test (fig. 16). In this case the calculated χ is larger than the tabulated value, thus the test fails. Consequently the program informs the user that the distribution is significantly different from a normal distribution.

Fig. 16. Screenshot of the command prompt during `grainsize` execution. Here the Chi-squared summary and results, together with the median (*phi50*) and sorting (*sigma*) values are displayed.

The median ϕ_{50} (*phi50*), together with ϕ_{84} (*phi84*) and ϕ_{16} (*phi16*) are listed, with the corresponding sizes in mm (*d50*, *d84* and *d16*). The sorting σ_ϕ is only in phi units.
All the outputs displayed in the command prompt during the execution are saved in a file named `log.dat`.

4.2.3. The log file

As explained in Section 4.2, PYFLOW continuously displays temporary results and residuals of numerical calculations. At the end of the execution it is usually not possible to go back to the first output messages, due to the space limitations of the prompt command shell. For this reason, all the output are stored in a log file, named `log.dat`, which can be examined by the user at any time.

4.2.4. Output files

PYFLOW opens the following output files:
- `results.dat`
- `log.dat`
- `conc_profile.dat`
- `pdyn_profile.dat`
- `vel_profile.dat`
- `dens_profile.dat`

`results.dat` reports the same results as shown in fig. 9, with the addition of the part relative to the probability functions; an example of this part is shown below.

```
###### PROBABILITY FUNCTIONS ######
 10 m dynamic pressure probability function
Symmetrization exponent  -0.452
Median  0.1232E+00
Standard deviation  0.7966E-01


 2 m particle concentration probability function
Symmetrization exponent    0.118
Median  0.3272E+00
Standard deviation  0.9491E-01


  5.00 dynamic pressure probability function
Symmetrization exponent  -0.378
Median  0.1684E+00
Standard deviation  0.9924E-01


  1.50 particle concentration probability function
Symmetrization exponent    0.132
Median  0.3015E+00
Standard deviation  0.8936E-01


 ###### CALCULATION OF FUNCTION VALUES ######
 Dynamic pressure 10 m
Percentile        0.900
Function value      5101.9745
 ###### CALCULATION OF FUNCTION VALUES ######
  1.50  Particle concentration
Percentile        0.600
Function value     0.1970E-03
```

The profiles files are organized in four columns. The first column is the height z in m, with a step-size of 0.01 m. To each height, the corresponding variable values for the three solutions (50th, 84th, 16th percentile) are written in the next three columns. Here a part of the file `pdyn_profile.dat` is given as an example:

Fig. 17. Screenshot of the `pdyn_profile.dat`.

Usually 50th, 84th and 16th percentiles correspond to the average, maximum and minimum solutions, but this is not always the case, especially in the basal part of the flow. Sometimes, at the chosen height, the 84th percentile does not show an higher value than the 50th or the 16th percentiles. This is due to the different gradient of the profiles of the different solutions, which intersect each other at some height, and to the shear stress solutions, which are always very close (fig. 10) and from which the subsequent solutions follow. This is the reason why the three solutions are named with the percentile values.

The file is organized in a way that it is easy to draw plots variable vs. height with the most used programs (e.g. Microsoft Excel, Grapher, Kaleidagraph, GnuPlot, etc.). Two examples drawn with Grapher are shown in fig. 18 and 19.
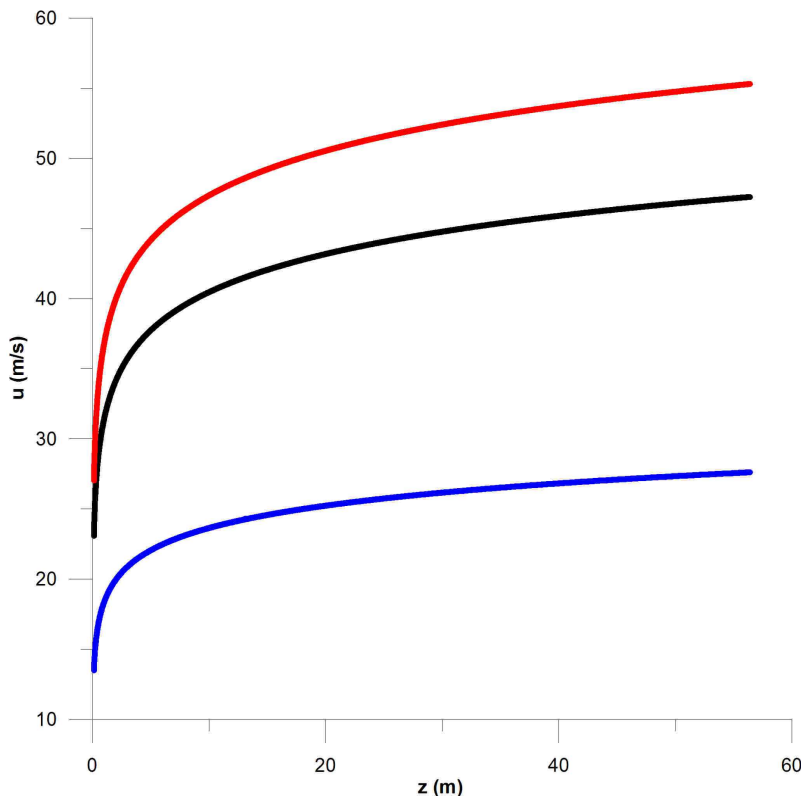
Fig. 18. Velocity *u* vs. height *z*. The black line is the 50th percentile solution, the blue and red lines are the 16th and 84th percentile solutions, respectively.
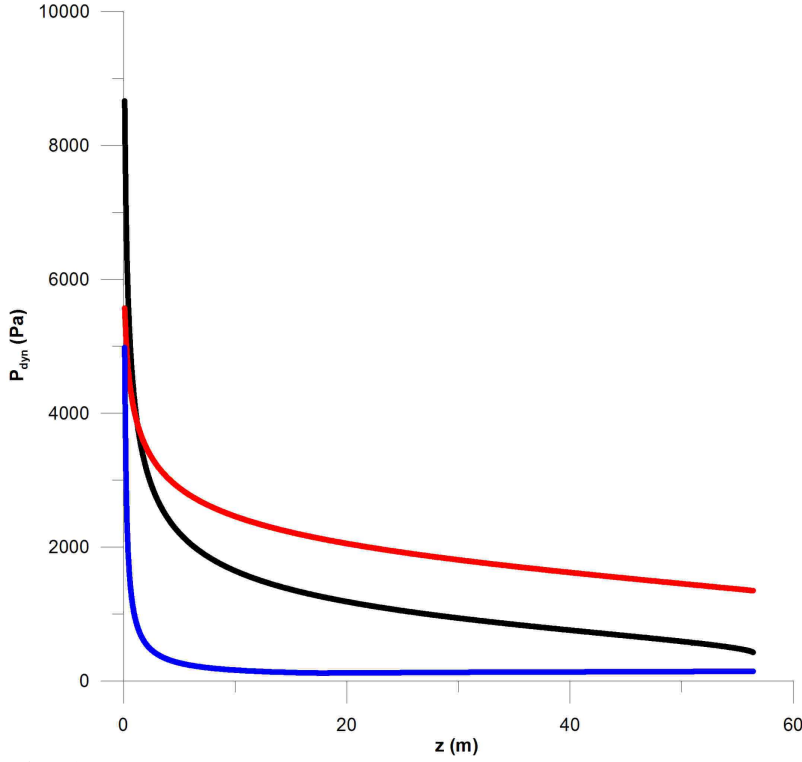
Fig. 19. Dynamic pressure P_{dyn} vs. height z. The black line is the 50th percentile solution, the blue and red lines are the 16th and 84th percentile solutions, respectively.

The velocity curves (fig. 18) follow a logarithmic trend, in agreement to the law of the wall (eq. 4). The dynamic pressure curves (fig. 19) show a steep gradient in the very basal part of the current, then the pressure decreases gently with the height. This is the expected strongly stratified characteristic of DPDCs.

Reference list

Alfano, F., Bonadonna, C., Delmelle, P., Costantini, L., 2011. Insights on tephra settling velocity from morphological observations. Journal of Volcanology and Geothermal Research 208, 86-98, doi:10.1016/j.jvolgeores.2011.09.013.

Branney, M. J., Kokelaar, P., 2002. Pyroclastic Density Currents and the Sedimentation of Ignimbrites. Geological Society, London, Memoirs, 27, 143 pp.

Davies, J. C., 1986. Statistic and Data Analysis in Geology, 2nd ed., John Wiley & Sons, 646 pp.

Dellino, P., Büttner, R., Dioguardi, F., Doronzo, D. M., La Volpe, L., Mele, D., Sonder, I., Sulpizio, R., Zimanowski, B., 2010. Experimental evidence links volcanic particle characteristics to pyroclastic flow hazard. Earth and Planetary Science Letters 295, 314-320. doi:10.1016/j.epsl.2010.04.022.

Dellino, P., Mele, D., Sulpizio, R., La Volpe, L., Braia, G., 2008. A method for the calculation of the impact parameters of dilute pyroclastic density currents based on deposit particle characteristics. Journal of Geophysical Research 113, B07206. doi:10.1029/2007B005365.

Dellino, P., Mele, D., Bonasia, R., Braia, G., La Volpe, L., Sulpizio, R., 2005. The analysis of the influence of pumice shape on its terminal velocity. Geophysical Research Letters 32, L21306. doi:10.1029/2005GL023954.

Dellino, P., Isaia, R., Veneruso, M., 2004. Turbulent boundary layer shear flows as an approximation of base surges at Campi Flegrei (Southern Italy). Journal of Volcanology and Geothermal Research 133, 211-228.

Dellino, P., La Volpe, L., 2000. Structures and grain size distribution in surge deposits as a tool for modelling the dynamics of dilute pyroclastic density currents at La Fossa di Vulcano (Aeolian Islands, Italy). Journal of Volcanology and Geothermal Research 96, 57–78.

Inman, D. L., 1952. Measures for describing the size distribution of sediments. Journal of Sedimentary Research 22-3, 125-145. doi: 10.1306/D42694DB-2B26-11D7-8648000102C1865D.

Furbish, D. J., 1997. Fluid Physics in Geology. Oxford University Press, New York, 476 pp.

Mele, D., Dellino, P., Sulpizio, R., Braia, G., 2011. A systematic investigation on the aerodynamics of ash particles. Journal of Volcanology and Geothermal Research 203, 1-11. doi: 10.1016/j.jvolgeores.2011.04.004.

Middleton, G. V., Southard, J. B., 1984. Mechanics of Sediment Movement, 2nd ed., Society of Economic Paleonologists and Mineralogists, Tulsa, OK, 401 pp.

Miller, M. C., McCave, I. N., Komar, P. D., 1977. Threshold of sediment motion under unidirectional currents. Sedimentology 24, 507–527.

Press, W. H., Teukolsky, S. A., Vetterling, W. T., Flannery, B. P., 1996. Numerical Recipes in Fortran 90. The Art of Parallel Scientific Computing. Volume 2 of Fortran Numerical Recipes. Second Edition, Cambridge University Press, 572 pp.

Rouse, H., 1939. An analysis of sediment transportation in the light of fluid turbulence, in Soil Conservation Services Report No. SCS-TP-25, USDA, Washington, D.C.

Schlichting, H., Gersten, K., 2000. Boundary-Layer Theory, Springer, Berlin, 801 pp.

Sulpizio, R., Dellino, P., 2008. Sedimentology, depositional mechanisms and pulsating behavior of pyroclastic density currents, In: Martì, J., Gottsman, J. (Eds.) Calderas Volcanism: Analysis, Modelling and Response, vol. 10, Developments in Volcanology, Elsevier, Amsterdam, pp. 57-96.

Symbol notation

Latin

Symbol	Description	Units
B	Beta function	-
C	Particle volumetric concentration	-
C_d	Drag coefficient	-
d	Particle equivalent diameter	mm
d_{mesh}	Mesh size in the hand-sieving analysis	mm
erf	Error function	-
g	Gravitational acceleration	m s^{-2}
j	Degrees of freedom in the Chi-squared test	-
k	Von Karman's constant	-
k_s	Roughness parameter of the substrate	m
m	Mass	kg
max	Maximum value of the variable for the probability function	Varying
Md_ϕ	Median size	ϕ
min	Minimum value of the variable for the probability function	Varying
ms	Symmetrization parameter	-
m_ϕ	Slope of the grain-size interpolation function	-
n	Degrees of freedom in the t-Student test	-
$n_{classes}$	Number of size classes in the grain-size distribution	-
p	Probability	-
P_{dyn}	Dynamic pressure	Pa
P_n	Average Rouse number	-
Re	Reynolds number	-
t	t-Student distribution parameter	-
u	Flow velocity	m s^{-1}
u_*	Shear velocity	m s^{-1}
u'	Fluctuating velocity in the stream (x) direction	m s^{-1}
w	Particle terminal velocity	m s^{-1}
w'	Fluctuating velocity in the vertical (z) direction	m s^{-1}
wt	Weight fraction	%
x	Stream direction	m
y	Variable value in the probability function	Varying
z	Vertical direction	m
Z	Standard normal distribution	-
z_{lam}	Thickness of the laminated layer in the DPDC deposit	m
z_{sf}	Shear flow thickness	m
z_{sf}	Shear flow thickness	m
Z_{std}	Standardized variable	-
z_{tot}	Total flow thickness of the DPDC	m

Greek

Symbol	Description	Units
α	Slope of the substrate	°
Γ	Gamma function	-
η	Gas viscosity	Pa s^{-1}
θ	Shield constant	-

μ	Median	-
ρ	Density	kg m^{-3}
σ	Standard deviation	-
σ_ϕ	Sorting	ϕ
τ	Shear stress	Pa
ϕ_{16}	16th percentile of the grain-size distribution	ϕ
ϕ_{50}	50th percentile of the grain-size distribution	ϕ
ϕ_{84}	84th percentile of the grain-size distribution	ϕ
χ	Chi distribution	-
Ψ	Particle shape factor	**-**

Subscripts

Symbol	Description
atm	Atmosphere
avg	Average value
f	Flow
g	Gas phase
max	Maximum value
min	Minimum value
mod	Model value
norm	Value normalized to real data
s	Solid phase (particles)
simm	Simmetryzed parameters
sp	Value specific to a certain height
sph	Equivalent sphere
xx	Crystals
0	Reference level in the DPDC
1	Entrained particle