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### **Calibration strategies of PDC kinetic energy models and their application to the construction of hazard maps**

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1 **Calibration strategies of PDC kinetic models: Implementation on two user-friendly**  
2 **programs (ECMapProb and BoxMapProb) and illustrative applications to El Misti (Peru),**  
3 **Merapi (Indonesia) and Campi Flegrei (Italy)**

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11 **Keywords:** Pyroclastic density currents, volcanic hazard assessment, numerical modeling,  
12 kinetic models, energy cone model, box model, branching formulation.

13 **Highlights**

- 14 • We present a set of structured and reproducible strategies to calibrate PDC kinetic models.  
15 • We implement these calibration strategies on two user-friendly programs: ECMapProb and  
16 BoxMapProb.  
17 • These calibration strategies reduce the biases derived from arbitrary user choices in the  
18 construction of hazard maps.

19 **Abstract**

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<sup>1</sup> **Authorship statement**

All co-authors contributed in the manuscript preparation and the identification of the study cases presented in this paper. AA programmed the models ECMapProb and BoxMapProb, run simulations and post-processed results. AA, AB, MdMV and TEO worked in the mathematical description of the models and the calibration strategies.

20 The availability of computer tools able to describe the behavior of pyroclastic density currents  
21 (PDCs) with uncertainty quantification is of primary importance for the assessment of volcanic  
22 hazard. A common strategy to assess the intrinsic variability of these phenomena is based on the  
23 analysis of large sets of numerical simulations with variable input parameters. The use of models  
24 fast enough to allow for a large number of simulations, such as the so-called kinetic models, is  
25 thus needed. However, due to the sensitivity of kinetic models on poorly constrained input  
26 parameters, the definition of their variation ranges is a critical step in the construction of hazard  
27 maps and a numerical calibration becomes necessary. In this work we present a set of  
28 reproducible and structured calibration procedures of kinetic models based either on a reference  
29 PDC deposit or on the distribution of runout distances or inundation areas of a number of  
30 documented PDCs. In the first case, various metrics can be adopted to compare the numerical  
31 results with the reference PDC deposit (Root mean square distance, Hausdorff distance and  
32 Jaccard index), facilitating the development of scenario-based hazard assessments. On the  
33 contrary, calibrations based on the distribution of runout distances or inundation areas allow  
34 constructing probabilistic hazard maps that are not conditioned on the occurrence of a specific  
35 scenario, but rather reflect the variability of the documented PDCs during the time window  
36 considered. Importantly, our calibration strategies allow setting the kinetic models input  
37 parameters considering their eventual interdependence. These procedures are implemented on  
38 improved, user-friendly versions of the programs ECMapProb and BoxMapProb, whose  
39 functionalities are presented for the first time in this paper. The different calibration strategies  
40 and the functionalities of our programs are illustrated by considering three case studies: El Misti  
41 (Peru), Merapi (Indonesia) and Campi Flegrei (Italy).

## 42 **1. Introduction**

43 Pyroclastic density currents (PDCs) are mixtures of pyroclasts, lithic fragments and gas typically  
44 produced by a lateral blast or by the collapse of an eruptive column or a volcanic dome (Druitt,  
45 1998; Roche et al., 2013; Dufek et al., 2015; Lube et al., 2020). These flows are denser than the  
46 surrounding atmosphere and propagate laterally due to the effect of gravity, being strongly  
47 influenced by the volcano topography. PDCs represent one of the major hazards associated with  
48 volcanic systems, which have been systematically assessed by adopting an approach based on  
49 numerical modeling (Malin and Sheridan, 1982; Neri et al., 2003; Sheridan et al., 2004; Patra et  
50 al., 2005; Kelfoun et al., 2009; Doyle et al., 2010; Esposti Ongaro et al., 2011; 2016; Kelfoun,  
51 2011; de' Michieli Vitturi et al., 2019; Aravena et al., 2020). PDCs pose important modeling  
52 challenges because of their complex propagation dynamics and the uncertainty in their initial  
53 conditions. Due to this uncertainty in the characteristics of future PDCs, a common strategy to  
54 assess the intrinsic variability of these phenomena is based on the analysis of a large number of  
55 simulations (e.g.  $10^4$ - $10^6$ ) with variable input parameters (Neri et al., 2015; Tierz et al., 2016a;  
56 Bevilacqua et al., 2017; Rutarindwa et al., 2019; Patra et al., 2020). Consequently, the use of  
57 tools fast enough to allow for large numbers of simulations, such as the so-called kinetic models  
58 (e.g. energy cone and box model), is required, enabling the quick production of statistically  
59 robust hazard maps without an excessive computational expense. However, because of the  
60 sensitivity of kinetic models on the often poorly constrained input parameters, the definition of  
61 their variation ranges is a critical step in the construction of hazard maps.

62 The absence of common strategies to set the input parameters of kinetic models often limits the  
63 capability to perform comparative analyses between the results derived from different studies  
64 and models. Inter-comparison of models is in fact a critical step in the validation of numerical  
65 tools, as discussed by Esposti Ongaro et al. (2020a), being particularly relevant when these tools

66 are used to define measures of volcanic risk mitigation. We stress that there are similar  
67 difficulties in any numerical model when it is adopted to describe a physical phenomenon  
68 characterized by significant uncertainty (Scollo et al., 2008; Worni et al., 2012; Biass et al.,  
69 2016; de' Michieli Vitturi and Tarquini, 2018; Bevilacqua et al., 2019; Yang et al., 2020), which  
70 appeals to the development of strategies to address this issue.

71 In this context, we present and apply to different case studies a set of reproducible and structured  
72 procedures to calibrate the input parameters of kinetic models based on geological information of  
73 the volcanic system of interest. These calibration strategies allow the reduction of the biases  
74 derived from arbitrary user assumptions in the construction of PDC hazard maps, which are often  
75 necessary due to lack of specific data. The geological information used in these calibration  
76 strategies can be described in terms of the inundation zone of a specific PDC or the distribution  
77 of runout distances or inundation areas of past PDCs. Importantly, these calibration procedures  
78 are implemented in the user-friendly programs EMapProb and BoxMapProb, which are based  
79 on the branching and traditional formulations of the energy cone and the box model, respectively  
80 (Aravena et al., 2020), and whose functionalities and user manuals are presented for the first time  
81 in this paper (see Supplementary Material).

82 This study acknowledges and aims at complementing many previous efforts to set the input  
83 parameters of numerical models based on the eruptive record of volcanoes (e.g. Neri et al., 2015;  
84 Tierz et al., 2016a; 2016b; Ogburn and Calder, 2017; Cioni et al., 2020). We remark that the  
85 purpose of this work is not to compare the suitability of different calibration procedures or  
86 provide new hazard maps for well-documented volcanoes, but to present a set of calibration  
87 strategies that can be used for the quick construction of PDC inundation probabilistic maps and  
88 describe the functionalities of the programs EMapProb and BoxMapProb. We illustrate these

89 calibration strategies by considering three volcanic systems: El Misti (Peru), Merapi (Indonesia)  
90 and Campi Flegrei (Italy).

91 This paper consists of five sections. In Section 2 we describe briefly the numerical models used  
92 in this work and their input parameters. In Section 3 we present a set of reproducible calibration  
93 strategies of the inputs of kinetic models. In Section 4 we show three illustrative applications of  
94 our calibration strategies and, finally, in Section 5 we present a summary and the conclusion of  
95 this paper.

### 96 **1.1 Setting the Input parameters of kinetic models: historical background**

97 In the case of the energy cone model, where input parameters are collapse position ( $Q_{0,0}$ ),  
98 collapse height ( $H_{0,0}$ , hereafter defined with respect to the topography) and the energy cone slope  
99 ( $\tan(\varphi)$ ), several efforts have been devoted to constrain  $\tan(\varphi)$  (Hsu, 1975). Sheridan and  
100 Macías (1995) studied the deposits of pyroclastic flows at Colima volcano (Mexico) showing  
101 that  $\tan(\varphi)$  is influenced by the pyroclastic flow size. Hayashi and Self (1992) also found a  
102 negative correlation between  $\tan(\varphi)$  and flow volume. The statistical correlation between flow  
103 volume and  $\tan(\varphi)$  was further investigated and quantified in Spiller et al. (2014) and Ogburn et  
104 al. (2016). These papers have allowed constraining only partially the expected variability of  
105  $\tan(\varphi)$ , and thus additional assumptions are needed to set this input parameter. Regarding the  
106 parameter  $H_{0,0}$ , it is worth noting that numerical simulations of 3D multiphase flow models (e.g.  
107 Esposti Ongaro et al., 2020b) have shown that column collapse height is virtually irrelevant in  
108 the determination of the flow runout. This is consistent with fieldwork evidence (Tadini et al.,  
109 2021) and results derived from integral inertial models. Consequently, the common interpretation  
110 of  $H_{0,0}$  as a measure of the collapse height may be misleading in PDCs derived from collapsing

111 columns, and thus  $H_{0,0}$  has to be considered as a model parameter for which a numerical  
112 calibration becomes necessary.

113 In practice, to deal with the problem of setting the input parameters of the energy cone model,  
114 many strategies have been applied during the last decades, and the use of vent opening maps is  
115 not uncommon. For instance, Alberico et al. (2002) adopted the energy cone model to study PDC  
116 propagation at Campi Flegrei (Italy) using a vent opening probability map to define a set of  
117 likely collapse positions. In these simulations, input parameters were arbitrarily imposed  
118 defining two scenarios that roughly reflect the typical runout distance of small and large-scale  
119 PDCs in this volcanic system. Other examples where  $H_{0,0}$  and  $\tan(\varphi)$  were imposed  
120 deterministically are Macías et al. (2008) and Ferrés et al. (2013). Among the examples where a  
121 Monte Carlo strategy was used to sample input parameters, it is worth mentioning Tierz et al.  
122 (2016b), who performed an analysis of the inundation area and runout distance of past PDCs at  
123 Vesuvius and Campi Flegrei, and defined independent probability distributions for the inputs of  
124 the energy cone model. Other examples where a Monte Carlo approach was applied are Sandri et  
125 al. (2018) and Clarke et al. (2020).

126 Regarding the definition of the box model input parameters, it is worth citing Neri et al. (2015),  
127 who studied the geological record of Campi Flegrei to define probability distributions of the  
128 inundation area of past PDCs and then they used these data to compute the input conditions (in  
129 particular, the flow volume) of a set of simulations through an iterative method of numerical  
130 inversion (Bevilacqua, 2016). In addition, Neri et al. (2015) used the vent opening probability  
131 maps from Bevilacqua et al. (2015) for the construction of fully probabilistic maps of PDC  
132 inundation at Campi Flegrei. Their findings were further extended by Bevilacqua et al. (2017),  
133 who detailed the joint effects of vent position, PDC scale, and temporal eruption rates. In

134 summary, both Neri et al. (2015) and Bevilacqua et al. (2017) considered the inundation area as a  
135 random variable whose definition is based on the vent location and the geological record of  
136 Campi Flegrei, which was therefore used as an input in the box model simulations performed.  
137 On the other hand, Tadini et al. (2021) constrained the input parameters of the box model for two  
138 significantly different PDC units of the AD 79 Vesuvius eruption, focusing on the average  
139 reconstruction of deposit thickness (Cioni et al., 2020) as a function of the distance from the  
140 collapse location.

141

## 142 **2. Input parameters of the models**

143 In this section, we briefly describe the input parameters of the traditional and branching  
144 formulations of the energy cone and the box model to frame the presentation of our calibration  
145 strategies. Further details of these models are presented in Huppert and Simpson (1980), Malin  
146 and Sheridan (1982), Sheridan and Malin (1983), Esposti Ongaro et al. (2016), Aravena et al.  
147 (2020) and in references therein.

### 148 **2.1 Energy cone model**

149 The energy cone model is a simple and widely used formulation to study PDC dispersal (Malin  
150 and Sheridan, 1982; Sheridan and Malin, 1983; Wadge and Isaacs, 1988). This model describes  
151 the evolution of the kinetic energy of a frictional flow by considering a constant rate of energy  
152 dissipation, which is compared with the potential energy needed to overcome the topographic  
153 obstacles the PDC faces. Consequently, this model suites to dense, frictional granular flows  
154 (Campbell, 2006; Pudasaini and Domnik, 2009). In addition to the collapse position  $Q_{0,0}$ , the  
155 input parameters of this model are: (a) collapse height ( $H_{0,0}$ ), and (b) energy cone slope



156  $(\tan(\varphi) = H/L$ , where  $H$  represents the height difference between the collapse point and the  
157 position of maximum runout and  $L$  is the distance travelled by the PDC). These parameters allow  
158 defining a vertical-axis cone whose interaction with the topography gives rise to an inundation  
159 area, as shown in Figure 1a-b. Because this model does not consider processes of pyroclasts  
160 channelization, an enhanced formulation was presented by Aravena et al. (2020), where a *root*  
161 energy cone is complemented with *branch* energy cones in the preferential channelization  
162 directions of pyroclastic material. *Root* and *branch* energy cones are organized in a tree-like  
163 structure that gives rise to a branching structure (Harris, 1963; Asmussen and Hering, 1983;  
164 Haccou et al., 2005), which is stopped when the *branch* energy cones are not able to increase the  
165 inundation zone of the modeled PDC (in Figure 1 we illustrate graphically how an iterative  
166 procedure is able to increase the inundation area and channelize pyroclastic material).  
167 Importantly, the branching formulation does not add new, unconstrained input parameters and  
168 thus the calibration procedures described below are valid both for the traditional and the  
169 branching formulations.

## 170 **2.2 Box model**

171 The box model integral formulation, based on the pioneering work of Huppert and Simpson  
172 (1980), allows to describe inertial flows such as dilute PDCs (particle concentration of the order  
173 of  $10^{-2}$  or less) and low aspect ratio ignimbrite-forming flows (Walker, 1983). In this model,  
174 friction is assumed to be negligible and the flow propagation dynamics is controlled by the  
175 hydrostatic pressure contrast and by the momentum dissipation due to particle sedimentation.  
176 The input parameters of the box model (Esposti Ongaro et al., 2016) are: (a) collapsing volume  
177 ( $V_0$ ), (b) initial concentration of solid particles ( $\phi_0$ ), (c) Froude number ( $Fr$ ), (d) sedimentation  
178 velocity ( $w_s$ ); (e) solid particles density ( $\rho_p$ ), and (f) ambient gas density ( $\rho_a$ ). These parameters

179 allow defining a vertical-axis conoid centered at the source position that is compared with the  
180 topography in order to calculate the inundation area. In this case as well, a new formulation  
181 based on the construction of additional (or *branch*) conoids in the zones of preferential  
182 channelization was presented by Aravena et al. (2020), which permits to improve the ability of  
183 the box model to reproduce channelization processes of pyroclastic material. The branching  
184 formulation does not involve the inclusion of additional input parameters and thus the calibration  
185 strategies described in this work are valid both for the traditional and the branching formulations  
186 of the box model.

### 187 **3. Calibration strategies**

188 Calibrating the input parameters of kinetic models is a critical step when they are used in the  
189 construction of PDC inundation probability maps, even if the Monte Carlo approach is adopted  
190 to sample the model inputs. This is because inundation probability maps are not only controlled  
191 by the variation range of the input parameters but also by their relative weights within the total  
192 number of simulations. In fact, the *probabilistic* nature of hazard maps computed from the  
193 invasion frequency within a set of numerical simulations is highly debatable if well-suited  
194 calibration procedures are not considered for their construction. For instance, Hyman et al.  
195 (2019) showed that selecting a non-uniform distribution over the input range can significantly  
196 enhance the robustness of numerical results.

197 In this section, we describe different strategies to calibrate the input parameters of kinetic  
198 models. To provide a common nomenclature, the calibrated input parameters are named  $\alpha$  and  $\beta$ .  
199 For the energy cone model,  $\alpha$  is defined as the collapse height ( $H_{0,0}$ ) and  $\beta$  represents the energy  
200 cone slope ( $\tan(\varphi)$ ). Instead, for the box model,  $\alpha$  represents  $\log(V_0)$  (with  $V_0$  representing the  
201 collapsing volume) and  $\beta$  is defined as the initial particle concentration ( $\phi_0$ ). The other input

202 parameters of the box model, whose expected variability typically exerts a lower influence on  
203 numerical results, are fixed. In any case, note that the six inputs of the box model are combined  
204 to define only two intermediate variables ( $L_{max}$  and  $C$ ; see Aravena et al., 2020) which fully set  
205 the characteristics of the box model conoids. Thus, a calibration based on only two variable  
206 parameters is enough to capture the variability in the numerical results of this model. To develop  
207 a reproducible calibration procedure, we need to define a similarity index (S) between the results  
208 of a set of calibration simulations and a reference scenario or set of reference scenarios. In this  
209 work and in the programs EMapProb and BoxMapProb, the latter can be defined in terms of a  
210 reference inundation polygon or a reference probability distribution of runout distance or  
211 inundation area.

212 Let consider a set of  $N \times N$  calibration simulations with fixed source position and the input  
213 parameters variable within the cross product of predefined ranges ( $\alpha \in [\alpha_1, \dots, \alpha_N]$  and  $\beta \in$   
214  $[\beta_1, \dots, \beta_N]$ ). Both sequences of inputs are increasing and their values equidistant. We name  $S_{m,n}$   
215 the similarity index between the modeled inundation polygon associated with the  $m$ -th value of  
216  $\alpha$  and the  $n$ -th value of  $\beta$  and the reference scenario or set of reference scenarios.  $S_{m,n}$  is  
217 assumed to be a non-negative number that increases as the consistency between the modeled  
218 inundation polygon and the reference scenario or set of reference scenarios increases. Thus, we  
219 can suppose that the ability of the pair of inputs  $(\alpha_m, \beta_n)$  to describe well the reference scenario  
220 or set of reference scenarios is an increasing function of  $S_{m,n}$ . This translates into a mathematical  
221 relationship between  $S_{m,n}$  and the sampling probability of a pair of inputs in the neighborhood of  
222  $(\alpha_m, \beta_n)$ :

$$P((\alpha, \beta) \approx (\alpha_m, \beta_n)) := c_p \cdot S_{m,n}^\gamma \quad (1)$$

223 where  $c_p$  is a proportionality constant and  $\gamma$  is a positive exponent. In our calibration strategies,  
 224 for metrics based on a reference inundation polygon (see Section 3.1), we assume a second-order  
 225 relationship ( $\gamma = 2$ ) to enhance the weight of the pairs of input parameters with high values of  
 226  $S_{m,n}$  in the calibration simulations. Otherwise, for metrics based on a reference probability  
 227 distribution of runout distance or inundation area (see Section 3.2), a first-order relationship is  
 228 considered ( $\gamma = 1$ ) in order to reproduce the predefined distribution of runout distance or  
 229 inundation area.

230 Considering known values for  $S_{m,n}$  we can define a probability function for sampling the model  
 231 inputs based on the reference scenario or set of reference scenarios. In practice, this means that  
 232 we can calculate  $c_p$  by assuming:

$$\begin{cases} P(\alpha \in [\alpha_1, \alpha_N]) = 1 \\ P(\beta \in [\beta_1, \beta_N]) = 1 \end{cases} \quad (2)$$

233 In this work we describe five different similarity indexes, which are already implemented in the  
 234 programs EMapProb and BoxMapProb. Three approaches are based on a reference inundation  
 235 polygon (i.e. the footprint over the topography of the inundation area of a given PDC; Section  
 236 3.1), and the other two approaches are based on predefined probability distributions of runout  
 237 distance and inundation area, respectively (Section 3.2). These probability distributions are  
 238 expected to be based on the geological record of the studied volcano.

239 Importantly, all the calibration strategies described in this work consider a possible statistical  
 240 dependence between the model inputs. For instance, in the case of the energy cone model, the

241 well-known relationship between PDC volume and  $\tan(\varphi)$  likely translates into a mathematical  
 242 relationship between  $H_{0,0}$  and  $\tan(\varphi)$  (see Section 4.1), which would imply that the input  
 243 parameters cannot be sampled independently for the construction of PDC hazard maps. On the  
 244 other hand, in the case of the box model, the product between  $V_0$  and  $\phi_0$  represents the  
 245 collapsing volume of pyroclasts, and thus the applicability of an independent sampling is highly  
 246 debatable (see Section 4.3).

### 247 **3.1 Metrics based on a reference inundation polygon**

248 Let consider two inundation polygons (A and B) defined by the sets of boundary points  $A_i$  and  
 249  $B_j$ , respectively ( $i = 1, \dots, n_a$  and  $j = 1, \dots, n_b$ ). Polygon A is given by the reference inundation  
 250 area (defined by the user in the programs EMapProb and BoxMapProb) and polygon B is  
 251 associated with a given calibration simulation (computed using  $\alpha = \alpha_m$  and  $\beta = \beta_n$ ). In our  
 252 programs, in order to reduce the numerical errors derived from the definition of these polygons  
 253 and to balance the weight given to the different portions of the polygons, their contour points are  
 254 re-sampled considering a large number ( $n_r = 1,000$ ) of equidistant points (with respect to the  
 255 arc length) named  $A_k$  and  $B_k$  ( $k = 1, \dots, n_r$ ). Below we describe the three different metrics  
 256 available to calculate  $S_{m,n}$  based on a reference inundation polygon (Fig. 2).

#### 257 **3.1.1 Root mean square distance (RMSD)**

258 This similarity index is based on the root mean square distance between the boundary points of  
 259 each polygon ( $A_k$  and  $B_k$ ) and the closest boundary point of the other one (Fig. 2a), i.e.:

$$RMSD_{m,n} = \frac{\sqrt{\left(\sum_{i=1}^{n_r} \left( \min_{j \in [1, n_r]} \left( d(A_i, B_j) \right)^2 \right)\right) + \left(\sum_{i=1}^{n_r} \left( \min_{j \in [1, n_r]} \left( d(B_i, A_j) \right)^2 \right)\right)}}{2n_r} \quad (3)$$

260

261 where  $RMSD$  is the matrix array containing the results of root mean square distance in the  
262 calibration simulations and the subscripts refer to the indices of this matrix. The lower the value  
263 of  $RMSD_{m,n}$ , the higher the similarity degree between the inundation polygons. From these  
264 results, the similarity index is:

$$S_{m,n}^{(1)} = \frac{1}{RMSD_{m,n} + \varepsilon_{DEM}} \quad (4)$$

265 where  $\varepsilon_{DEM}$  is the cell size of the DEM used in the calibration simulations, representing a  
266 measure of the DEM resolution-derived uncertainty in the calculation of the distance-based  
267 similarity metrics. We found that the effect of  $\varepsilon_{DEM}$  was negligible in all the tested cases, but it is  
268 still incorporated in Eq. 4 to avoid division by zero in any simulation condition (note that the  
269 minimum value computed for  $RMSD_{m,n}$  in the studied cases is much larger than  $\varepsilon_{DEM} \approx 30$  m).

### 270 3.1.2 Hausdorff distance (HD)

271 The second similarity index is defined by (Fig. 2b):

$$HD_{m,n} = \max \left\{ \max_{i \in [1,n_r]} \min_{j \in [1,n_r]} d(A_i, B_j), \max_{i \in [1,n_r]} \min_{j \in [1,n_r]} d(B_i, A_j) \right\} \quad (5)$$

272 where  $HD$  is the matrix array containing the Hausdorff distances associated with the calibration  
273 simulations and the subscripts refer to the indices of this matrix. The resulting similarity index is:

$$S_{m,n}^{(2)} = \frac{1}{HD_{m,n} + \varepsilon_{DEM}} \quad (6)$$

274 where  $\varepsilon_{DEM}$  is incorporated to avoid division by zero in any simulation condition.

275 **3.1.3 Jaccard index (JI)**

276 This similarity index compares the areas defined by the inundation polygons, and is given by  
277 (Fig. 2c):

$$JI_{m,n} = \frac{|A \cap B|}{|A \cup B|} \quad (7)$$

278 where  $JI$  is the matrix array containing the results of Jaccard index associated with the  
279 calibration simulations and the subscripts refer to the indices of this matrix. The Jaccard index  
280 ranges between 0 and 1, and is considered equal to the derived similarity degree (i.e.,  $S_{m,n}^{(3)} =$   
281  $JI_{m,n}$ ).

282 **3.2 Metrics based on a reference probability distribution of runout distance or inundation**  
283 **area**

284 **3.2.1 Runout distance-based calibration**

285 Since in some cases likely eruption scenarios have been defined by adopting the expected runout  
286 distance (e.g. Ferrés et al., 2013), we consider this parameter as a measure potentially useful to  
287 calibrate the inputs of kinetic models. In this case, no reference inundation polygon is needed  
288 and calibration is only based on a predefined distribution of runout distances. If  $F_{RD}$  is the  
289 cumulative distribution function of runout distance, we can compute a measure of the weight that  
290 must be assigned to a calibration simulation characterized by a runout distance  $RD_{m,n}$  in order to  
291 reproduce the predefined distribution of runout distance:

$$S_{m,n}^{(4)} = \int_0^1 \frac{(|RD_{m,n} - F_{RD}^{-1}(x)| + \varepsilon_{DEM})^{-1}}{\sum_{a=1}^N \sum_{b=1}^N (|RD_{a,b} - F_{RD}^{-1}(x)| + \varepsilon_{DEM})^{-1}} dx \quad (8)$$

292 where  $RD$  is the matrix array containing the runout distances of the calibration simulations, and  
 293 the subscripts indicate the indices of this matrix. Let consider a specific integration step defined  
 294 by the cumulative probability  $x_s$  and thus associated with a specific runout distance  $F_{RD}^{-1}(x_s)$ .  
 295 The numerator of Eq. 8 is a measure of the consistency degree between  $F_{RD}^{-1}(x_s)$  and  $RD_{m,n}$ ,  
 296 while the denominator is a normalization factor that considers the consistency degree between  
 297  $F_{RD}^{-1}(x_s)$  and the runout distance in all the elements of the matrix  $RD$  (i.e. all the calibration  
 298 simulations).  $\varepsilon_{DEM}$  is incorporated to avoid division by zero in any simulation condition.

### 299 3.2.2 Inundation area-based calibration

300 Finally, because likely eruption scenarios have been also defined using the expected inundation  
 301 area (e.g. Bevilacqua et al., 2017), we also consider the use of this variable to calibrate the input  
 302 parameters (in this case as well, no reference inundation polygon is needed to develop the  
 303 calibration simulations). If we define the cumulative distribution function of inundation area by  
 304  $F_{IA}$ , we can compute the weight that must be assigned to a calibration simulation characterized  
 305 by the inundation area  $IA_{m,n}$  with the aim of reproducing the predefined probability distribution  
 306 of inundation area:

$$S_{m,n}^{(5)} = \int_0^1 \frac{(|IA_{m,n} - F_{IA}^{-1}(x)| + \varepsilon_{DEM}^2)^{-1}}{\sum_{a=1}^N \sum_{b=1}^N (|IA_{a,b} - F_{IA}^{-1}(x)| + \varepsilon_{DEM}^2)^{-1}} dx \quad (9)$$

307 where  $IA$  is the matrix containing the inundation area of the calibration simulations and the  
 308 subscripts refer to the indices of this matrix. The reason for including  $\varepsilon_{DEM}^2$  is equivalent to that  
 309 presented previously.

310 In EMapProb and BoxMapProb, the number of simulations to be performed in the calibration  
 311 step is defined by the user. However, in order to mitigate discretization errors, the comparison



312 metrics (i.e. *RMSD*, *HD*, *JI*, *RD* and *IA*) are interpolated in the input space, giving rise to a  
313 sufficiently large matrix, which considers  $N = 100$  and preserves the limits of the ranges defined  
314 by the user for  $H_{0,0}$  and  $\tan(\varphi)$ . It is worth noting that, as an alternative to the described  
315 calibration strategies, our programs also allow the user to define *a priori* the probability  
316 distributions adopted to sample the input parameters. Various options are available to set the vent  
317 position as well, including pointwise, linear and radial geometries or a set of positions expressly  
318 defined by the user, which can be flexibly adopted for testing the influence of collapse position  
319 in PDC propagation.

#### 320 **4. Test cases: Results and discussion**

321 Here we present three applications of our calibration strategies. In particular, El Misti volcano  
322 (Peru) was adopted to show the use of calibrations based on a reference inundation polygon for  
323 constructing probability maps of PDC inundation, through the branching energy cone model. On  
324 the other hand, Merapi volcano (Indonesia) was adopted to illustrate the use of calibrations based  
325 on the expected distribution of runout distance, while Campi Flegrei (Italy) was selected to show  
326 the use of calibrations based on the expected distribution of inundation area. Because most of the  
327 PDCs generated at Merapi volcano are derived from dome collapses (i.e. they are frictional  
328 flows), we used the branching energy cone model. Instead, since Campi Flegrei eruptions tend to  
329 produce dilute, inertial PDCs, they are better described by the box model (Esposti Ongaro et al.,  
330 2016). In the latter case, we adopted the traditional formulation instead of the branching one  
331 because minor channelization processes are expected in such a flat topography and because this  
332 choice allows performing comparisons with the most recent PDC hazard assessments at Campi  
333 Flegrei (Neri et al., 2015; Bevilacqua et al., 2017).

#### 334 **5.1 El Misti volcano**

335 El Misti volcano (5,822 m a.s.l.) is located at 13 km NE from Arequipa city (>1 million  
336 inhabitants, at an altitude 3,500 m lower than the summit of El Misti). These factors and its  
337 potential to develop PDC-forming eruptions (Legros, 2001; Thouret et al., 2001; Harpel et al.,  
338 2011; Sandri et al., 2014; Charbonnier et al., 2020) justify the use of this volcano as a case study  
339 for illustrating the application of our calibration strategies. In fact, at least three sub-Plinian and  
340 Plinian eruptions occurred at El Misti during the last 10,000 years, intercalated with small-  
341 magnitude Vulcanian events (Cobeñas et al., 2012). Following Cobeñas et al. (2012) and  
342 Charbonnier et al. (2020), we adopted the 2070 cal yr BP Plinian eruption as a reference event to  
343 assess PDC hazard at El Misti volcano, which corresponds to a VEI 4 event for which the  
344 recurrence rate has been estimated between 2000 and 4000 years (Charbonnier et al., 2020). We  
345 stress that the presentation of updated hazard maps is beyond the objectives of this work (for  
346 which the reader can consult the official hazard map for El Misti; Mariño et al., 2008). Instead,  
347 we aim at presenting an illustrative application of our calibration strategies. For this, we used the  
348 inundation polygon of the PDCs derived from the 2070 cal yr BP Plinian eruption (Fig. 3a;  
349 Charbonnier et al., 2020) to calibrate the input parameters, considering a fixed collapse position  
350 at the summit crater (Fig. 3a),  $H_{0,0}$  from 100 m to 2,000 m, and  $\tan(\varphi)$  ranging between 0.2 and  
351 1.0.

352 We performed 400 calibration simulations using the branching energy cone model. Figure 3b-d  
353 shows the pseudo-color plots derived from the calibration simulations, based on the following  
354 metrics: RMSD, HD and JI. This figure highlights the strong correlation between  $H_{0,0}$  and  
355  $\tan(\varphi)$  in determining the different similarity indexes and shows that the best-fit conditions of  
356 RMSD are quite similar to those of JI, while best-fit conditions of HD tend to show lower values  
357 of  $\tan(\varphi)$  at equal  $H_{0,0}$ .

358 Then, calibration results were used to sample three sets of input parameters, each one derived  
359 from the application of a different metric (RMSD, HD and JI, respectively; Fig. 3e-g). With this  
360 information, we performed three additional sets of simulations aimed at constructing scenario-  
361 based probability maps of PDC inundation. Here we also introduced a small variability in vent  
362 position, which was sampled uniformly within a 200 m-radius circle centered in the collapse  
363 position used in the calibration simulations (Fig. 3a).

364 The resulting probability maps of PDC inundation (Fig. 4) are highly consistent between them  
365 and with Cobeñas et al. (2012) and Sandri et al. (2014). They show a preferential propagation  
366 direction toward NW (i.e., toward the basin and the city of Arequipa, reaching in many cases its  
367 suburbs). Runout distance typically ranges between 6 km and 15-17 km (mean value of about 10  
368 km and median value of ~9 km; Fig. 4 and supplementary Table C1). The branching energy cone  
369 model predicts non-negligible channelization processes through river Chili, which agrees with  
370 the geological record at El Misti volcano, influencing sensibly the inundation probability in the  
371 northern portion of Arequipa (Fig. 4). Depending on the adopted calibration procedure, results  
372 show probabilities between ~5% and ~10% that a PDC caused by an event similar to the  
373 reference eruption will reach the district of Chiguata and probabilities of up to 20% for the NE  
374 suburbs of Arequipa (~10-20% for Alto Selva Alegre and ~5-10% for Miraflores; Fig. 4). On the  
375 other hand, significant channelization processes toward NE and SE are not apparent in the  
376 numerical results. Figure 4 shows that the 50% isolines of the resulting probabilistic maps tend to  
377 present a behavior similar to the reference scenario (indicated by a green line in Fig. 4), but it  
378 presents shorter propagation distances in the channelization zones. However, the 10% isolines  
379 envelope most of the inundation area of the reference scenario also in the channelization  
380 domains.

381 Importantly, channelization through the San Lázaro catchment is significant at proximal and  
382 medial zones and small at distal domains, and very weak channelization is modelled along the  
383 Huarangal catchment. This is apparently inconsistent with Charbonnier et al. (2020), who  
384 recognized these catchments as relevant for the channelization of pyroclastic material to  
385 Arequipa. However, we stress that our simulations were calibrated using a specific reference  
386 deposit with very limited channelization through these catchments and, more importantly, our  
387 collapse positions are located in the summit zone, while the simulations performed by  
388 Charbonnier et al. (2020) were developed considering the collapse of already channelized  
389 pyroclastic material (in particular, the collapsing material was initially located at the apex of two  
390 specific drainage networks, at  $>2$  km from the summit crater). Consequently, as Charbonnier et  
391 al. (2020) indicate, their probabilistic maps are not only conditioned on the occurrence of a VEI  
392 4 eruption, but also on the entrance of large volumes of pyroclastic material in two specific  
393 drainage networks that threaten Arequipa; while our probabilistic maps are conditioned  
394 exclusively on the occurrence of a VEI 4 event. These differences in the objectives and thus in  
395 the criteria adopted in the calibration step hinder the development of further comparisons with  
396 Charbonnier et al. (2020), and highlight the necessity of considering separately the PDCs  
397 initiated from the summit and near the drainage networks at El Misti volcano. In any case, to  
398 show that this difference derive from the adoption of different calibration criteria instead of  
399 limitations of the branching energy cone model to channelize pyroclastic material, we performed  
400 additional simulations with a vent located on the flanks of the volcano, which are displayed in  
401 the supplementary Figure C1. These simulations show the potential of the branching energy cone  
402 model to predict highly channelized flows along the main drainage networks of El Misti volcano,  
403 eventually threatening the city of Arequipa.

## 404 4.2 Merapi volcano

405 Merapi stratovolcano (~2,930 m a.s.l.) is located at ~25 km north of the metropolitan area of  
406 Yogyakarta, Central Java, Indonesia. This basaltic-to-basaltic andesitic volcano has presented  
407 frequent dome-forming activity during the last centuries. Several of these eruptions have  
408 generated PDCs (“*Merapi-type*” *nuées ardentes*) and subsequent lahars (Boudon et al., 1993;  
409 Voight et al., 2000; Voight and Davis, 2000; Bourdier and Abdurachman, 2001; Thouret et al.,  
410 2001; Lube et al., 2011; Gertisser et al., 2012; Suroño et al., 2012; Charbonnier et al., 2013;  
411 Komorowski et al., 2013; Kelfoun et al., 2021). The topography of Merapi, characterized by  
412 numerous radial valleys, has exerted a significant effect in the propagation of PDCs, and also the  
413 crater configuration and collapse position have influenced the transport direction of recent PDCs  
414 (e.g. Charbonnier and Gertisser, 2008). For instance, because of the topographic barriers present  
415 at the NE of the volcano summit, most of the recent PDCs propagated towards S, SW and W  
416 (Solikhin, 2015).

417 The frequent occurrence of dome-forming eruptions and the presence of densely populated cities  
418 in the surroundings of Merapi justify the use of this volcano as a study case to illustrate the  
419 application of our calibration procedures. Moreover, the dynamics of this type of PDCs is  
420 dominated by gravitational acceleration on the volcanic slopes and granular frictional dissipation,  
421 making them suitable for the use of the branching energy cone model. We remark that the  
422 presentation of new hazard maps is beyond the objectives of this article, for which the reader can  
423 consult the wide volcanological literature at Merapi (Andreastuti et al., 2000; Itoh et al., 2000;  
424 Lavigne et al., 2000; Thouret et al., 2000; Charbonnier and Gertisser, 2012; Mei et al., 2013;  
425 Lavigne et al., 2015; Kelfoun et al., 2017) and the official hazard map of this volcano (Sayudi et

426 al., 2010). Instead, we adopt this case study to illustrate the application of calibrations based on  
427 the distribution of runout distance.

428 In fact, the availability of detailed information about the dispersion of PDCs in the past (e.g.  
429 Bourdier and Abdurachman, 2001; Solikhin, 2015) allows us to consider the expected  
430 distribution of runout distance to calibrate our numerical model. To do this, first we performed  
431 400 calibration simulations using the branching energy cone model and considering a fixed  
432 collapse position at the summit crater,  $H_{0,0}$  ranging from 40 m to 200 m, and  $\tan(\varphi)$  ranging  
433 between 0.2 and 1.0. The small range adopted for collapse height is justified by the generation  
434 mechanism of most of the PDCs at Merapi, i.e. dome collapse.

435 Figure 5a-b presents the pseudo-color plots of runout distance and inundation area in the  
436 calibration simulations. Because of the high slope that characterizes the volcano flanks in the  
437 proximal area ( $>30^\circ$ ), a significant gap is observed in the simulated runout distances between  
438  $\sim 0.2$  km (i.e. inside the crater limits) and  $\sim 2.5$  km (Fig. 5a). In other words, all the simulations  
439 that exceeded the crater limits were able to travel at least  $\sim 2.5$  km from the source due to the high  
440 slopes encountered by the PDC in this zone of the volcano.

441 To define the input probability distribution of runout distance, we adopted the information  
442 summarized by Solikhin (2015), who compiled the runout distances of 55 PDCs between 1900  
443 and 2010 (Fig. 5c-d). In particular, the runout distances of these events were fitted considering  
444 both gamma and lognormal probability functions (Fig. 5c-d). Although a bimodal distribution  
445 could be hypothesized to describe the data, we decided to keep the discussion simpler and focus  
446 on the calibration features. The coupling of calibration simulations and the two predefined  
447 distributions of runout distance give rise to two sampling probability distributions of input  
448 parameters (Figure 5e-f). It is worth noting that the absence of runout distances between  $\sim 0.2$  km

449 and ~2.5 km in the calibration simulations necessarily translates into the absence of these values  
450 of runout distances in the resulting PDC invasion maps. With the two sampling probability  
451 distributions of input parameters described previously (Fig. 5e-f), we performed two sets of 500  
452 simulations to construct PDC inundation probability maps. To carry out these simulations,  
453 collapse positions were sampled uniformly from a 300 m-radius circle centered in the collapse  
454 position used for the calibration simulations (i.e. the volcano summit).

455 The resulting inundation maps are displayed in Figure 6. Even though we sampled the collapse  
456 positions uniformly, results reproduce well the preferential propagation directions observed at  
457 Merapi volcano (i.e. S, W, NW and SW), which are also observed in hazard maps derived from  
458 the geological record of Merapi volcano (e.g. Figure 4 of Thouret et al., 2000). It is worth noting  
459 that the small inundation probabilities simulated at distances of the order of 15 km, which are  
460 present in the geological record of Merapi (Newhall et al., 2000), is a consequence of the dataset  
461 adopted in the numerical calibration (i.e. PDCs between 1900 and 2010), which implies that our  
462 probability maps are conditioned on the occurrence of an eruption that follows the eruption  
463 variability of the last century (Solikhin, 2015).

464 Differences between the results associated with the gamma and lognormal fits are negligible  
465 (Fig. 6, Fig. 7a and supplementary Table C2). In these simulations, mean runout distance is 5.8-  
466 5.9 km, with 90% confidence intervals of [3.2, 12.1] km and [3.1, 11.5] km for the results  
467 associated with gamma and lognormal fits, respectively (supplementary Table C2). The low  
468 values of  $IA/(\pi \cdot R_{\max}^2)$  in numerical simulations, where IA is the inundation area and  $R_{\max}$  is  
469 the runout distance, highlights the capacity of the branching energy cone model to reproduce the  
470 strong channelization effects related to Merapi's topography (supplementary Table C2). In fact,  
471 the branching energy cone model predicts non-negligible channelization processes through

472 different river valleys such as Senowo, Apu, Woro, Opak and Gendol, which agrees with the  
473 recent activity at Merapi volcano (Fig. 6). Interestingly, although the last major PDC at Merapi  
474 was channelized through the Gendol catchment, our results suggest a dominant channelization  
475 effect in Woro and Opak catchments to the south. This apparent inconsistency with the last  
476 eruption is instead coherent with the geological record of the last century (Solikhin, 2015).

477 Figure 7a presents the comparison between the CDFs of the predefined distributions of runout  
478 distance, which derive from two fits based on the geological record of Merapi (gamma and  
479 lognormal; dashed lines), and the resulting distributions of runout distance in the simulations  
480 presented in Figure 6 (continuous lines). The empirical CDF of 55 documented PDCs is also  
481 included (Solikhin, 2015). The main contrast between the predefined and resulting CDFs derives  
482 from the absence of simulations with runout distances lower than 2.5 km. We speculate that low-  
483 runout distance PDCs observed at Merapi can be related to volume-limited block-and-ash flows  
484 (or simply a rock-fall rather than a PDC), whose dynamics cannot be modeled by the branching  
485 energy cone model. The presence of different families of PDCs at Merapi could be responsible  
486 for the bimodal behavior of documented runout distances (Fig. 5c-d). Additional differences  
487 between the predefined and resulting CDFs presented in Figure 7a may derive from the use of a  
488 calibration based on simulations performed using a single collapse position, while a small  
489 uncertainty in collapse position was introduced for the construction of the hazard maps presented  
490 in Figure 6.

491 A major challenge to evaluate the hazard associated with dome collapse at Merapi is the frequent  
492 occurrence of changes in the eruption site (Thouret et al., 2000). To demonstrate the model  
493 capability to simulate the effect associated with collapse position, we performed four additional  
494 sets of simulations considering collapse positions in different zones of the volcano. In particular,



495 collapse positions were sampled uniformly within different regions of a 300 m-radius circle  
496 centered in the volcano summit. Four regions were considered: NW, NE, SW and SE. On the  
497 other hand,  $H_{0,0}$  and  $\tan(\varphi)$  were sampled considering the gamma fit used previously (Fig. 5e).  
498 Results are presented in Figure 8, indicating that small differences in the collapse position (e.g.  
499 of the order of hundreds of meters) are able to change dramatically the expected propagation of  
500 PDCs and the valleys involved. In particular, PDCs derived from collapsing domes located in the  
501 NW flank of Merapi volcano tends to be channelized through the valleys Apu and Senowo, and a  
502 significant part of these PDCs is propagated toward SW (Fig. 8a). Importantly, volcano  
503 topography at the NE flank tends to redirect PDCs mainly through the valleys Apu (i.e. NW) and  
504 Woro (i.e. SSE; Fig. 8b). This is consistent with the geological record of Merapi. On the other  
505 hand, PDCs produced from collapsing domes situated in the SW flank tend to be channelized  
506 through the valleys Senowo, Putih, Bebeng, Krasak, Boyong, Opak and Gendol (Fig. 8c).  
507 Finally, collapses at the SE flank of Merapi tend to be channelized through the valleys Opak,  
508 Gendol and Woro. Figure 7b shows the empirical CDFs of the runout distances modelled in the  
509 simulations presented in Fig. 8, with only minor differences between the different sets of  
510 simulations.

511 We remark that these maps are conditioned on the occurrence of a PDC derived from the  
512 collapse of a summit dome, which is not the only mechanism able to produce PDCs at Merapi. In  
513 fact, this volcano has presented large explosive eruptions in historic times, such as the 1872  
514 eruption (Hartmann, 1934). Another limitation is related to the absence of numerical simulations  
515 able to produce runout distances lower than 2.5 km. Despite this, our results highlight the model  
516 capability to capture the strong control exerted by collapse position in the propagation of PDCs.  
517 A more extensive analysis of the dependence between the location of collapsing domes and

518 transport of the resulting PDCs may provide key information for the design and implementation  
519 of effective, focalized measures for volcanic hazard mitigation.

### 520 **4.3 Campi Flegrei**

521 Campi Flegrei, located on the Campanian plain in Southern Italy, is a 12 km wide caldera that  
522 includes a highly urbanized area and a significant portion of the city of Naples. The volcanic  
523 activity of Campi Flegrei during the last 15 kyr has been separated in three epochs of temporally  
524 clustered eruptions, which include at least 70 explosive events (e.g. Di Vito et al., 1999; Smith et  
525 al., 2011; Bevilacqua et al., 2016; Isaia et al., 2019). Among the products of these eruptions,  
526 PDCs represent the main volcanic hazard at Campi Flegrei (Lirer et al., 2001; Alberico et al.,  
527 2002; Orsi et al., 2004; Rossano et al., 2004; Todesco et al., 2006; Orsi et al., 2009; Alberico et  
528 al., 2011; Neri et al., 2015; Tierz et al., 2016b; Bevilacqua et al., 2017) but their assessment is  
529 made more challenging by the large uncertainty in the position of future vents (Alberico et al.,  
530 2002; Orsi et al., 2004; Selva et al., 2012; Bevilacqua et al., 2015; Bevilacqua et al., 2017;  
531 Rivalta et al., 2019; Bevilacqua et al., 2020). We adopted this case study to show the application  
532 of a calibration based on the distribution of inundation area.

533 In fact, the availability of detailed information about the dispersion of PDCs in the past allows  
534 considering the expected distribution of inundation area to calibrate the box model. To do this,  
535 we performed two sets of 900 calibration simulations each? by adopting the traditional  
536 formulation of the box model, with the collapsing volume ranging from  $10^6$  to  $10^{11}$  m<sup>3</sup> and the  
537 initial concentration of solid particles between 0.5 vol. % and 4.0 vol. %. The other input  
538 parameters of the box model were fixed (sedimentation velocity of 0.6 m/s, Froude number of  
539 1.1, pyroclasts density of 1500 kg/m<sup>3</sup> and ambient gas density of 1.1 kg/m<sup>3</sup>). These two sets of  
540 simulations differ in their collapse positions, which were set at Monte Nuovo and Agnano,

541 respectively (Fig. 9a), and allow to calculate the inundation area as a function of the two variable  
542 input parameters (Fig. 9b-c). It is worth noting that, although the uncertainty in vent position in  
543 this volcanic field may hinder the use of a fixed vent position for calibration purposes, the  
544 absence of major topographic barriers at Campi Flegrei (with the exception of the caldera rim of  
545 ~160 m height and the boundary of the Agnano plain of ~110 m height) produces only small  
546 differences in the calibration results as a function of the collapse position. In particular, we  
547 adopted the calibration data of Monte Nuovo and Agnano as representative of the western and  
548 eastern sectors of Campi Flegrei, respectively. In the following we further evaluate the validity  
549 of this assumption.

550 Because the calibration procedure described in Section 3.2.2 needs the input of a probability  
551 distribution of inundation area, we used the information summarized by Neri et al. (2015), which  
552 relies largely on Orsi et al. (2004). In particular, we followed the strategy of Neri et al. (2015)  
553 and Bevilacqua et al. (2017) to consider the variability of inundation area in 47 documented  
554 PDCs, the effect of eventual underestimations of the area of PDC deposits, and the presence of  
555 “lost” deposits in the dataset, considering the western and eastern domains of Campi Flegrei  
556 separately because significant differences have been recognized in the typical scale of their  
557 eruptions (for additional details, see Bevilacqua et al., 2017). This allowed us to define the  
558 expected distribution of inundation area in the two regions of Campi Flegrei, which are displayed  
559 as cumulative curves in Figure 9d-e. These results show that the inundation area of PDCs  
560 generated at the eastern sector of Campi Flegrei tends to be significantly larger than that  
561 expected in the western portion of this volcanic field.

562 The coupling of the calibration simulations (Fig. 9b-c) and the expected distributions of  
563 inundation area (Fig. 9d-e) gives rise to two sampling probability distributions of input

564 parameters, which are displayed in Figure 10. These results show a strong correlation between  
565 the two input parameters in the calculation the sampling probability of the model inputs,  
566 suggesting that interdependent sampling strategies of the model inputs should be preferred (Fig.  
567 10). As expected, the peak of sampling probability for the western sector of Campi Flegrei  
568 (computed for collapsing volumes of  $V_0 = 10^7 - 3 \cdot 10^8 \text{ m}^3$  and volumes of pyroclasts of  
569  $V_0\phi = 4 \cdot 10^5 - 1.6 \cdot 10^6 \text{ m}^3$ ) is associated with much smaller PDCs than that predicted for the  
570 eastern zone of this caldera (computed for collapsing volumes of  $V_0 = 3 \cdot 10^8 - 2 \cdot 10^9 \text{ m}^3$  and  
571 volumes of pyroclasts of  $V_0\phi = 8 \cdot 10^6 - 1.2 \cdot 10^7 \text{ m}^3$ ), with differences of one order of  
572 magnitude (Fig. 10).

573 With this information, we performed two sets of 3,000 simulations to construct PDC inundation  
574 probability maps for the two sectors of Campi Flegrei. To carry out these simulations, collapse  
575 positions were sampled using the vent opening probability map presented by Bevilacqua et al.  
576 (2015). Note that this map includes uncertainty ranges but, for simplicity, in this work we  
577 adopted the mean value map. We also resampled all the vents located offshore and considered  
578 separately the western and eastern sectors of Campi Flegrei, using the limits adopted by  
579 Bevilacqua et al. (2017). On the other hand, the sea surface has been considered as a flat  
580 topography with no consideration of water influence in the PDC propagation dynamics.

581 Numerical results, visualized in a GIS environment, are displayed in Figure 11a-b. We remark  
582 that these maps are conditioned on the occurrence of a PDC-forming eruption in the western and  
583 eastern sectors of Campi Flegrei, respectively, without assumptions associated with its  
584 magnitude or intensity, in contrast to the maps obtained for El Misti volcano. We also include the  
585 combined probabilistic map of PDC inundation (Fig. 11c), defined using the relative weights of  
586 the two sectors of Campi Flegrei in the vent opening maps of Bevilacqua et al. (2015), i.e. 30.7%

587 for the western sector and 69.3% for the eastern sector. For an eruption located in the western  
588 sector of Campi Flegrei, our simulations show a peak of PDC inundation probability of about  
589 30% at Averno, being strongly consistent with Bevilacqua et al. (2017). Instead, for an eruption  
590 located in the eastern portion of this volcanic system, numerical results show a maximum PDC  
591 inundation probability of ~60% at Astroni and Agnano, with probabilities around 15-20% of  
592 having a PDC able to overcome the Posillipo Hill, again in agreement with the results presented  
593 by Bevilacqua et al. (2017). Note that the differences in the maximum values of PDC inundation  
594 probability between the two sectors of Campi Flegrei are mainly derived from the scale of the  
595 PDCs expected, which are much larger in the eastern sector. The combined probability map of  
596 PDC inundation, which is not conditioned on the sector of the source position, presents a  
597 maximum value of ~43% at Agnano and Astroni, and a probability of ~10-15% of overcoming  
598 the Posillipo Hill. The consistency between our results and Bevilacqua et al. (2017) can be  
599 considered an expected result because we used the same geological dataset to calibrate the  
600 models. However, it is worth stressing that the calibration procedures are completely different,  
601 showing that a calibration based on a single source point can be enough in volcanic contexts  
602 characterized by small scale topographic barriers as Campi Flegrei.

603 Finally, Figure 12 presents the comparison between the CDFs of the predefined distributions of  
604 inundation area (continuous red lines) and the resulting distributions of this variable in the  
605 simulations of the probability maps presented in Figure 11a-b (dashed blue lines). The empirical  
606 CDF of inundation area in the geological record of Campi Flegrei is also displayed (black line).  
607 The strong agreement between the prescribed and the resulting distributions of inundation area  
608 further confirms that a calibration procedure based on simulations performed using a single

609 source point is able to capture well the dependence between the box model input parameters and  
610 the resulting inundation area in this volcanic system, where the topographic roughness is small.

## 611 **5. Summary and conclusions**

612 Although numerical models have become a fundamental aspect in the assessment of volcanic  
613 hazard and in the design of volcanic risk mitigation strategies (e.g. Ferrés et al., 2013; Sandri et  
614 al., 2014; Bevilacqua et al., 2017; Charbonnier et al., 2020; Clarke et al., 2020; Esposti Ongaro et  
615 al., 2020b), the large variety of criteria used to calibrate their input parameters often limits the  
616 development of comparisons between different numerical models, which is a critical step for  
617 their validation (Esposti Ongaro et al., 2020a). In this work we propose a set of structured and  
618 reproducible procedures to calibrate the input parameters of numerical models, which are based  
619 on the characteristics of past PDCs in the studied volcanic system. This information can be  
620 described in terms of:

621 (a) A reference inundation polygon derived from a specific eruption. Three parameters to  
622 compute the similarity index between this polygon and a set of calibration simulations have  
623 been considered (RMSD, Hausdorff distance, and Jaccard Index). These results can be used  
624 to define different sampling probability distributions of the input parameters, which in turn  
625 can be adopted to extract a set of calibrated inputs to use in numerical simulations. The  
626 application of these calibrations enables the construction of probabilistic maps of PDC  
627 inundation conditioned on the occurrence of an event similar to the reference scenario (i.e.  
628 scenario-based hazard assessment, see Section 4.1).

629 (b) The distribution of runout distance or inundation area of past PDCs. This information, along  
630 with the results of the calibration simulations, allows sampling a set of input parameters able  
631 to reflect the eruptive history of the volcano. These two procedures, whose application

632 involves a large knowledge of the characteristics of the studied volcanic system, are able to  
633 produce PDC inundation probabilistic maps conditioned on the occurrence of a PDC-forming  
634 eruption without assumptions associated with its characteristics (e.g. magnitude or intensity,  
635 see Sections 4.2 and 4.3).

636 The suitability of the different calibration procedures will be naturally controlled by the  
637 availability of detailed information of the studied volcanic system and by the approach used to  
638 assess the hazard derived from PDCs (e.g. based on a specific scenario or not). All these  
639 strategies allow considering the interaction of the input parameters in controlling the numerical  
640 results (in other words, input parameters are not sampled independently). In fact, all the tested  
641 cases exhibit a strong interdependence between the input parameters in the resulting functions of  
642 sampling probability, suggesting that calibration strategies that consider interdependent sampling  
643 should be preferred for the construction of probabilistic maps of PDC inundation. Thereby,  
644 through the use of these calibration strategies, we reduce the biases derived from arbitrary user  
645 choices/assumptions in the construction of PDC hazard maps, which have been often necessary  
646 due to lack of ad-hoc data.

647 We have illustrated our calibration strategies by applying them to three volcanoes: El Misti,  
648 Merapi and Campi Flegrei. In particular, the El Misti example illustrates the use of calibrations  
649 based on a reference inundation polygon related to a specific eruption; the Merapi example  
650 shows the use of a calibration based on the expected distribution of runout distance, and the  
651 analysis of Campi Flegrei was developed by using a calibration based on the expected  
652 distribution of inundation area. In general terms, results are strongly consistent with previous  
653 hazard assessments and with the geological record of these volcanic systems (e.g., Cobeñas et  
654 al., 2012; Sandri et al., 2014; Neri et al., 2015; Solikhin, 2015; Bevilacqua et al., 2017). In any

655 case, we stress that our results are not intended to represent updated hazard maps of these well-  
656 documented volcanoes, for which the reader can consult the official maps and other recent  
657 studies of volcanic hazard (e.g. Mariño et al., 2008; Sayudi et al., 2010; Sandri et al., 2014; Neri  
658 et al., 2015; Bevilacqua et al., 2017; Charbonnier et al., 2020).

659 The different calibration procedures described here were implemented on improved, user-  
660 friendly versions of the programs EMapProb and BoxMapProb, whose functionalities and user  
661 manuals are presented for the first time in this article. These open-source and freely  
662 downloadable programs adopt the traditional and branching formulations of the energy cone and  
663 the box models (Aravena et al., 2020), respectively, and thus they present different applicability  
664 fields (frictional and inertial flows, respectively). In addition to the presented calibration  
665 procedures, we stress that EMapProb and BoxMapProb allow the user to define *a priori*  
666 different probability distributions to sample the model inputs. Different modalities are also  
667 available to set vent position, which can be adopted for coupling kinetic models with vent  
668 opening probability maps (Bevilacqua et al., 2021), as shown in Section 4.3. We also note that  
669 the traditional and branching formulations of kinetic models do not involve large computational  
670 requirements and allow constructing PDC inundation maps on simple CPU computers. All these  
671 characteristics make our programs useful tools for the early assessment of PDC volcanic hazards,  
672 allowing for the construction of probabilistic inundation maps considering reproducible  
673 calibration procedures, able to reduce the biases introduced by user choices.

674

675 **Code availability**



676 ECMapProb is available in <https://github.com/AlvaroAravena/ECMapProb> (Apache 2.0 license).  
677 BoxMapProb is available in <https://github.com/AlvaroAravena/BoxMapProb> (Apache 2.0  
678 license).

679

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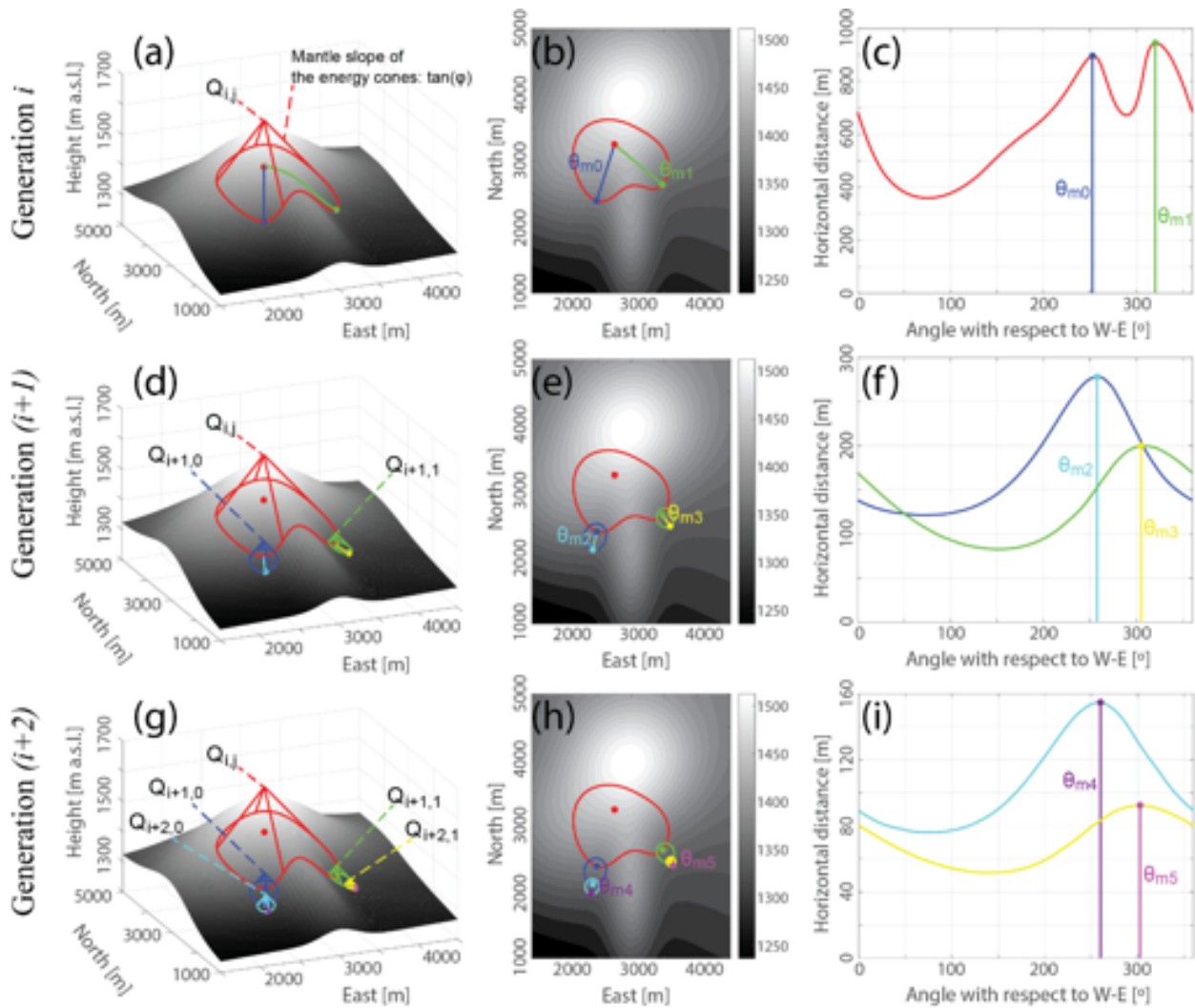
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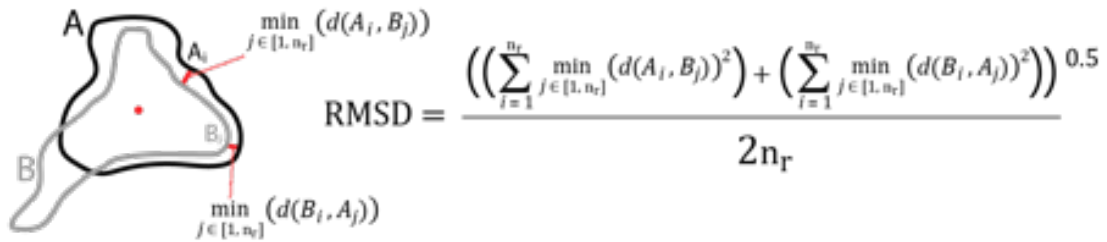
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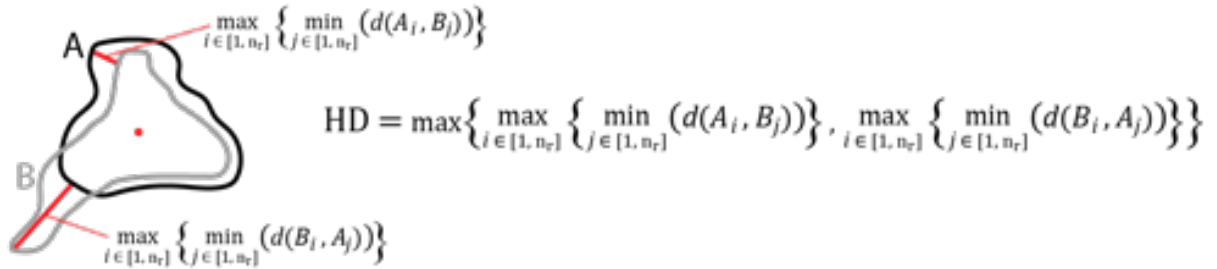
**Figure 1.** Illustrative example of the tree-like structure used in the branching energy cone model. More details can be found in Aravena et al. (2020). Left-hand side: surface plots of the energy cones and the topography. Central column: contour plots of the energy cones and the topography. Right-hand side: functions of horizontal distance (i.e. run-out distance as a function of the polar angle) of the different generations of energy cones. The number of generations increases from top to bottom.



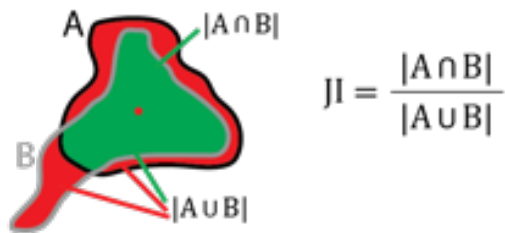
(a) Root mean square distance (RMSD)



(b) Hausdorff distance (HD)



(c) Jaccard Index (JI)

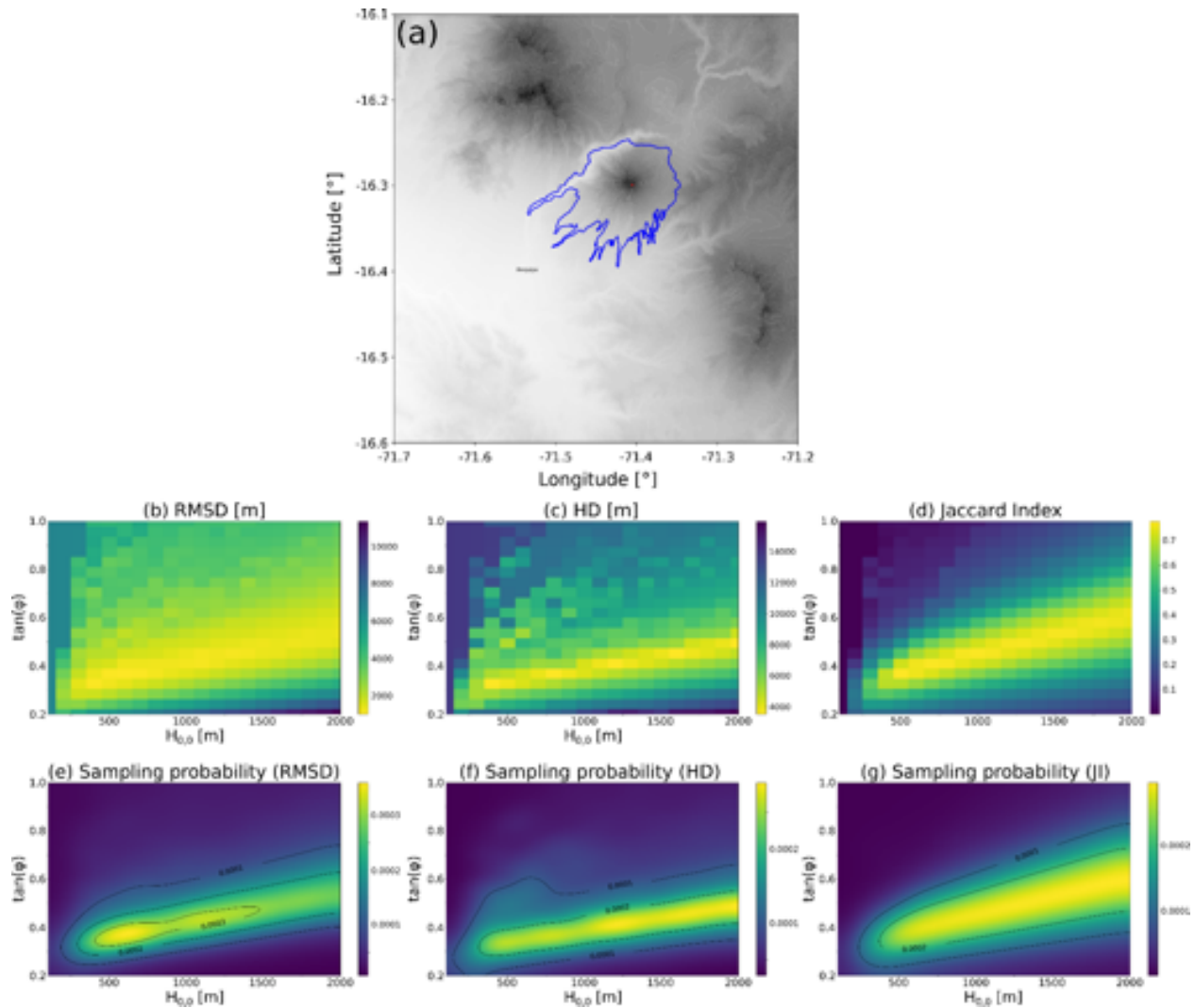


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981 **Figure 2.** Illustrations of the different metrics used to calculate the similarity index between a reference scenario,  
 982 defined by the reference inundation polygon A, and a given calibration simulation characterized by the inundation  
 983 polygon B (see Section 3.1).

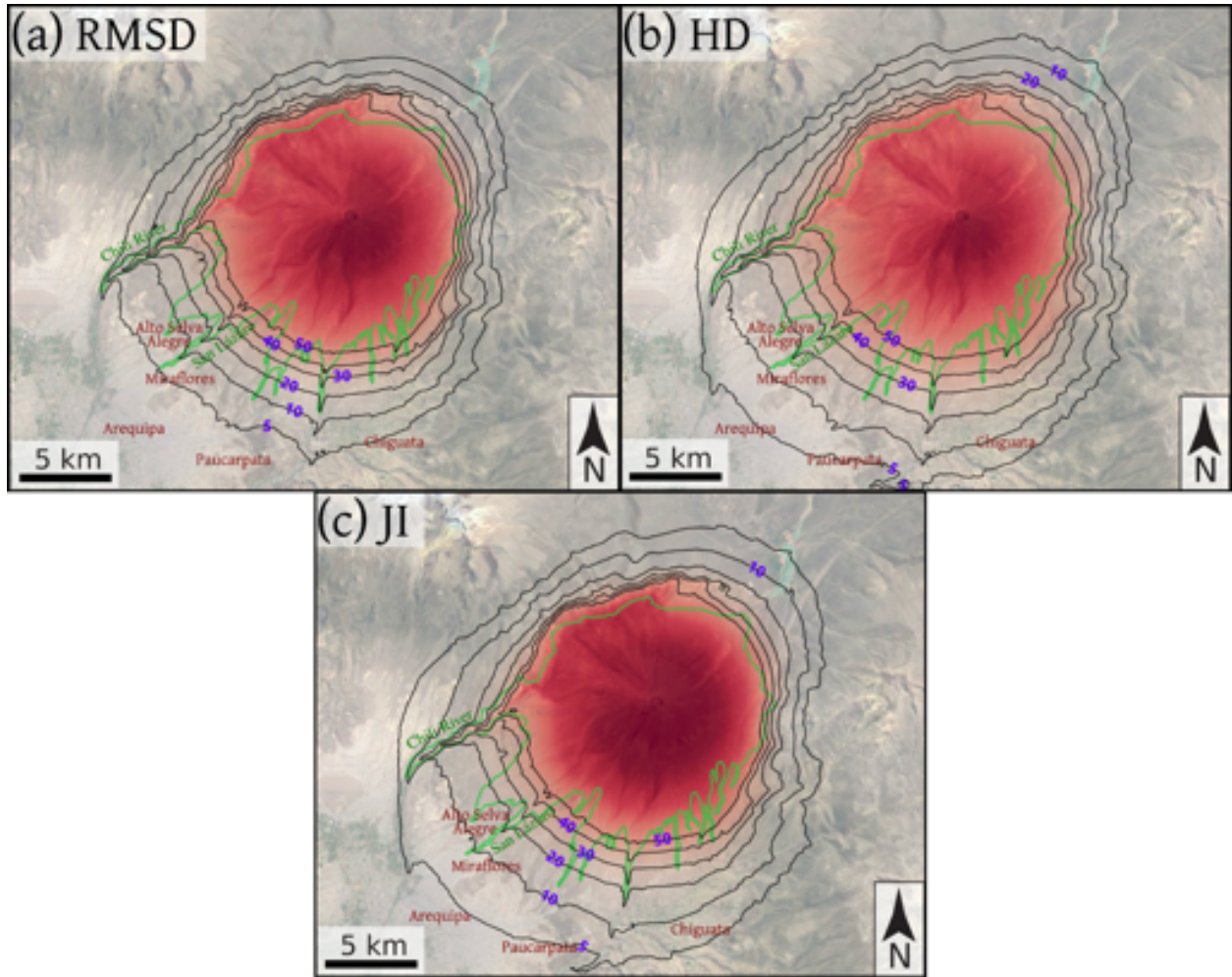
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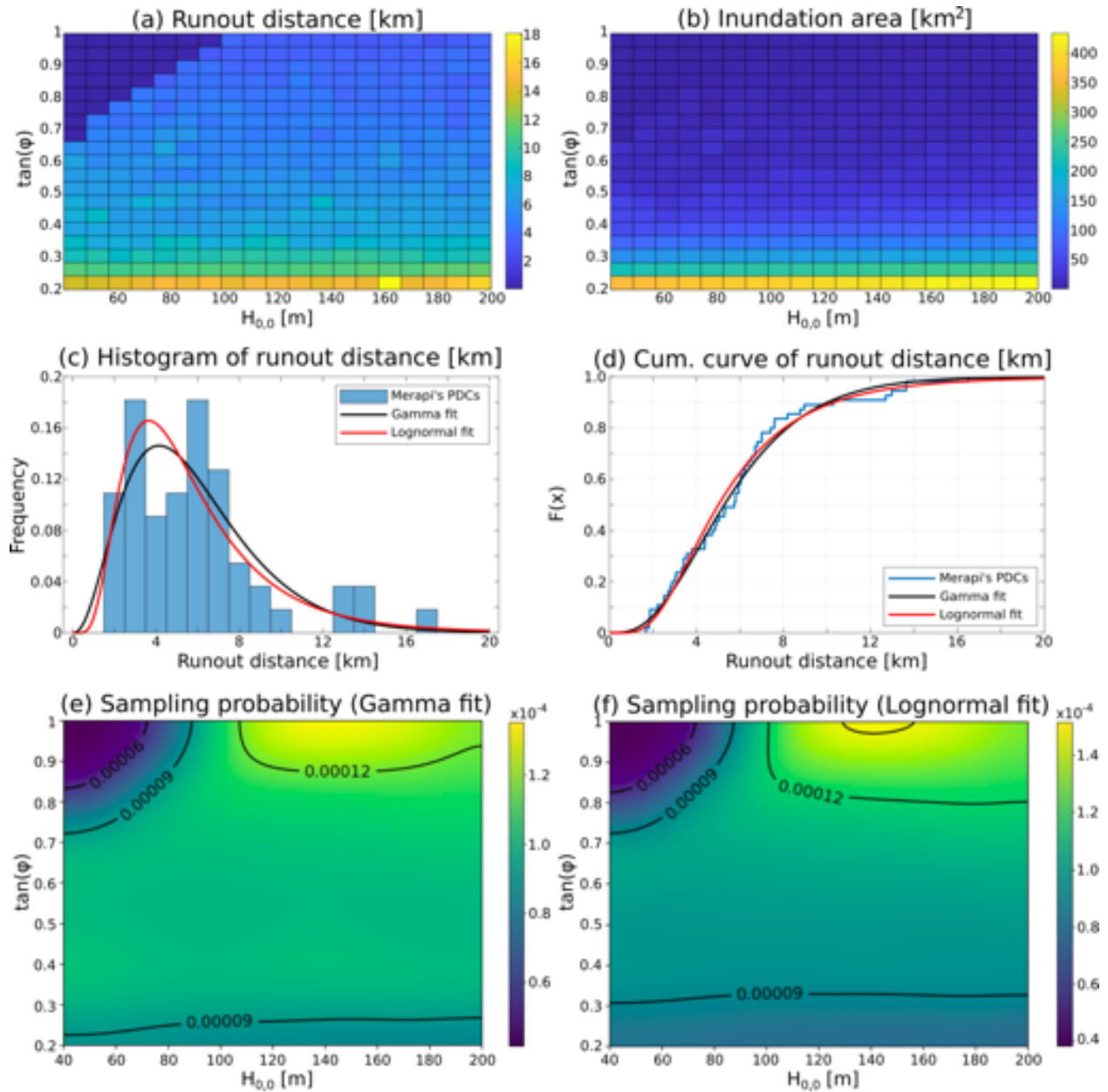
987 **Figure 3.** (a) Elevation map of El Misti volcano (Peru) including the PDC inundation area associated with the 2070  
 988 cal yr BP eruption (Charbonnier et al., 2020), used to calibrate the branching energy cone model. The red point  
 989 represents the collapse position used in the calibration simulations. These simulations took  $\sim 170$  min on an Intel  
 990 Core i5-2320 CPU at 3.00 GHz ( $\sim 25$  s per simulation). (b-d) Pseudo-color plots of the different coincidence  
 991 parameters (RMSD, HD and JI) computed from the calibration simulations. In these panels, yellow pixels are  
 992 associated with high similarity indexes between the calibration simulations and the reference inundation polygon,  
 993 and blue pixels indicate low degrees of similarity between the computed invasion zones in the calibration  
 994 simulations and the reference inundation polygon. (e-g) Sampling probability distributions of input parameters ( $H_{0,0}$   
 995 and  $\tan(\varphi)$ ) used in different sets of simulations for El Misti volcano (see Fig. 4), which derive from the  
 996 calibrations simulations displayed in panels b-d.



997

998 **Figure 4.** Maps of PDC inundation probability at El Misti volcano imported in a GIS environment. Results are  
 999 expressed in percent. Each set of simulations took ~480 min on an Intel Core i5-2320 CPU at 3.00 GHz (~29 s per  
 1000 simulation). The input parameters used in these simulations derive from the calibrations displayed in Figure 3. The  
 1001 reference PDC deposit used for the numerical calibration of input parameters is displayed in green (2070 cal yr BP  
 1002 eruption; Charbonnier et al., 2020).

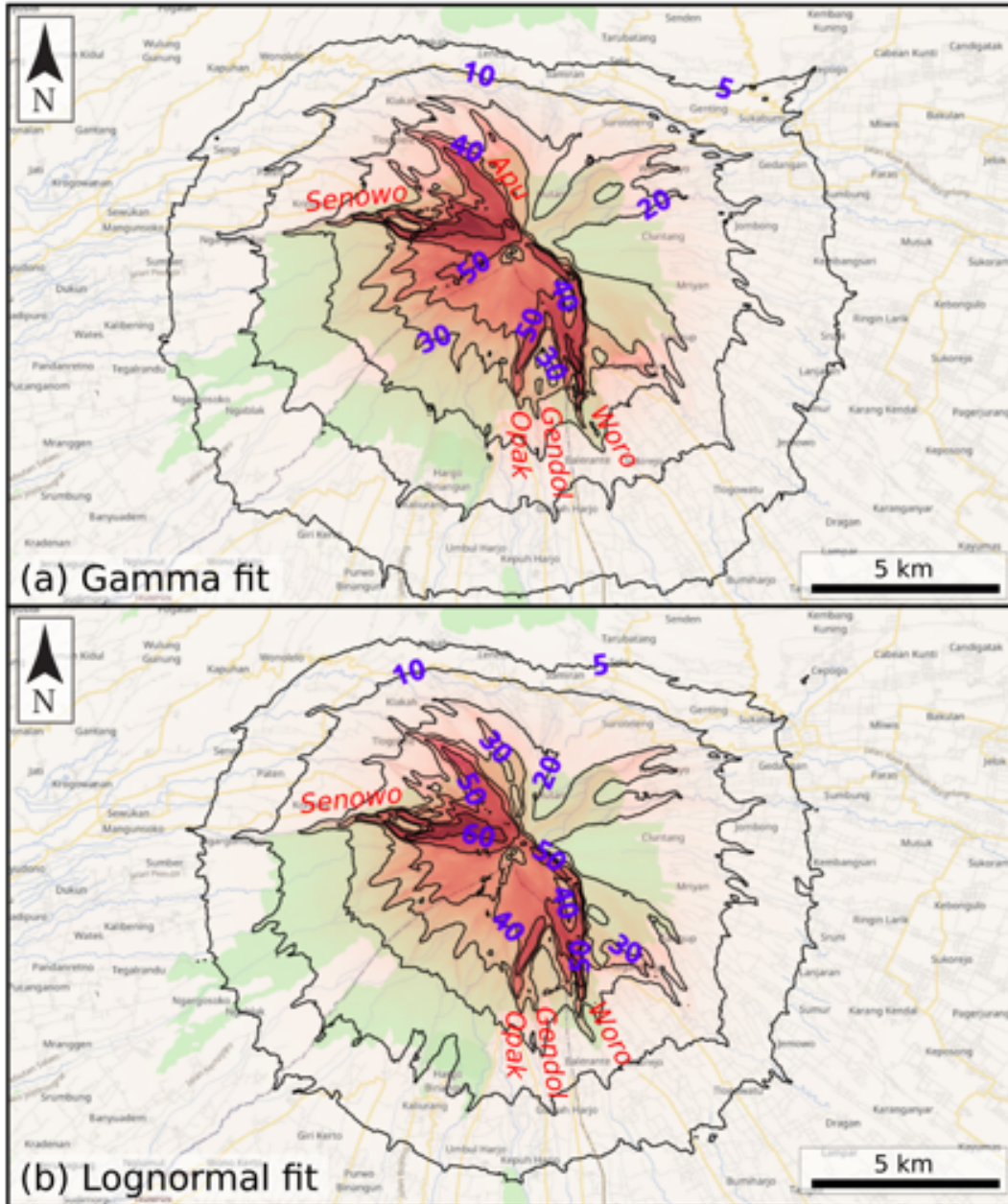
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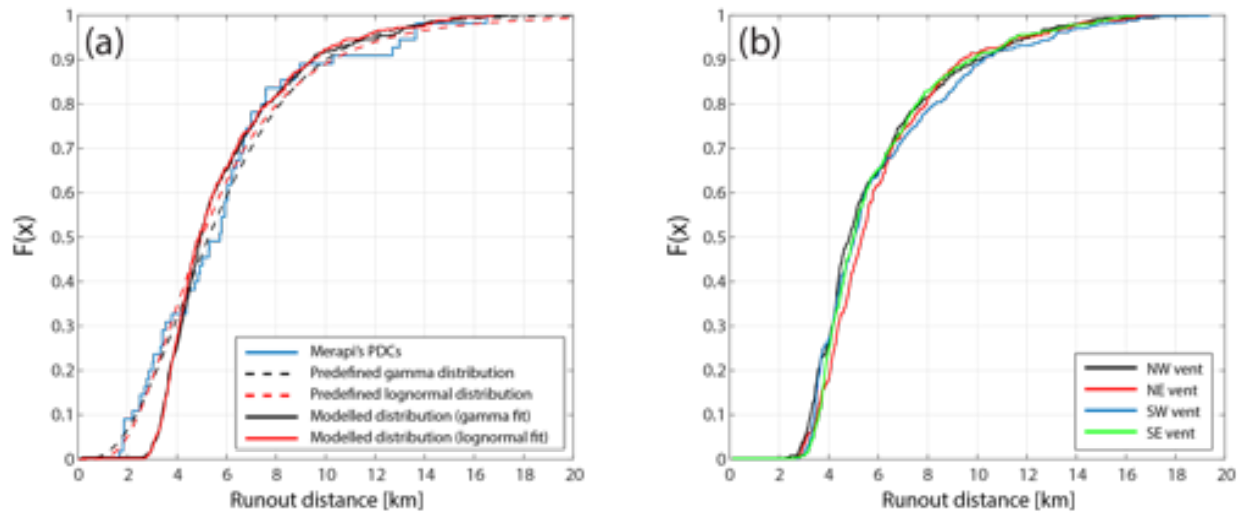
1005 **Figure 5.** (a-b) Pseudo-color plots of runout distance and inundation area derived from the set of calibration  
 1006 simulations performed for Merapi volcano. These calibration simulations took  $\sim 140$  min on an Intel Core i5-2320  
 1007 CPU at 3.00 GHz ( $\sim 21$  s per simulation). (c-d) PDF and CDF of the predefined probability distributions of runout  
 1008 distance used for the calibration of input parameters used in Merapi simulations. These distributions derive from  
 1009 fitting the data of 55 PDCs (Solikhin, 2015), which is displayed as a histogram (c) and an empirical cumulative  
 1010 curve (d), using gamma and lognormal probability distributions. (e-f) Sampling probability distribution of input  
 1011 parameters (collapse height and  $\tan(\phi)$ ) used in two sets of simulations performed for Merapi volcano (see Fig. 6).





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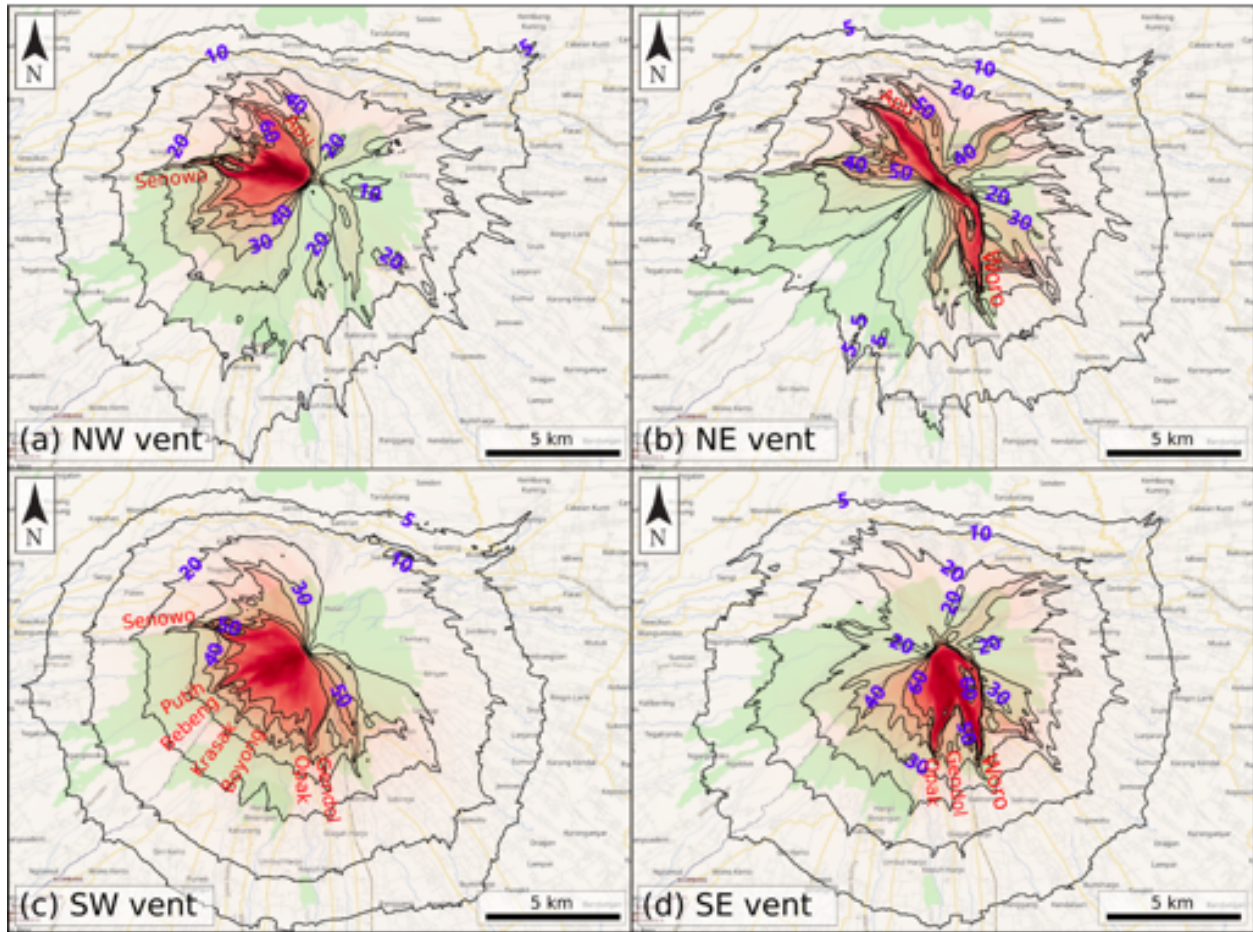
1014 **Figure 6.** Probability maps of PDC inundation at Merapi volcano constructed using the branching energy cone  
 1015 model. Collapse positions were sampled uniformly within a 300 m-radius circle in the volcanic summit while  
 1016 collapse parameters (i.e. collapse height and  $\tan(\varphi)$ ) were sampled considering the distribution of runout distance  
 1017 observed in the geological record (Solikhin, 2015). This data was fitted using gamma (a) and lognormal (b)  
 1018 probability distributions (Fig. 5c-f). Each set of simulations took ~120 min on an Intel Core i5-2320 CPU at 3.00  
 1019 GHz (~14 s per simulation). Results are expressed in percent.



1020

1021 **Figure 7.** (a) Empirical cumulative curves of runout distance in documented PDCs at Merapi and in the simulation  
 1022 sets presented in Figure 6. The predefined probability functions of runout distance, derived from fitting the data of  
 1023 documented PDCs (Solikhin, 2015) using both gamma and lognormal probability functions, are included. The  
 1024 differences between these curves are mainly related to the absence of runout distances lower than 2.5 km in the  
 1025 modeling results. (b) Empirical cumulative curves of runout distance in the simulation sets presented in Figure 8.

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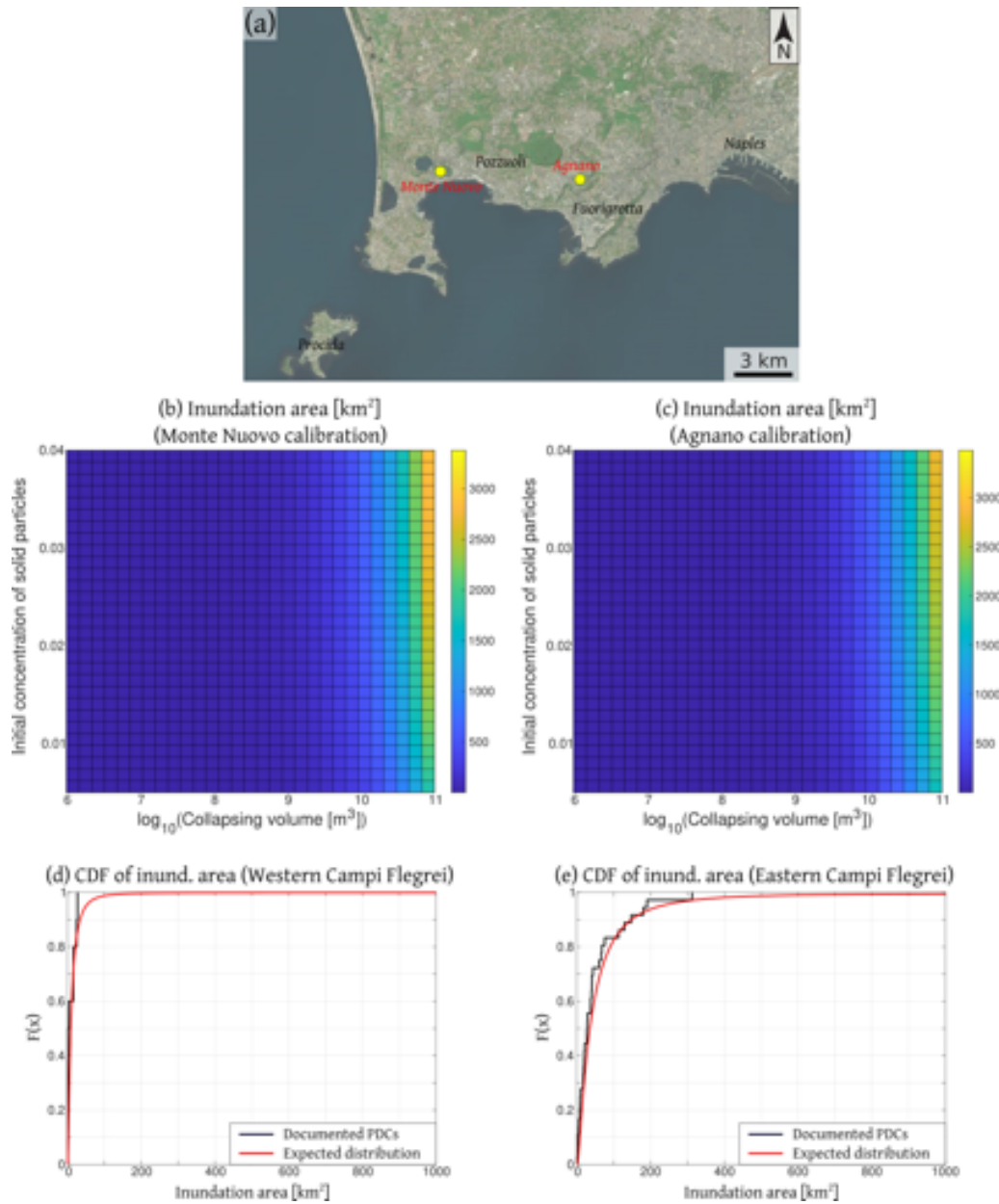


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1028 **Figure 8.** Probability maps of PDC inundation at Merapi volcano considering collapse positions in different flanks  
 1029 of the volcano. These maps were constructed using the branching energy cone model. Collapse positions were  
 1030 sampled uniformly within different regions of a 300 m-radius circle centered in the volcano summit. Four regions  
 1031 were considered: NW (a), NE (b), SW (c), and SE (d). Collapse parameters (i.e. collapse height and  $\tan(\varphi)$ ) were  
 1032 sampled considering the distribution of runout distance observed in the geological record (Solikhin, 2015). This data  
 1033 was fitted using a gamma probability distribution (Fig. 5c, e). Results are expressed in percent.

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1036 **Figure 9.** (a) Map of Campi Flegrei showing the points used as the collapse position in the calibration simulations.

1037 (b-c) Pseudo-color plots of inundation area derived from the set of calibration simulations performed for Campi

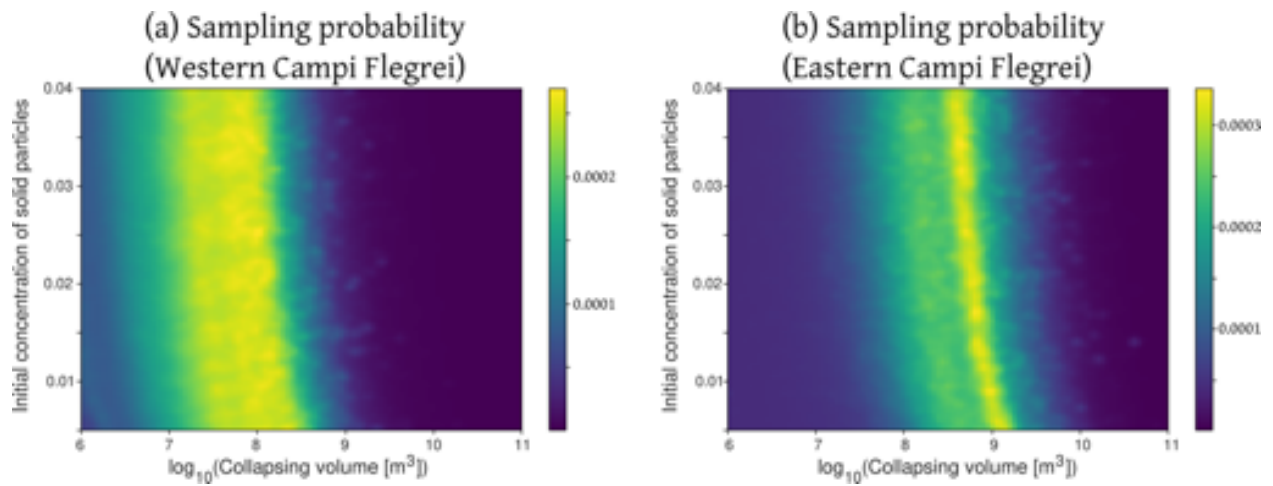
1038 Flegrei. (d-e) CDFs of the inundation area in documented PDCs at the western and eastern domains of Campi

1039 Flegrei and the expected probability distributions of this parameter, computed following Neri et al. (2015) and

1040 Bevilacqua et al. (2017) in order to consider the effect of eventual underestimations of the area of PDC deposits and

1041 the presence of “lost” deposits in the dataset.

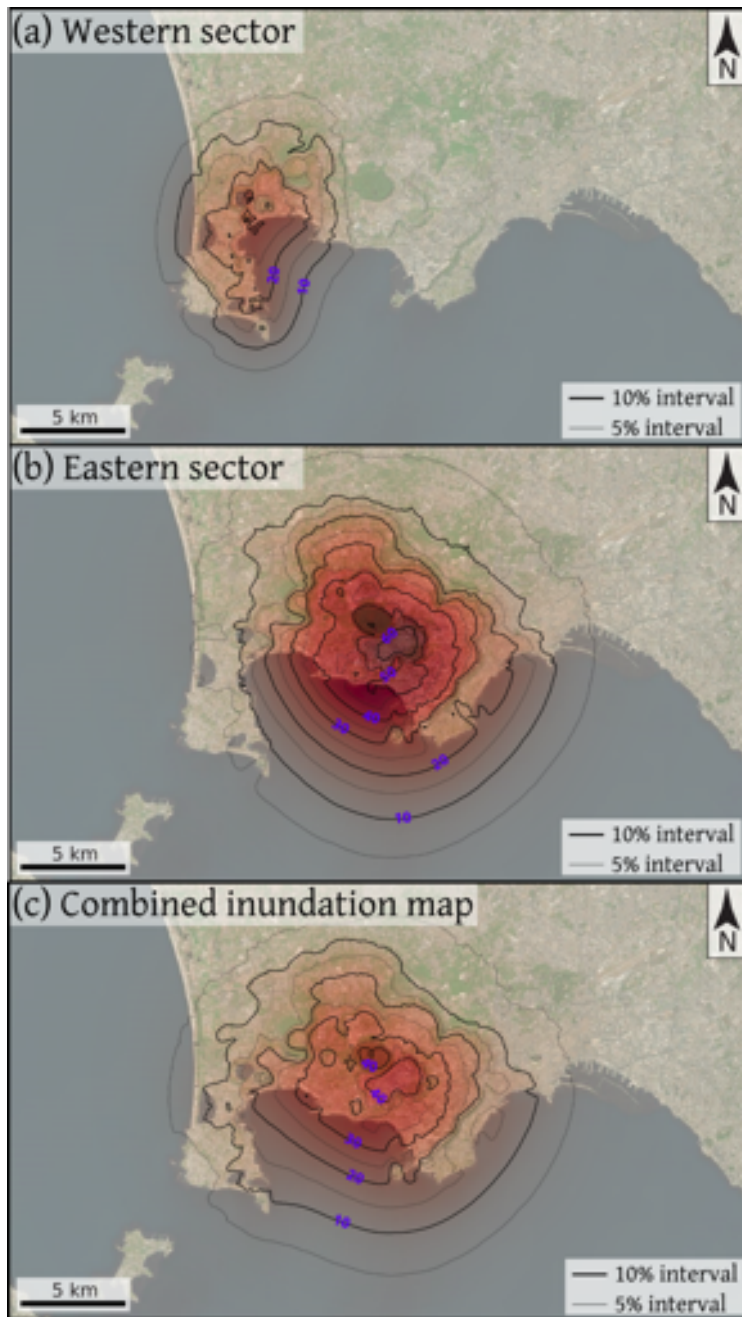
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1044 **Figure 10.** Sampling probability distributions of input parameters (collapsing volume and initial concentration of  
1045 solid particles) in two sets of simulations performed for Campi Flegrei (see Fig. 11).

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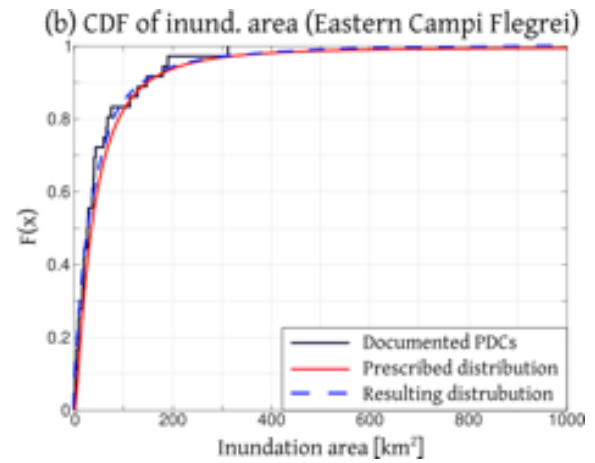
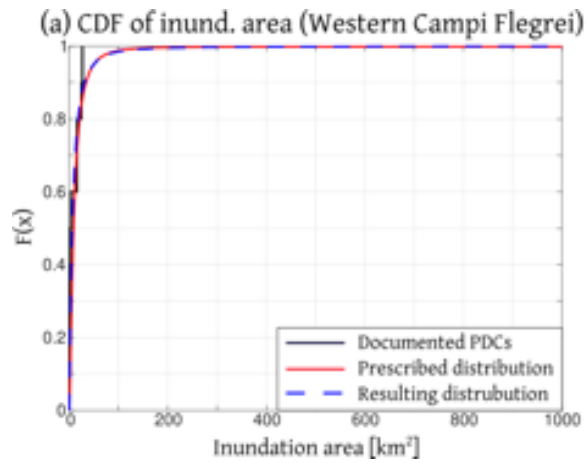
1048 **Figure 11.** Probability maps of PDC inundation at Campi Flegrei constructed using the traditional box model.

1049 Collapse positions were sampled from published vent opening probability maps (Neri et al, 2015; Bevilacqua et al.,

1050 2017), while the other model inputs were sampled considering calibrations based on the expected distribution of

1051 inundation area.

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1054 **Figure 12.** CDFs of the inundation area in documented PDCs at the western and eastern domains of Campi Flegrei,  
 1055 the expected probability distributions of this parameter (i.e. prescribed in our numerical simulations), and the  
 1056 resulting distributions of inundation area in the simulations presented in Figure 11.

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