

1 **A study on the influence of internal structures on the shape of pyroclastic particles**
2 **by X-ray microtomography investigations**

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27 **Abstract**

28 X-Ray computed microtomography is a non-destructive 3D imaging technique that can be used for
29 the investigation of both the morphology and internal structures of a solid object. Thanks to its
30 versatility, it is currently of common use in many research fields and applications, from medical
31 science to geosciences. The latter includes volcanology, where this analytical technique is becoming
32 increasingly popular, in particular for quantifying the shape as well as the internal structure of
33 particles constituting tephra deposits. Particle morphology plays a major role in controlling the
34 mobility of pyroclastic material in the atmosphere and particle-laden flows, while the internal

35 structure (e.g. vesicles and crystal content) is of importance in constraining the processes that
36 occurred in magmatic chambers or volcanic conduits.

37 In this paper, we present results of X-Ray microtomography morphological and textural analyses on
38 volcanic particles carried out to study how particle shape is influenced by internal structures. Particles
39 were selected from tephra generated during explosive eruptions of different magnitudes and
40 compositions. Results show that particle morphology is strongly influenced by internal structure,
41 which is characterized by textural features like vesicularity, vesicle and solid structure distribution,
42 vesicle inter-connectivity and distance between adjacent vesicles. These have been found to vary with
43 magma composition, vesiculation and crystallization history. Furthermore, our results confirm that
44 X-Ray microtomography is a powerful tool for investigating shape and internal structure of particles.
45 It allows us to both characterize the particle shape by means of tridimensional shape parameters and
46 relate them to their internal structures.

47

48 **Key words:** 3D sphericity, 3D fractal dimension, volcanic particles, particle shape,
49 microtomography, textural properties, vesicularity.

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52 1. INTRODUCTION

53 During explosive eruptions, particles of variable size, shape and density are injected into the
54 atmosphere and, depending on the eruptive size and style, can have an impact on human beings,
55 infrastructure and activities from local up to global scale [Blong, 1984; Casadevall 1994; Horwell
56 and Baxter, 2006; Bonadonna et al., 2012; Wilson et al. 2012, 2014; Beckett et al., 2015]. The
57 physical properties of pyroclastic particles (size, shape, density) affect their aerodynamic behavior,
58 i.e. the aerodynamic drag force. Many studies have been carried out over the past few decades
59 focusing on the dependency of the aerodynamic drag on particle shape, especially in the field of
60 multiphase flow dynamics [Sneed and Folk, 1958; Wilson and Huang, 1979; Haider and Levenspiel,
61 1989; Swamee and Ojha 1991; Ganser 1993; Rodrigue et al., 1994; Chien 1994; Taylor, 2002; Tran-
62 Cong et al., 2004; Dellino et al., 2005; Pfeiffer et al. 2005; Loth; 2008; Hölzer and Sommerfeld, 2008;
63 Mele et al., 2011; Dioguardi and Mele, 2015; Bagheri and Bonadonna, 2016; Dioguardi et al., 2017,
64 2018]. In these studies, several shape-dependent drag laws have been proposed, which depend on one
65 or more shape descriptors that are generally functions of 1D and 2D parameters. More recently, the
66 use of X-Ray microtomography (μ X-CT) has enabled improvements in the ability to investigate the
67 internal structures and morphologies of materials with a non-destructive and three-dimensional (3D)
68 visualization and quantification [Song et al., 2001; Ersoy et al., 2010; Voltolini et al., 2011; Baker et

69 al., 2012; Cnudde and Boone, 2013; Rausch et al., 2015; Vonlanthen et al. 2015; Bagheri et al., 2015;
70 Polacci et al., 2018]. In particular, 3D shape descriptors quantified by means of μ X-CT analyses have
71 been introduced and applied to predict the aerodynamic drag of volcanic particles [e.g. Dioguardi et
72 al. 2017].

73 Recently, Mele and Dioguardi [2018] presented a study on the dependency of particle shape on the
74 size of vesiculated volcanic juvenile particles analyzed with μ X-CT. The study proved how the shape
75 of these particles, which are commonly generated during explosive eruptions fed by evolved
76 vesiculated magmas, is the result of the interaction between particle size and the size distribution of
77 vesicles. This means that the general assumption made when simulating the transport of volcanic ash
78 in the atmosphere by means of dispersion models [e.g. Costa et al. 2006; Jones et al., 2007; Mastin et
79 al., 2013], i.e. assuming a size-independent particle shape, does not hold for these types of eruptions.
80 This is the assumption made, for example, by London VAAC when using the standard grainsize
81 distribution for operational forecasts [see Beckett et al. 2015]. Particle shape plays a crucial role in
82 the multiphase flows occurring on Earth's surface, including sandstorms [e.g. Kok et al., 2012,
83 Doronzo et al. 2015] and turbulent density currents [e.g. Branney and Kokelaar, 2002; Dufek, 2016;
84 Dioguardi and Mele, 2018; Dellino et al. 2018]. In fact, Dioguardi et al. [2014] showed how
85 implementing shape-dependent drag parametrizations into multiphase computational fluid dynamic
86 models improve their performance in predicting the particle trajectories and fall velocity.

87 With the aim of further investigating the dependency of particle shape on the internal texture of
88 volcanic particles, we carried out a systematic quantification of different internal textural properties
89 of volcanic particles collected from tephra fallout deposits of eruptions of different magnitudes, styles
90 and magma composition. In this paper, we first describe particle samples and the employed technique,
91 and then we present results of the analysis on the relationship between particle morphology and
92 internal structural characteristics, namely the fraction of vesicles and how these are inter-connected
93 and/or distributed.

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96 **2. MATERIALS AND METHOD**

97 In order to investigate the influence of internal texture on particle shape, we used the same set of
98 juvenile particles employed in Dioguardi et al. [2017]. The samples were from the juvenile
99 component of fallout deposits emplaced by the following eruptions: 1) Eyjafjallajökull 2010 [Dellino
100 et al., 2012] and Grímsvötn 2004 [Jude-Eton et al., 2012], eruptions of trachybasalt and basaltic
101 composition in Iceland, respectively; 2) Mt. Etna 2001 [Scollo et al., 2007], of basaltic composition
102 (trachybasalt); 3) Pomici di Avellino Plinian eruption of Vesuvius (3900 BP; Sulpizio et al., 2010),

103 of tephritic-phonolitic composition; 4) AD 472 (Pollena) sub-Plinian eruption of Vesuvius [Sulpizio
104 et al., 2005] of tephritic-phonolitic composition; 5) Agnano Monte-Spina Plinian eruption of Campi
105 Flegrei (4500 BP; de Vita et al., 1999), of trachytic composition. In this work, all particles were
106 generated during explosive eruptions driven by dry magmatic fragmentation [Dellino et al., 2001;
107 Sulpizio et al., 2005; Scollo et al., 2007; Sulpizio et al., 2010; Dellino et al., 2012], with the exception
108 of particles from the Grímsvötn 2004 eruption, which were the product of magma-water interaction
109 [Jude-Eton et al., 2012].

110 We used particles of the same grain-size interval, i.e. 0.500-0.355 mm because, as shown in Mele et
111 al. [2011] and Mele and Dioguardi [2018], they have a more irregular contour, including a significant
112 number of vesicles on the particle surface.

113 For each sample suite, the 3D external morphology and internal texture of 15 particles were
114 reconstructed by means of μ X-CT imaging with a Bruker Skyscan 1172 high-resolution μ X-CT
115 scanner. Particles were cleaned in an ultrasonic bath and mounted on a graphite rod holder using vinyl
116 glue. The parameters used for the acquisition of μ X-CT radiograph are shown in Table 1. In order to
117 detect vesicles across the widest possible range of sizes, particles were scanned with a pixel size of
118 1.02 μ m, which, as shown in Mele and Dioguardi [2018], is enough to sample the fine vesicle
119 population.

120 Bruker's NRecon software [Liu and Sasov, 2005] was used to reconstruct μ X-CT projection images
121 into two-dimensional cross sections (slices) by applying the Feldkamp algorithm [Feldkamp et al.,
122 1984]. Cross-section reconstruction parameters are shown in Table 1.

123 3D quantitative image analysis of shape and internal textures of particles was performed using
124 Bruker's CTAn software [Skyscan, 2009]. Each particle was segmented from the background (holder,
125 glue and air) using a global threshold [Otsu, 1979]. It is to be noted that by internal texture we mean
126 both vesicles and the solid structure. The latter is represented by both glass and crystals due to the
127 difficulty of discriminating between these two components using the microtomographic technique
128 since, in most cases, they have a similar X-Ray attenuation coefficient [Arzilli et al. 2016].

129 To quantify particle shape, the sphericity Φ_{3D} and Fractal dimension D_{3D} [Dioguardi et al. 2017] were
130 calculated.

131 Sphericity is defined by:

$$132 \quad \Phi_{3D} = \frac{A_{sph}}{A_p} = \frac{\sqrt[3]{(6V_p)^2}}{A_p} \quad (1)$$

133 where A_{sph} is the surface area of the sphere equivalent to the particle of volume V_p and A_p is the
134 particle surface area. The calculation of particle volume, i.e. the number of voxels of the binarised
135 solid object times the volume of one voxel, is carried out by means of the hexahedral marching cubes

136 volume model [Lorensen and Cline, 1987]. The 3D particle surface area calculation is based on the
137 faceted surface of the marching cubes volume model [Lorensen and Cline, 1987]. By definition, Φ_{3D}
138 ranges between 0 and 1, being 1 the value of a perfect sphere.

139 Fractal dimension (D_{3D}) is defined by:

$$140 L = ks^{-D_{3D}} \quad (2)$$

141 where L is the length of the fractal line approximating the contour of the object with ever-decreasing
142 segments of length scale s , D_{3D} is the fractal dimension and k is a number. Graphically D_{3D} is the
143 slope of the line in the plot $\log(L)$ vs. $\log(s)$. D_{3D} was calculated by an algorithm based on the “box
144 counting” method [Chappard et al., 2001], by which the 3D digital object is approximated by an array
145 of equal-sized cubes, which are counted. The procedure is repeated over a range of cube sizes, and
146 the number of cubes is plotted against cube size in a log-log plot. D_{3D} is the slope of the regression
147 line. D_{3D} is equal to 2 for a sphere. The more D_{3D} is larger than 2, the more a particle is irregular in
148 shape

149 As far as the internal structure analysis is concerned, for each particle a Volume of Interest (VOI)
150 with the same shape of particle without vesicles was created by a shrink-wrap operation (Figure 1).
151 The latter was necessary in order to investigate the total size-range of vesicles inside particles.

152 The following parameters were then evaluated: vesicularity, vesicle-size distribution, solid structure
153 distribution, surface convexity index of vesicles and structure linear density of vesicles.

154 Vesicularity (%) is defined as the fraction of the total volume of a sample occupied by vesicles or
155 voids, encompassing open and closed vesicles, i.e. the volume of all open plus closed pores as percent
156 of the total VOI volume.

157 Vesicle-size or solid structure distribution (mm) are the fractions of vesicle or solid structure volume
158 that are within a specific range of vesicle size. Its calculation involves two steps: skeletonisation,
159 which identifies the medial axes of all vesicles or solid structures, and sphere-fitting that measures
160 the local thickness for all the voxels lying along this axis [Remy and Thiel, 2002]. The average
161 diameter and standard deviation of vesicle and solid structure size distribution were also calculated.

162 Surface convexity index of vesicles (mm^{-1}), also known as Fragmentation index, is characterized by
163 the rupture of connectivity [Hahn et al., 1992; Promentilla et al. 2009]. It is calculated by comparing
164 volume and surface of binarised vesicles before and after a single voxel image dilation, i.e.

$$165 FI = \frac{S_1 - S_2}{V_1 - V_2} \quad (3)$$

166 where S and V are vesicle surface and volume and the subscript numbers 1 and 2 mean before and
167 after image dilation. The more negative the surface convexity index is, the greater is the vesicle
168 connectivity.

169 Structure linear density of vesicles (mm^{-1}), also known in medical sciences as the trabecular number,
170 is the number of vesicles per unit length on a linear path through the structure, given by the inverse
171 of the mean distance between the medial axes of the vesicle structure [Hildebrand et al., 1999]. High
172 structure linear density value means that the thickness of solid structure, which separates vesicles, is
173 small; i.e. vesicles are very close together.

174

175 3. RESULTS

176 The averages and standard deviations of all the measured parameters are listed in Table 2; Figure 2
177 shows the typical morphologies of representative particles chosen from each sample suite illustrated
178 by 3D volume rendering. Data show that the Avellino and Grímsvötn particles represent the two end-
179 members of both vesicularity and particle shape measured ranges. Grímsvötn particles display the
180 lowermost vesicularity and the highest sphericity and the lowermost fractal dimensions (Table 2)
181 whereas particles sampled from the Avellino eruption deposits are the most irregular of the analyzed
182 samples.

183 We then determined the vesicle size distribution of all the particles of every sample suite; the
184 distributions are shown in Figure 3. Two different groups can be clearly discerned by a simple first
185 qualitative analysis of the vesicle size distribution: Avellino, Pollena and Agnano Monte Spina on
186 one side (Group 1), Eyjafjallajökull, Grímsvötn and Etna particles on the other (Group 2). Group 1
187 particles show a finer vesicle population and a narrower distribution than particles of Group 2.
188 Interestingly, samples from eruptions of similar composition tend to group together: Group 1 include
189 samples of eruptions fed by tephritic-phonolitic and trachytic vesiculated magmas; Group 2 is made
190 by particles from basaltic and trachybasaltic eruptions. A similar trend can be inferred from the plots
191 of the solid structure distribution (Figure 3). Particles from Group 1 are characterized by a thinner
192 solid structure than basaltic and trachybasaltic particles, which on the contrary show a very variable
193 thickness of the solid structure (Figure 3). Comparing the average size of both vesicles and solid
194 structures (Figure 2), we can observe that particles of Group 1 are characterized by both smaller
195 vesicles and a less thick solid structure than basaltic particles (Group 2), although few particles of
196 Avellino, Pollena and Agnano Monte Spina eruptions have a thick solid structure. This can be
197 attributed to:

- 198 - the presence of large phenocrysts (Figure 2), which are characterized by a solid structure
199 histogram with a different population (for example grey and black solid structure histograms
200 of Pollena particles and green histogram of Avellino particles; Figure 3);
- 201 - poorly vesiculated particle with tubular vesicles (Agnano Monte Spina particles, Figure 2 and
202 light blue histogram of Figure 3) or;

203 - highly vesiculated particle with a portion of poorly vesiculated glass (Agnano Monte Spina
204 particles, Figure 2; orange histogram of Figure 3).

205 Eyjafjallajökull and Etna particles show coarser vesicles than Avellino, Pollena and Agnano Monte
206 Spina particles, and display a wide range of solid structure size (Figures 2, 3). However,
207 Eyjafjallajökull particles have smaller structure thickness values than those of Etna, except for three
208 particles, which have a thick solid structure due to the presence of large phenocrysts (Figure 2). In
209 general, for Etna particles, the thick solid structure is mainly related to a higher content of large
210 phenocrysts than Eyjafjallajökull particles (Figure 2). Grímsvötn particles show the largest range
211 of vesicle size with a thick solid structure, which is mainly represented by glass (Figure 2).

212 It was also observed that the solid structure is well correlated with particle vesicularity (Figure 4); in
213 particular, the thinner the solid structure, the greater the particle vesicularity. This behavior is further
214 corroborated by the significant correlation between structure linear density of vesicles and
215 vesicularity (Figure 4), i.e. the distance between vesicles decreases (i.e. the structure linear density
216 value increases) with increasing particle vesicularity. The latter show also a negative correlation with
217 the surface convexity index, i.e. vesicularity increases as surface convexity index decreases, meaning
218 that vesicles are better inter-connected (Figure 4).

219 Concerning the influence of internal texture on particle shape, Figure 5 shows that with increasing
220 vesicularity, Φ_{3D} decreases and D_{3D} increases, i.e. particles are more irregular. Furthermore, a
221 particle's irregularity increases with decreasing thickness of the solid structure, hence decreasing the
222 distance between vesicles and with increasing inter-connection of vesicles (Figure 5). It is notable
223 that particle shape is well-constrained by a thorough analysis of all parameters related to the internal
224 structure. For example, Avellino particles tend to be more irregular than Agnano Monte Spina
225 particles, despite having a similar vesicle and solid structure distribution (Figure 3) and the same
226 vesicularity range (Figure 5). This difference of shape can instead be attributed to a higher inter-
227 connectivity and lower distance between vesicles of Avellino particles than Agnano Monte Spina
228 particles (Figure 5).

229 In addition, results suggest how particles produced by magma of the same composition and by similar
230 fragmentation processes (Group 1 and 2 above) might not display similar shape parameters. For
231 example, Avellino and Pollena particles have different shapes (Table 2, Figure 5) that can be related
232 to both a different vesiculation and crystallization history as shown by the vesicularity, surface
233 convexity index, solid structure thickness and structure linear density parameters (Figure 5).
234 Furthermore, these particles display the same vesicle size (Figures 2, 3) but Pollena particles are less
235 vesiculated with a poor inter-connectivity of vesicles than Avellino particles (Figure 5). Finally,
236 Pollena particles have a thicker solid structure, which is reflected in a greater distance between

237 vesicles (Figures 4, 5), caused by both a greater thickness of the glass and a greater presence of
238 phenocrysts (Fig. 6).

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240

241 4. CONCLUSIONS

242 The use of μ X-CT has allowed us to demonstrate that particle shape, which is here described by
243 sphericity Φ_{3D} and fractal dimension D_{3D} , is strongly influenced by the internal structure of particles,
244 here quantified by means of vesicularity, vesicle and solid structure distribution, vesicle inter-
245 connectivity and distance between adjacent vesicles. These textural features have been found to vary
246 with magma composition and show that volcanic particles collected from tephra fallout deposits of
247 eruptions of different magnitudes, styles and magma composition show different shapes.

248 This work highlights that, for modelling purposes, the assumption that particles of different eruptions,
249 which are produced by magma of the same composition and by similar fragmentation processes, have
250 the same shape, might not be correct. Therefore, it is necessary to obtain particle shape for each case
251 study.

252 Furthermore, our results confirm that μ X-CT is a powerful tool for investigating the shape and
253 internal structure of particles. It both allows us to characterize the shape of irregular particles by
254 means of tridimensional shape parameters and to relate them to the internal structures of particles.

255

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515 **Tables**

516

μX-CT scanner parameters		Reconstruction parameters	
Pixel Size (μm)	1.02	Smoothing	1
X-ray Voltage (kV)	48	Ring Artifact correction	6
X-ray Current (μA)	208	Beam Hardening Correction (%)	56
Rotation Step (degrees)	0.37	-	

Filter	No filter	-
Frame averaging	5	-

517 Table 1. Scan parameters of the μ X-CT scanner and cross-section reconstruction.
518
519

	unit	Eyjafjallajökull	Grímsvötn	Etna	Avellino	Agnano M. Spina	Pollena
Object volume	mm ³	0.041±0.014	0.039±0.013	0.041±0.009	0.035±0.011	0.041±0.021	0.047±0.010
Vesicularity	%	23.8±11.9	16.0±6.4	16.2±9.5	48.0±9.9	39.3±14.0	24.9±7,6
Solid structure size	mm	0.052±0.024	0.062±0.024	0.069±0.032	0.016±0.011	0.019±0.010	0.027±0.017
Vesicle size	mm	0.029±0.016	0.042±0.021	0.029±0.017	0.018±0.010	0.017±0.010	0.018±0.011
Surface convexity index	1/mm	107.5±28.7	104.2±16.8	133.5±35.2	31.8±46.6	93.6±64.0	167.6±47.2
Structure linear density	1/mm	8.38±4.71	4.31±2.62	5.64±2.97	27.35±3.51	21.96±5.49	14.40±4.96
D_{3D}	-	2.288±0.095	2.165±0.058	2.230±0.093	2.564±0.057	2.445±0.154	2.288±0.141
Φ_{3D}	-	0.244±0.096	0.383±0.075	0.314±0.102	0.073±0.040	0.151±0.134	0.316±0.139

520
521 Table 2. Average values and standard deviations of 3D parameters of all analyzed particles.
522

523
524 **Figure Captions**

525 Figure 1. Two examples of segmentation and creation of VOI (Volume of interest) by means of
526 shrink-wrap operation. a, b and c: raw, binary and ROI (Region of Interest) images of one cross
527 section of a Grímsvötn particle. d, e and f: raw, binary and ROI (Region of Interest) images of one
528 cross section of a Agnano Monte Spina particle.

529
530 Figure 2. Solid structure size vs. vesicle size diagram. 3D surface rendering and cross section images
531 of few particles are also insert. The red line inside the reconstructed particles indicates the position
532 of the displayed cross section image.

533
534 Figure 3. Vesicle and solid structure distribution histograms of all analyzed particles.

535
536 Figure 4. Structure linear density, solid structure size and surface convexity index vs. vesicularity
537 diagrams of all analyzed particles. -

538

539 Figure 5. Sphericity Φ_{3D} and fractal dimension D_{3D} vs. vesicularity, surface convexity index, solid
540 structure size and structure linear density diagrams of all analyzed particles.

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542 Figure 6. 3D surface rendering (with Maximum intensity projection function) and cross section image
543 of two particles of Avellino and Pollena eruption. The red line inside the reconstructed particles
544 indicates the position of the displayed cross section image.

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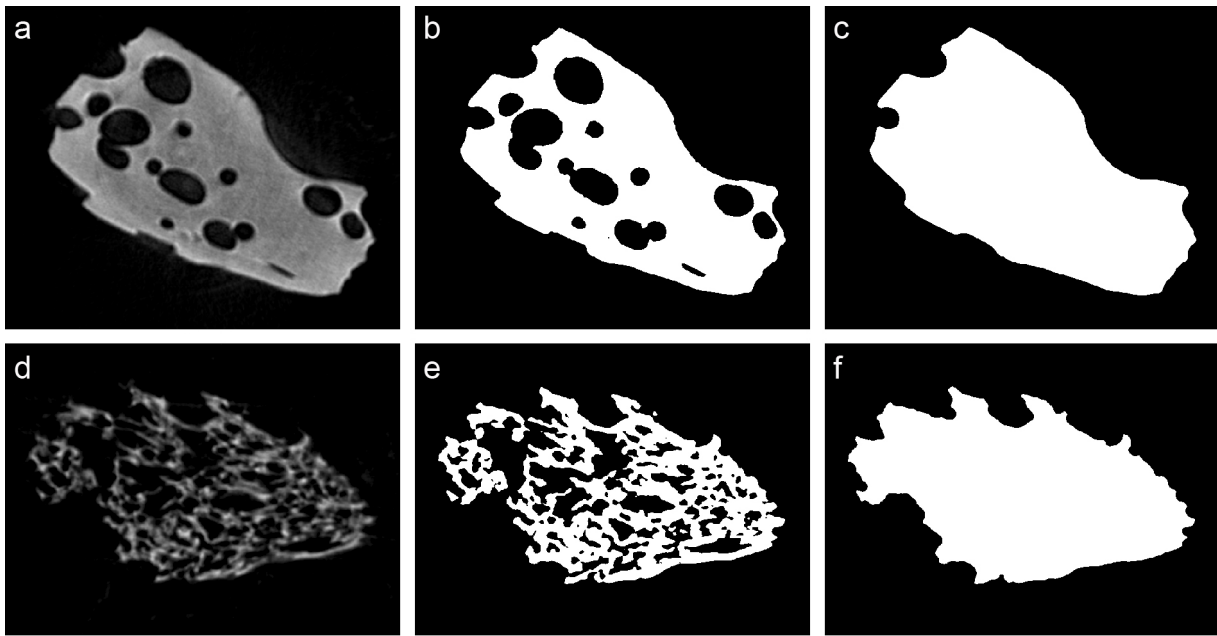
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572 Figure 1

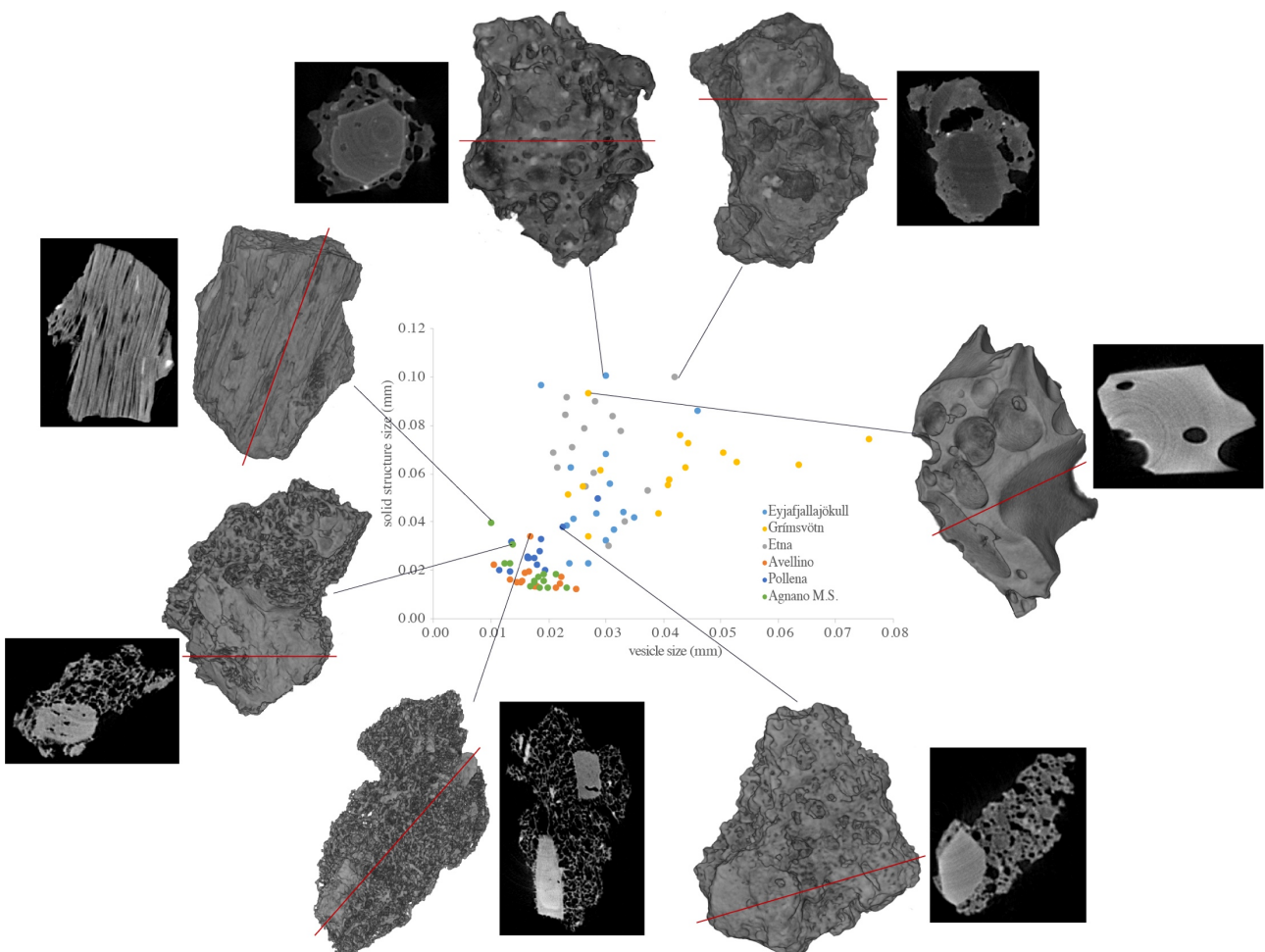


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575 Figure 2

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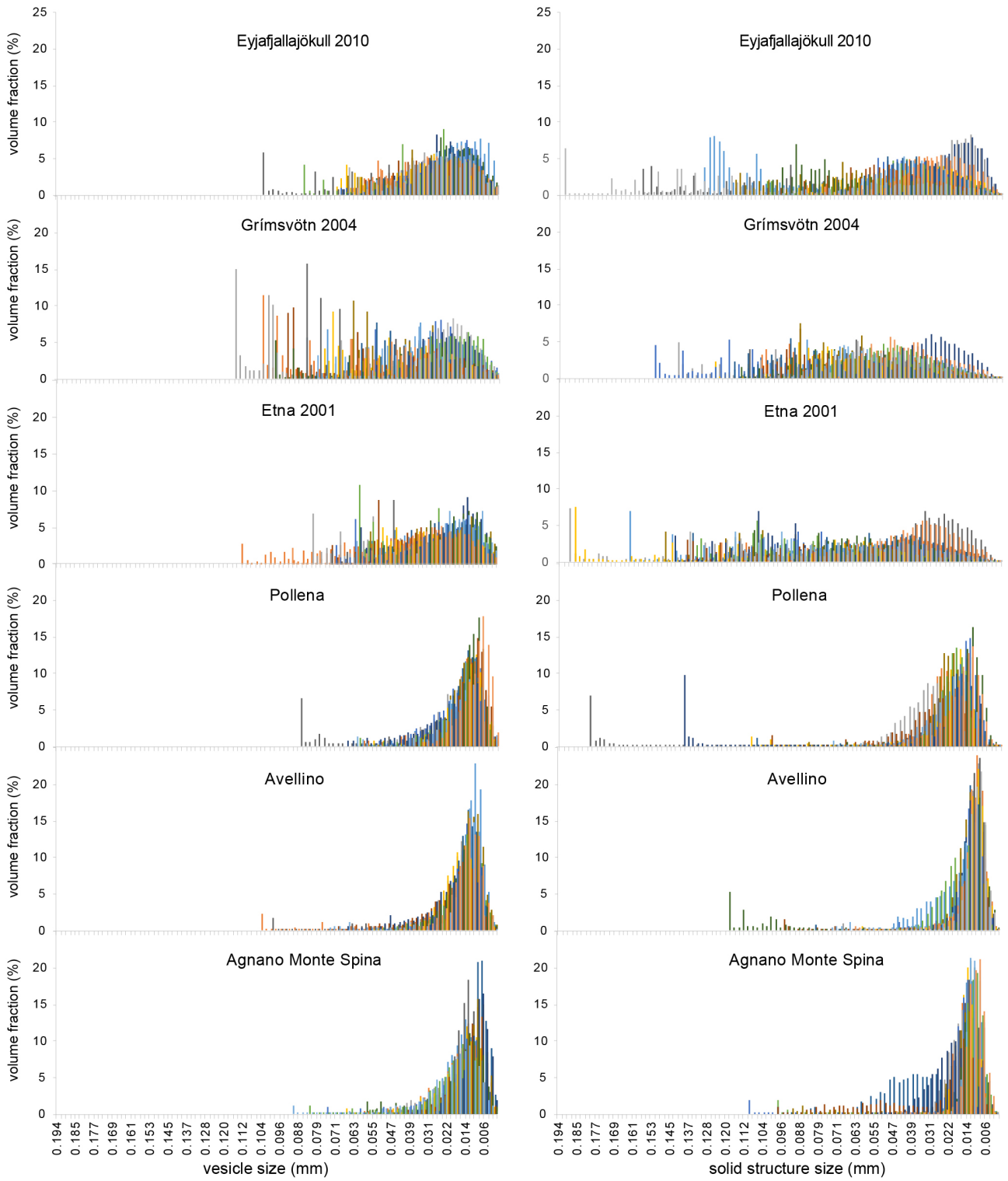


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579 Figure 3

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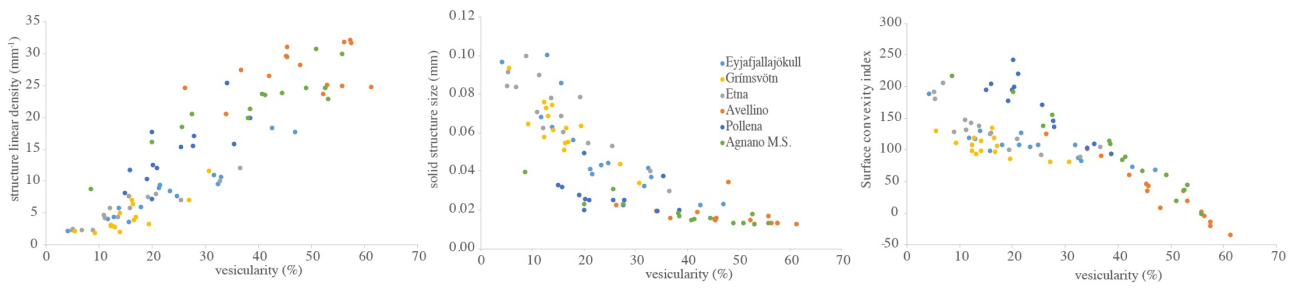
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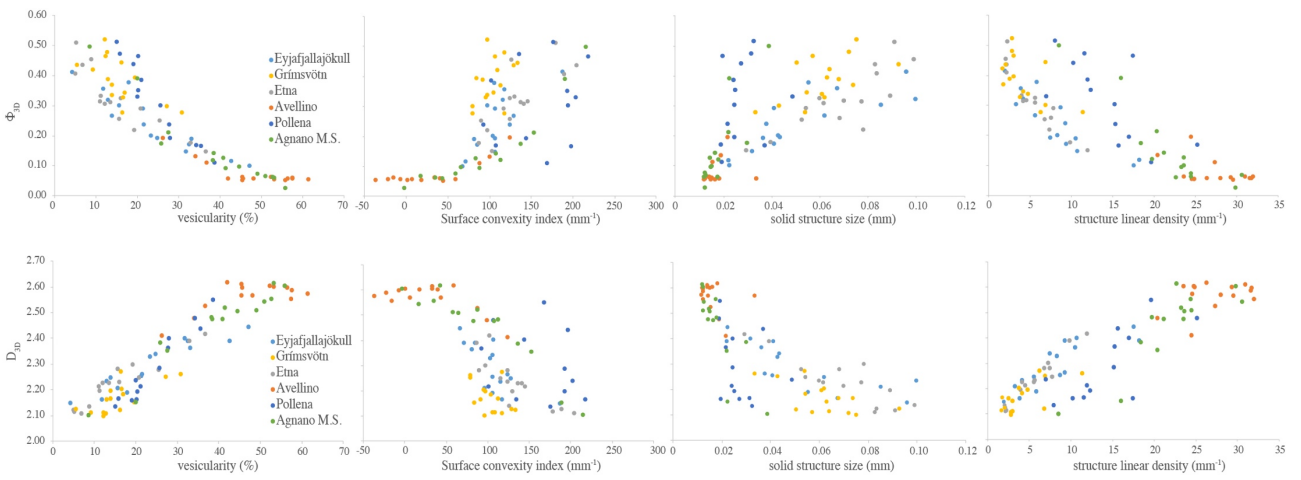
587 Figure 4



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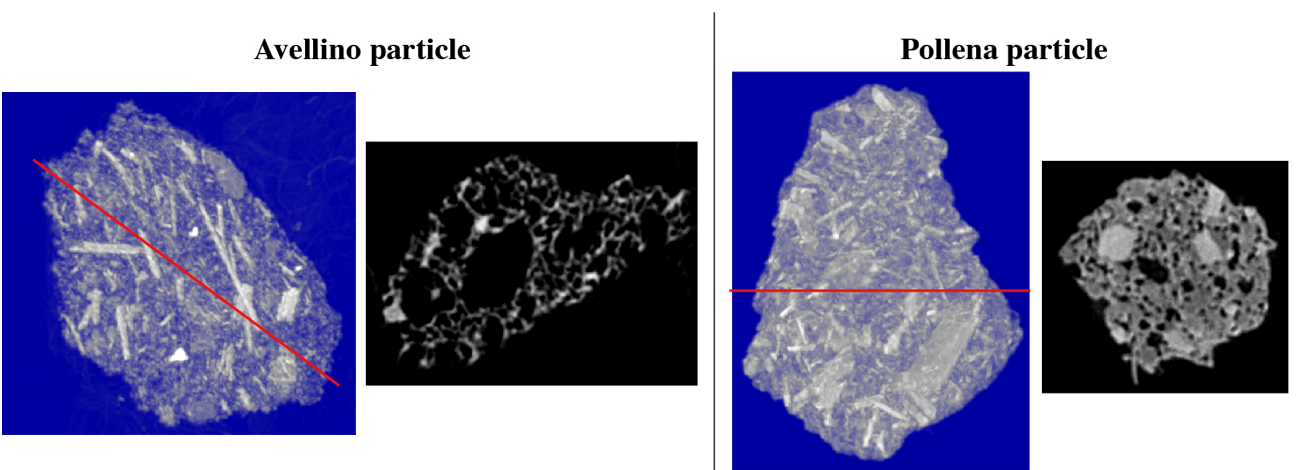
590 Figure 5



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593 Figure 6



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