1   **Fluid-dynamics of the 1997 Boxing Day volcanic blast on Montserrat, W.I.**

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9   **Abstract.** *Directed volcanic blasts* are powerful explosions with a significant laterally-

10   directed component, which can generate devastating, high-energy pyroclastic density currents

11   (PDCs). Such blasts are an important class of eruptive phenomena, but quantified

12   understanding of their dynamics and effects is still incomplete. Here we use 2D and 3D

13   multiparticle thermofluid dynamic flow codes to examine a powerful volcanic blast that

14   occurred on Montserrat in December 1997. Based on the simulations, we divide the blast

15   into three phases; an initial burst phase lasts roughly 5 s and involves rapid expansion of the

16   gas-pyroclast mixture, a gravitational collapse phase which occurs when the erupted material

17   fails to mix with sufficient air to form a buoyant column and thus collapses asymmetrically,

18   and a PDC phase which is dominated by motion parallel to the ground surface and is

19   influenced by topography. We vary key input parameters such as total gas energy and total

20   solid mass to understand their influence on simulations, and compare the simulations with

21   independent field observations of damage and deposits, demonstrating that the models

22   generally capture important large-scale features of the natural phenomenon. We also

23   examine the 2D and 3D model results to estimate the flow Mach number and conclude that

24   the range of damage sustained at villages on Montserrat can be reasonably explained by the

25   spatial and temporal distribution of the dynamic pressure associated with subsonic PDCs.

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1. Introduction

Directed volcanic blasts are powerful explosions with a significant laterally-directed component, which can generate devastating, high-energy pyroclastic density currents. Volcanic blasts have had violent consequences at Bezymianny, Russia, in 1956 [Belousov, 1996], and Mt. St. Helens, USA in 1980 [Hoblitt et al., 1981; Moore and Sisson, 1981; Waitt, 1981; Fisher et al., 1987; Fisher, 1990; Druitt, 1992]. They represent an important and extremely hazardous class of eruptive phenomena, and consideration of blasts and their associated pyroclastic density currents (PDCs) is necessary for modern volcanic hazard zonation at stratovolcanoes [Crandell and Hoblitt, 1986]. However, quantified prediction of their dynamics and effects is still possible only at a generalized level, often involving simplifying assumptions, such as one- or two-dimensional, steady, and/or choked flow [e.g., Kieffer, 1981; Woods et al., 2002].

The term "*directed volcanic blast*" was suggested for the first time by Gorshkov [1959], who studied the eruption of Bezymianny volcano in Kamchatka in 1956. This directed blast was observed only from large distances, and thus the main conclusions about mechanisms of the event were based on interpretations of the effects and deposits of the eruption. The very similar explosive eruption of Mount St. Helens in 1980 [Lipman and Mullineaux, 1981] rekindled a worldwide interest in directed blasts, and the mass and variety of observations, monitoring data, photo-documentation, and detailed geologic studies at Mount St. Helens enabled a quantum improvement in understanding of the basic causative mechanisms. It was observed that the large-scale collapse of the volcanic edifice, which transformed into a debris avalanche, was the event that triggered a directed explosion by suddenly exposing a pressurized body of magma and gas to atmospheric pressure [Voight, 1981; Voight et al., 1981, 1983; Glicken, 1998]. This explosion, and the pyroclastic density current that it generated, devastated a large area of complex topography and left deposits closely resembling those of Bezymianny [Hoblitt et al., 1981; Moore and Sisson, 1981; Waitt, 1981; Kieffer, 1981; Walker and McBroome, 1983; Brantley and Waitt 1988; Fisher et al., 1987; Fisher, 1990; Druitt, 1992; Sisson, 1995; Bursik et al., 1998; Belousov et al., 2007].

Through deposit studies and field observations, it has been generally recognized that an initially-pressurized lava dome or cryptodome, suddenly depressurized by a slope failure, can create a directed blast. However, controls on the strength, direction and physics of the initial explosion, its subsequent transformation to a PDC, and propagation of the PDC across incised volcanic topography, require further analysis, with 3D analysis required to capture

60 full interaction with topography.   This capability has been lacking in the past in
61 computational fluid dynamics modeling of explosive volcanic phenomena.

62   The recent directed blast from the Soufrière Hills volcano (SHV), Montserrat,
63 provides the opportunity to further improve our understanding of blast dynamics. This blast
64 and associated PDC eradicated the village of St. Patricks and substantially damaged much of
65 the southern part of the island, on 26 December (Boxing Day) 1997 (Figures 1, 2). In this
66 case, despite the severity of the event, no lives were lost because a pre-emptive evacuation
67 was enforced, based on recognition of flank instability and the anticipation of a blast [Young
68 et al., 2002]. The resulting deposits and destructive effects have been well studied [Sparks et
69 al., 2002; Ritchie et al., 2002; Voight et al., 2002; Baxter et al., 2005], and thus despite
70 certain limitations, and apart from the images recorded uniquely at Mount St. Helens, the
71 database for this event is unsurpassed for eruptions of this type.

72   Here we perform a preliminary study using a 2D cylindrical-coordinate model, which
73 allows us to efficiently parameterize the effect of the initial dome mass and energy on the
74 blast behavior and to constrain appropriate initial conditions for later implementation in the
75 3D model. We then apply a fully 3D multiphase flow model incorporating realistic 3D
76 topography, using initial conditions constrained by field observations. We compare these
77 runs against the field observations of the Montserrat event, in order to demonstrate broad-
78 scale similarity between natural phenomena and our model results. We also use the 3D
79 results to demonstrate relationships between the flow dynamics and initial conditions,
80 topography, spatial location, and time, within the context of the model assumptions.

81   The effects of gas compressibility and shock waves on the eruption dynamics was
82 first investigated by Nairn [1976] and Nairn and Self [1978] for vertical explosions. Some
83 authors modeled the directed blast at Mount St. Helens as a quasi-steady-state overpressured,
84 supersonic jet, accompanied by internal shock structures and compressibility effects [Kieffer,
85 1981, 1984; Kieffer and Sturtevant 1984, 1988; Wohletz and Valentine, 1990]. Here, we use
86 *directed blast* simply to denote an explosion, caused by decompression of a cryptodome or
87 lava dome, with a significant initial lateral component and an asymmetric deposit distribution
88 due to an asymmetric source geometry and/or edifice morphology. A contested question is
89 whether the preponderance of strong damage observed in volcanic directed blasts should be
90 attributed to air shocks [Wohletz et al., 1984; Wohletz 1998], supersonic flow within an
91 overpressured jet [Kieffer 1981, 1984], or flow dynamic pressure [Sparks et al., 2002; Baxter
92 et al., 2005; Esposti Ongaro et al., 2005] and (possibly) shocks within the energetic collapse
93 and PDC (gravity current) phases. Exploring this issue is an additional goal of this paper.

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2. Observational constraints on the Boxing Day blast

At Soufrière Hills Volcano (SHV) in December 1997, an andesite dome and talus cone with a volume of 113×10^6 m^3 was growing above the hydrothermally altered and unstable south flank of the volcano. Gravitational collapse of the flank on 26 December triggered an explosive decompression of the dome's interior, to form a violent blast and PDC that traveled >4 km overland, and then continued >3 km over the sea surface [Voight et al., 2002; Sparks et al., 2002; Hart et al., 2004]. The volume of material (dense rock equivalent, DRE) involved in the failure was estimated from the dimensions of the failure scars and by comparison with pre-collapse topography [Sparks et al., 2002; Voight et al., 2002]: c. 20-30 $\times$ 10^6 m^3 from the south flank hot spring area, c. 5×10^6 m^3 from the old crater rim, c. 25×10^6 m^3 from the lava dome that had grown between 6 November and 26 December, and about 30 $\times 10^6$ m^3 of lava talus. We take the volume of dome lava participating in the blast as ~25 $\times$ 10^6 m^3 (DRE), exclusive of additional materials that may have been incorporated through erosion. The lava volume is relatively well constrained, but the volume of entrained material is not well constrained due to offshore deposition [Hart et al., 2004]. The total duration of strong activity was ~11.6 min but occurred in several pulses. The volatile components in the blast came from the andesite, and the material comprising the blast was a complex multiphase vapor-liquid-solid mixture.

Seismic data suggest 6 pulses [Sparks et al., 2002], and stratigraphy reveals clearly only two depositional events, and at least two erosional events resulting from relatively large pulses [Ritchie et al., 2002]. Thus two seismic events are not accounted for in the stratigraphy. It is possible they were both largely erosional onshore or perhaps early deposits were eroded by later pulses, leaving no record observed on land. The individual pulses were short lived, lasting but a few minutes. Only 2-3 $\times 10^6$ m^3 DRE was deposited on land with the remainder entering the sea or elutriated by co-PDC plumes. Our constraints are poor but we estimate the small pulse volumes to be ~1 to 5×10^6 m^3 DRE, with the minimum value bounded by the volume per pulse deposited on land. The large pulses were two or three times the volume of the small pulses, based on seismic magnitudes, with the sum of all pulses being about 25×10^6 m^3 DRE plus eroded and entrained materials. Co-PDC plumes reached a height ~15 km asl, with two separate parts, an ash-rich upper part, and an ash-poor lower part rich in condensed steam [Pace et al., 1998; Mayberry et al., 2002]. The latter is inferred to be a consequence of the PDC entering the sea. The airborne ash was about 15-20% of the original PDC volume [Sparks et al., 2002].

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The area devastated on land was ~10 km^2 with some pulses affecting a 70° sector and a much smaller pulse depositing mainly over only a 35° sector (Fig. 2). The damage varied from complete destruction in the central axial region, to lesser physical effects such as blown out windows and roofs, and fire damage, in peripheral areas [Sparks et al., 2002; Baxter et al., 2005]. The destruction was complete in the axial area of the blast near the village of St. Patricks where structures were razed to their foundations, with detached structural components (including building walls) flattened to the ground or carried to the sea along with loose debris. Buildings swept away include stone-built structures and those with poured reinforced concrete walls. Trees with trunks up to 1m in diameter were removed entirely leaving only abraded stumps and roots [Sparks et al., 2002]. Entrained boulders and pieces of destroyed buildings added to the destructive capability of the PDCs in addition to dynamic pressure [Baxter et al., 2005]. East of the axial area of the blast zone and the White River valley, the blast zone is dominated by erosional features across the raised shoulder of an older volcanic edifice. The severity of damage decreases systematically, but with local variability, from the axis of the PDC towards the lateral periphery. One kilometer west of the axial zone, the top floors of houses were blown down and scattered 50 m down slope, impact marks from saltating boulders occur on house walls facing the volcano, and trucks and a bulldozer were flung over a cliff onto the beach [Sparks et al., 2002; Baxter et al., 2005]. Although trees up to 50 cm in diameter were broken a few meters above ground, smaller trees (<10 cm trunks) and shrubs were merely bent over with branches stripped and the trunk tip sharpened by abrasion. Still farther from the axis, house walls were damaged, roofs were partially or entirely removed, and cars were crumpled and displaced tens of meters. At the western lateral limit of damage, 200-m from source, damage was limited to in-blown windows and displaced roof tiles and blown-down wooden sheds [Sparks et al., 2002]. Dynamic pressures estimated from the damage ranged from >25 kPa in the central axial region to 1-3 kPa near the periphery, with local fluctuations of about ~1-5 kPa associated with localized sheltering and topographic effects [Baxter et al., 2005].

There are several other constraints on the dynamics of the Boxing Day event. The upper part of the current climbed almost to the summit of South Soufrière Hills (SSH), from the saddle between Galways Mountain and South Soufrière Hills [Fig. 2; Sparks et al., 2002]. The trimline representing the upper surface of the current descends the side of Galways Mountain to the saddle at about 600 m a.s.l., where the current collided with the South Soufrière Hills and climbed 150 m further. Converting kinetic to potential energy for the

162 height climbed in the Galways-SSH peripheral zone results in 55 m s^{-1} for the upper part of
163 the current in this region [Sparks et al., 2002].

164   A reliable but limited constraint on dynamics is given by the St Patricks seismic
165 station, MSPT, about 3.4 km from the dome [Voight et al., 2002; Sparks et al., 2002]. The
166 initial collapse began about 03:01.0 LT (the signal is emergent, making it difficult to pick
167 onset time), the first stronger seismic pulses began at 03:01.8 LT and 03:02.8 LT,
168 respectively, and MSPT was destroyed at 03:03.3 LT [Sparks et al., 2002]. If one assumes
169 that the blast pulse that destroyed MSPT began during the first seismic pulse, the implication
170 is that average frontal speeds were 38-56 m s^{-1}. An alternative interpretation is that the first
171 seismic pulse represented mainly edifice collapse and debris avalanche movement, and that
172 the second, sharp, seismic pulse represented the blast initiation. This interpretation yields an
173 average frontal blast velocity of 113 m s^{-1}. Nevertheless, focusing exclusively on *average*
174 velocities could be misleading since modeling presented here and observations at SHV
175 [Sparks et al., 2002] and Mount St Helens [Voight, 1981; Moore and Rice, 1984; Hickson,
176 1990; Hoblitt, 2000; Belousov et al., 2007] illustrate that velocities were not constant. We
177 therefore discuss temporal and spatial distribution of blast characteristics from both an
178 observational and modeling perspective later in the text.

179   Dynamic pressure estimates for the pyroclastic density current presented above
180 [Sparks et al., 2002] were calculated from building damage following the approach of
181 Valentine [1998a], where dynamic impact pressures in pyroclastic currents were compared
182 with pressures required to damage structures in atomic explosions. The dynamic pressure P_d
183 is half the product of current mixture density and velocity squared, so that velocity can be
184 calculated if current density is known. Sparks et al. [2002] assumed a mass fraction of gas in
185 the flow and calculated a current density of 6 kg m^{-3}. Using this density, about five times that
186 of ambient air, they concluded that maximum velocities could have been ~30-40 m s^{-1} in the
187 peripheral area near Kinsale, >40 m s^{-1} near Germans Ghaut, and >>60 m s^{-1} at St. Patricks.

188

189 **3. Blast modeling**

190   Previous steps toward conceptual and quantified understanding of directed blast
191 behavior illuminated many features of the phenomenon. For example, the lateral blast at
192 Mount St. Helens was modeled as a horizontal quasi-steady-state, underexpanded, supersonic
193 jet with perfect coupling between gas and solid phases [Kieffer, 1981]. These results found
194 limited support in numerical simulations by Wohletz and Valentine [1990], who also
195 explored shock effects in vertical explosions. For Montserrat, modeling of decompression

196 and dome fragmentation [Woods et al., 2002] were combined with an analytical 1D ash-flow

197 model to illustrate basic controls on runout distance and dynamic pressure of the directed

198 blast [Sparks et al., 2002]. Here we assume the model of lava dome pressurization presented

199 by Woods et al. [2002], and apply 2D and 3D unsteady multiphase models of pyroclastic

200 dispersal to the rapid decompression of that dome.

201 Our approach builds upon that of Woods et al. [2002] and effectively extends it in

202 several ways. First, flow in volcanic blasts is highly unsteady and the source conditions are

203 reported to be impulsive. We therefore calculate the rapid decompression of a lava dome with

204 finite mass and gas energy, which creates an impulsive source for our blast model. Second,

205 we relax the assumption of perfect coupling between the gas and solid phase (pseudogas

206 assumption) and thus treat the multiphase aspects of the blast (discussed in the model section

207 below). The perfect coupling assumption is reasonable only for particles ≤30 microns in

208 diameter [Woods, 1995; Neri et al., 2003], while recent work synthesizing deposit data shows

209 that ~88% of directed-blast clasts exceed 30 microns [Belousov et al., 2007]. Furthermore,

210 high acceleration in the initial phases of blasts is likely to produce high levels of decoupling

211 between solid and gas phases. Both conditions make relaxing the pseudogas assumption

212 desirable and potentially important. Third, we treat the system in 3D allowing the effects of

213 complex topography on flow propagation to be explicitly explored. In a directed-blast the

214 exposed vent and lava- or cryptodome geometry direct much of the momentum at angles

215 highly oblique to the vertical [Voight, 1981; Belousov et al., 2007]. Moreover, flow

216 channeling and azimuthal variations in topography have particular importance in evolution of

217 the flow [Belousov, 1996; Hoblitt et al., 1981; Ritchie et al., 2002]. Evidence of flow

218 channeling at distances from the vent greater than several km was observed at SHV [Sparks

219 et al., 2002; Druitt et al., 2002] and Mount St. Helens [Hoblitt et al., 1981; Kieffer, 1981;

220 Waitt, 1981], revealing that channels allowed dangerous flows to move far from the blast

221 axis, and cause destruction in locations that would not necessarily have been predicted by

222 intuition or by 2D simulations. Furthermore, tree blowdown patterns at MSH [Waitt, 1981;

223 Kieffer, 1981] provide evidence of topography-initiated flow separation and formation of

224 large-scale eddies. As a result of rugged topography, damage was highly variable over

225 relatively short spatial scales.

226

227 **3.1. Physical and numerical model**

228 Motivated by the aforementioned factors, our model describes the dynamics of

229 directed blasts by adopting the multiphase transport theory [Gidaspow, 1994; Valentine

230   1998b; Dartevelle, 2004]. Accordingly, each phase of the mixture (gas, liquid, and solid with

231   specific characteristics) is described separately from the others by solving the corresponding

232   mass, momentum, and energy balance equations. The model thus describes the kinetic and

233   thermal disequilibrium of the gas and particles, and the interphase momentum and energy

234   exchange. In detail, we adopted the PDAC (*Pyroclastic Dispersal Analysis Code*) code

235   [Esposti Ongaro et al., 2007; Neri et al., 2007], which solves the multiphase flow equations

236   on two and three-dimensional domains with topography imported from a digital elevation

237   model (DEM). This code is an evolutionary advance from the KFIX code developed at the

238   Los Alamos National Laboratory (USA) in the mid 70's [Rivard and Torrey, 1977], and

239   further developed along one evolutionary branch at the Illinois Institute of Technology (US)

240   for fluidization engineering studies [Gidaspow, 1994]. The basic model formulation and

241   algorithm derive from the work of Harlow and Amsden [1975], in which classical iterative

242   methods for subsonic flows were extended to the compressible and supersonic regime and to

243   multiphase flows. The details of these models are given by Neri et al. [2003], Dartevelle

244   [2004], and Esposti Ongaro et al. [2007].

245   This approach makes it possible to investigate the dispersal of pyroclasts in the

246   atmosphere and along the volcano flanks without the need of *a priori* assumptions and *ad-hoc*

247   parameterizations of the flow features (e.g., the transient 3D feature allows effective

248   description of flow characteristics in the different regions of the system, the turbulent

249   entrainment is explicitly simulated through the large eddies of the flow and only

250   parameterized at the subgrid scale, the particle settling velocity is computed explicitly by the

251   model as a function of flow properties and need not be specified *a priori*). Moreover, the

252   possibility of using different particle classes gives us the opportunity to investigate the

253   different dispersal pattern of each particle size as well as the effect of their relative proportion

254   on the flow behavior.

255   Nevertheless, several limitations to our model formulation still exist. Present model

256   formulation is limited to solid volume fraction less than about 50 vol.%. Above this

257   threshold, the flow likely enters a frictional regime requiring a different set of constitutive

258   equations. Moreover, although the model describes the sedimentation and stratification

259   within the flow (as well as particle elutriation) through the settling of different particle

260   classes, an explicit deposition model (i.e. particle loss from the ground boundary condition) is

261   not included at this time in the formulation, so that particles are assumed to remain fluidized

262   at all times. A recent study by Dufek and Bergantz [2007] has shown that deposition through

263   a leaky boundary can significantly decrease runout distance, therefore our estimates should

264 be considered liberal in this respect. However, on Montserrat on land, because of the steep

265 slopes there was little deposition and the stronger pulses were erosive. So for the modeling in

266 this paper, the lack of a deposition subroutine seems unimportant. Similarly, erosion and

267 entrainment of substrate material into the density current are not explicitly considered in our

268 model. The thermal interactions between the hot PDCs and the sea surface, and phase

269 changes (condensation) of water vapor, are not specifically treated. However, water vapor

270 condensation is possible only in the upper region of the computational domain, as verified by

271 computing *a posteriori* the water vapour saturation pressure as a function of local pressure,

272 temperature and concentration.

273 Full model verification and validation is an ongoing endeavor, especially for 3D

274 flows, including "validation" against natural events, with new regimes and dynamic

275 conditions being tested continually. To this aim, several applications of the PDAC code in 2D

276 have been successfully carried out in the last decade to assess the model's ability to capture

277 the behavior of compressible, dilute, turbulent multiphase flows. Neri and Gidaspow [2000]

278 have compared 2D cylindrical and Cartesian model solutions to fluidization experiments in

279 order to test the formulation of the particulate phase. Similarly, the gas turbulence subgrid

280 model has been validated against experiments of gas flow around a bluff-body [Barsotti,

281 2002]. The accuracy of compressible flow simulations was also tested for both one- and two-

282 dimensional shock tubes and supersonic jets by comparison against analytical solutions and

283 well-validated results obtained by other codes [Esposti Ongaro et al., 2006, 2007]. Clarke et

284 al. [2002a,b] compared solutions of PDAC2D against well-documented Vulcanian explosions

285 on Montserrat in 1997.

286

287 **3.2 Initial conditions for the multiphase flow model**

288 Initial source conditions are as follows. The dome is represented as a hemisphere on a

289 sloping base with uniform gas volume fraction of 0.1, based on measurements given by

290 Robertson et al. [1998] and Melnik and Sparks [2002]. During the effusive phase, the dome

291 grows as degassed magma reaches the interior or surface of the dome, while the exsolved

292 volatiles separate from the magma and travel through the permeable dome to the atmosphere

293 [Melnik and Sparks, 1999; Sparks et al., 2002]. Models of viscous conduit flow with gas

294 escape show that overpressures of several MPa can develop near the conduit exit, where

295 overpressure is taken as the difference between gas pressure and local lithostatic pressure

296 [Sparks, 1997; Melnik and Sparks, 2002]. The overpressure is only partially dissipated by gas

297 escape through the permeable dome. We use the Woods et al. [2002] permeable hemisphere

298   model to determine initial pressure profiles within the lava dome prior to the blast, for a

299   steady gas (steam) flux of ~400 kg s^{-1} and dome permeability K. The gas flux is consistent

300   with measured magma extrusion rates of ~8 m^3 s^{-1} for December 1997 [Sparks et al., 1998],

301   and bulk volatile content ~2 wt% [Barclay et al., 1998]. No COSPEC measurements were

302   made during December 1997, but this result is conservative with correlated SO_2 flux with

303   magma output, ~680 g SO_2 per tonne of magma [Young et al., 1998] and H_2O/SO_2 ratios of

304   200-1000 [Woods et al., 2002]. Measurements of dome rock suggest permeability values in

305   the range K = 10^{-14} to 10^{-12} m^2, including the effects of pervasive fractures [Melnik and

306   Sparks, 2002]. Gas is assumed to be steam with a temperature of 850° C and vapor viscosity

307   2×10^{-5} Pa s [Woods et al., 2002]. These results yield overpressures of the order 5-10 MPa

308   throughout much of the dome for K = 10^{-12} m^2, and higher values for lower permeability. For

309   the range of permeabilities considered, the mass of solid fraction ranges from 12 to 25×10^9

310   kg, whereas the net mass of exsolved gas (water vapor) in the dome ranges from 3 to 15×10^6

311   kg. This is an important result that constrains the dynamics of the fragmenting mixture. Such

312   pressurized domes have two to three orders of magnitude less exsolved volatiles per mass of

313   magma than is present in a typical Plinian eruption, and this leads to a substantially greater

314   density of the pyroclastic currents produced [Woods et al., 2002].

315   The particle size distribution of the Boxing Day blast deposit was estimated by

316   Ritchie et al. [2002] using well-established sedimentological techniques, although much

317   uncertainty remains in the characterization of pyroclastic mixtures, particularly when large

318   portions of the flow are lost to sea. Based on these deposit studies and additional field work

319   of our own, we use three particle sizes (5000 μm; 500 μm; 50 μm) to represent particle

320   classes >2000 μm, ~125 μm, and <125 μm, respectively, yielding the bulk proportions 25,

321   40, 35 wt%. A density of 2300 kg m^{-3} is used for the largest particle size, otherwise particle

322   density is 2600 kg m^{-3}. Although the three populations cannot cover the full spectrum of

323   grain sizes in the deposits, particularly the coarse tail, our choice was dictated by both

324   computational efficiency and the physical model (constitutive equations) which cannot treat

325   clasts larger than several mm. Furthermore, the model does not treat changes in grain size

326   due to aggregation and secondary fragmentation, processes which have yet to be

327   quantitatively characterized. We refer the reader to previous work which explicitly explores

328   the effects of grain size simplifications on 2D model results [Neri and Macedonio, 1996; Neri

329   et al., 2003] and leave the corresponding 3D study for future work.

330   The volume of dome lava involved in the blast and its associated high-energy PDC

331   was ~25×10^6 m^3 dense rock equivalent (DRE). This value is relatively well constrained, but

332   because the total duration of strong activity was ~11.6 min and occurred in several pulses, we

333   partitioned the total volume into smaller quantities representing individual pulses. Our main

334   constraint is on the *total* volume of original dome, which limits the sum of individual pulse

335   volumes, apart from additional materials entrained. For our models we therefore consider

336   representative volumes of ~5 and 10×10^6 m^3 DRE, representing relatively small and large

337   pulses, according to arguments outlined in Section 2.

338

339   **4. 2D Simulation results**

340   Before conducting the 3D simulations, we performed a number of 2D sensitivity runs

341   using PDAC. Here we present three of these, illustrating the influence of solid mass (or

342   volume), and gas energy (via the influence of permeability on dome pressurization), on flow

343   evolution. The first comparison between simulations examines the influence of mass released

344   by varying volume DRE (5 and 10×10^6 m^3), independently of permeability, which remains

345   constant at K = 10^{-12} m^2. The second comparison examines the effects of gas pressure and

346   energy, by varying pre-blast dome permeability (K = 10^{-12} m^2 and 10^{-14} m^2), while keeping

347   volume constant at 5×10^6 m^3 (Table 1). The computational domain extends 10 km radially

348   and 8 km vertically, with a non-uniform mesh resolution increasing very gradually, from 10

349   m close the left boundary axis of symmetry and above the topography, to 100m on the right

350   edge and the top atmospheric boundaries. The non-uniform mesh allowed us to increase the

351   resolution in the regions near the source and the ground, where we observe the largest

352   gradients in the flow variables. The location of the topographic profile used in all 2D

353   simulations is shown in Fig 2 (A-A') and includes the offshore sea surface. Although the

354   dense basal portion of pyroclastic flows can travel underwater, pyroclastic surges on

355   Montserrat have been observed gliding over the sea [Montserrat Volcano Observatory,

356   unpublished data; Hart et al., 2004].

357

358   **4.1 Large-scale features**

359   Simulation A-2D uses a high permeability value of K = 10^{-12} m^2 resulting in internal

360   gas pressures from 10 MPa at the base of the dome to atmospheric at the surface   The solids

361   volume $V_{DRE} = 5 \times 10^6$ m^3 assumed for the ~70° sector corresponded to a mass per unit angle

362   of ($5 \times 10^6/2\pi$) × (360/70) m^3/radiant for input in the cylindrical coordinate simulation. An

363   estimate of the volatile energy stored in the dome is given by the specific work, and the range

364   of values (see Table 1) correspond to purely adiabatic (lower limit) or purely isothermal

365   (upper limit) expansions [Woods et al., 2002]: E_s = 320-490 J kg^{-1}. Simulation B-2D uses a

366   greater dome volume of 2X that of A-2D (V_{DRE} = 10 × 10^6 m^3 for the 70° sector; E_s = 390-

367   610 J kg^{-1}), but is otherwise nearly identical to A-2D. The specific energy is slightly greater

368   in B-2D due to the non-linearity of the pressure distribution within the dome. Simulation C-

369   2D uses K = 10^{-14} m^2, which results in greater interior pressures and much higher gas energy:

370   E_s = 1880-3380 J kg^{-1}. The volume is identical to A-2D.

371   In simulation A-2D (Figure 3), an initial quasi-spherical expansion occurred, reaching

372   maximum gas velocity of ~160 m s^{-1} at 0.2 s. Corresponding peak particle velocities varied

373   with particle size; 75, 125, and 155 m s^{-1} for particle diameters of 5000, 500, and 50 μm,

374   respectively. Lateral velocities were greater than vertical by 0.3 s. At 2 s, the vertical mixture

375   speed was ~120 m s^{-1}, and horizontal speed was 170 m s^{-1}. We call this first stage the burst

376   phase, in which the dynamics are primarily controlled by gas expansion and associated

377   particle acceleration, and are strongly affected by the initial total specific gas energy.

378   Velocities in the burst phase are generally higher than the sound speed of the pyroclast

379   mixture, which is much lower than the atmospheric sound speed because of the relatively

380   high particle concentration. Nevertheless, we propose that any leading atmospheric pressure

381   wave was weak [(p_{after}/p_{before}) < 1.5] for three reasons; the initial velocities of the pyroclast

382   mixture were much less than sound speed in atmosphere, ~330 m s^{-1} at standard ground

383   conditions, the pressurized fluid was a solid-gas mixture with a low gas volume fraction, and

384   the pressure ratio between the dome's interior and the atmosphere prior to blast initiation was

385   less than 100 [Chojnicki et al., 2006].

386   The erupted material fails to mix with sufficient air to form a buoyant column and

387   thus, at t > 5 s, collapses below the source, initiating the collapse phase (Fig. 3a). The

388   material then moves parallel to the ground surface in the PDC phase beginning between 15

389   and 20 s after onset (Fig. 4). The transition from initial burst to PDC phase is highlighted by

390   the trajectories of the fluid parcels from 0 to 15 s (Fig. 3b). The trajectories are characterized,

391   in the first seconds, by ballistic paths, where the outermost portions of the dispersed dome

392   pyroclasts reach the maximum height (>1300 m a.s.l., 250 m above the dome). We interpret

393   the start of the collapse phase as the point in time when a preponderance of "ballistic" paths

394   have passed peak height and are inclined downward and outward. The phases defined here

395   are to some extent gradational.

396   The transformation to the PDC was mostly complete by 15-20 s, with the flow front

397   ~1 km from source, and PDC velocity about 70 m s^{-1}. The evolution of the PDC is illustrated

398   by the isocontours of the total particle volumetric fraction at selected times in Fig. 4. At 40 s

399   the PDC head has reached a distance of about 2700 m from the source where particles start to

400   be elutriated by vertical convection. Mixing of the PDC with the atmospheric air occurs

401   mainly through the entrainment at the flow head, as evidenced by the thickened nose. At 90s

402   the flow head has reached 5 km and has grown by air entrainment and expansion. A vertical

403   convective plume is rising above the vent and small co-PDC clouds are developing where

404   topographic slope abruptly changes and because of vortex instability in the tail. At 180s the

405   elutriation of particles by co-PDC plumes is more developed, while the velocity of the PDC

406   head is greatly reduced, and now consists of a dilute ash current overlying a dense basal flow.

407   Nevertheless, it is worth recalling that the boundary condition at the bottom does not account

408   for the interaction of the PDC with the sea surface or for the loss of particles by deposition so

409   that the run-out of this thin basal flow could be overestimated, especially using a coarse mesh

410   [Neri et al., 2003; Dartevelle et al., 2004; Appendix]. At 240 s the PDC head has stopped and

411   an intense co-PDC plume develops at 6 km, while a dense basal flow has reached the distance

412   of 10 km. The animation of the results better represents the temporal evolution of the burst

413   and PDC propagation and can be seen on Movie S1 in the on-line auxiliary material.

414   In simulation A-2D, more than 95% of the total solid mass fed into the PDC. A small

415   fraction (less than 5%) of the mass fed the plume above the dome (Fig 4 at 90s). Co-PDC

416   plumes developed downslope after ~80 s, reflecting gravity segregation of fine versus coarse

417   particles in the PDC, and development of mixture buoyancy by air entrainment; the plumes

418   elutriated about 50% of 50 μm, 20% of 500 μm, and a negligible fraction of 5000 μm

419   particles. The mass in the PDC was computed by integrating the particle bulk density in the

420   sub-domain where R > 1 km and Z < 0.9 km, whereas elutriation by the co-PDC was

421   calculated over the sub-domain where Z > 0.9 km.

422   Simulation B-2D begins with double the dome volume of A-2D, with parameters

423   otherwise the same. B-2D produced the longest runout PDC of all 2D simulations due to its

424   higher mass. Initial quasi-spherical expansion in the burst phase achieved peak gas velocities

425   ~160 m s^{-1} at 0.2 s, but peak particle velocities varied with particle size. The burst phases of

426   A-2D and B-2D are very similar, because the specific gas expansion energy is of the same

427   order of magnitude (Table 1). At 2 s, vertical mixture speed was ~115 m s^{-1}, and horizontal

428   speed was 200 m s^{-1} (Fig. 5a). The erupted material failed to become buoyant and at t > 5 s,

429 and collapsed below the vent. The current then moved parallel to the ground surface in the
430 PDC phase at t > 10 s, with the flow front ~1 km from source, and slope-parallel velocities of
431 roughly 80 m s^{-1}. The trajectories of the fluid particles are similar to A-2D, with a very short
432 expansion phase followed by the sudden collapse of the stream (Fig. 5b).

433   The temporal evolution of the B-2D PDC is similar to A-2D up to 90s (Fig. 6 and
434 Movie S2 in auxiliary material), although the flow front moves faster due to higher inertia.
435 The main differences can be observed after 130s when the flow head does not significantly
436 slow down while the co-PDC plumes begin to develop in the flow tail. Instead, at 180s the
437 PDC head structure is preserved without showing significant deceleration and has reached a
438 distance of 10 km. The elutriation of particles occurs only in the PDC tail, so that it exerts a
439 negligible effect.

440   Next we examine simulation C-2D, which begins with a dome volume identical to A-
441 2D but K has been reduced to 10^{-14} m^2. The lower permeability results in greater interior
442 pressures of several tens of MPa and much higher gas energy than A-2D. Because these
443 magnitudes exceed previous estimates of conduit pressures [Clarke et al., 2002a,b; Voight et
444 al., 1999], we consider this an extreme upper-bound case but useful to explore the effects of
445 high dome overpressures on the blast. As a consequence of the higher gas energy (compared
446 to A-2D) the initial quasi-spherical expansion reached a maximum gas velocity of 175 m s^{-1},
447 with corresponding peak particle velocities of 80, 145, and 175 m s^{-1} for particle diameters of
448 5000, 500, and 50 μm, respectively. At 2 s, vertical speed was ~140 m s^{-1} and horizontal
449 speed was 188 m s^{-1}, and at 5 s, the average speeds were 106 m s^{-1} vertically, and 150 m s^{-1}
450 horizontally (Fig.7a). The erupted material again failed to mix with sufficient air to form a
451 buoyant column and thus, in the gravity collapse phase at t > 5 s, collapsed downslope in a
452 stream of ash, blocks, and gas. The material then moved parallel to the ground surface in the
453 PDC phase at t > 20 s (Fig. 9). The burst phase of C-2D is characterized by a violent radial
454 expansion of the mixture, with fluid parcels following almost ballistic trajectories up to 10 s
455 and greater than 500 m above the dome (Fig. 7b). Despite the high internal dome pressure,
456 even in this case the atmospheric pressure perturbation rapidly decays with distance from
457 source. Perturbations of the atmospheric pressure in the first 10 s at different distances from
458 the dome are shown in Figure 8. Values are sampled at 5 m above the ground. The plots
459 clearly identify the arrival of the pressure wave caused by the burst. The overpressure is
460 about 15 kPa at 1 km, creating a weak pressure wave of strength (p_{after}/p_{before}) < 1.2, and
461 decreases to only a few kPa at 3.5 km. Overpressures >2 kPa are sufficient to cause tree

462   blowdown [Valentine, 1998a], although the interior dome pressures assumed for C-2D are

463   extreme.

464   The transition from collapse phase to PDC phase occurs at ~15-20 s. PDC front

465   speeds are ~90 m s^{-1} at the transition. The temporal evolution of the PDC (Fig. 9, Movie S3

466   in auxiliary material) is similar to A-2D except that co-PDC plume development is more

467   vigorous due to the greater initial expansion of the mixture associated with higher dome

468   pressure. An intensely buoyant co-PDC plume develops from the flow head at a distance of 5

469   km at about 150 s and is then pulled vent-ward by the strong vertical convection above the

470   vent (Figure 9, 180 s). At 240s the co-PDC plume extends to about 4 km from the source

471   while a dense, thin basal flow has reached the distance of 10 km. The co-PDC plumes

472   elutriated about 65% of 50 μm, 30% of 500 μm and <5% 5000 μm particles.

473

474   **4.2. PDC dynamics**

475   Figure 10 shows the PDC front positions vs. time and the PDC front velocity vs.

476   distance from the source. The front is tracked by measuring the most advanced part of the

477   PDC, without distinguishing between the flow head and the thin basal layer. The "low

478   energy" blasts (A-2D and B-2D) display nearly parallel trends, with B-2D's flow velocity

479   systematically higher than that of A-2D. The slight change in slope of the A-2D distance-time

480   curve occurs where the current becomes positively buoyant and decelerates as a result. The

481   more energetic blast (C-2D), on the contrary, attains the highest initial PDC velocity of all

482   three 2D simulations (Fig. 10b) but decelerates rapidly due to extensive entrainment of

483   atmospheric air and subsequent development of positive buoyancy in portions of the flow. As

484   a result, the final PDC run-out is comparable with that of A-2D.

485   The trends of the front velocity vs. distance (Fig. 10b) are very similar for A-2D and

486   B-2D even though the former shows more pronounced changes in the front velocity at 4 km

487   (corresponding to the break-in-slope) and 6 km (where the co-PDC plume forms). On the

488   other hand, the PDC front of C-2D developed a very high lateral velocity in the burst phase

489   (please note that the front velocity does not necessarily coincide with the maximum flow

490   velocity) while it decreased more rapidly corresponding to breaks-in-slope and subsequent

491   entrainment.

492   Figure 11 compares mixture density, mixture velocity, and dynamic pressures, as a

493   function of time, at 10 m above the ground surface at sampling positions 2, 3, and 4 km from

494   the source. The left plots refer to simulations with lower dome volume (A-2D and C-2D),

495　　whereas the right plots refer to the higher volume (B-2D). The dynamic pressure is computed

496　　from the mixture density $\rho_m = \varepsilon_g \dfrac{P\overline{\mu}}{RT_g} + \sum_s \varepsilon_s \rho_s$ and the horizontal and vertical mixture

497　　velocity components $(u_m, v_m) = \dfrac{1}{\rho_m}\left[\varepsilon_g \dfrac{P\overline{\mu}}{RT_g}(u_g, v_g) + \sum_s \varepsilon_s \rho_s (u_s, v_s)\right]$, according to

498　　$P_d = \dfrac{1}{2}\rho_m \sqrt{(u_m{}^2 + v_m{}^2)}$. In the preceding equations, $\overline{\mu}$ is the averaged molecular weight of

499　　the gas mixture, P and T_g are the gas pressure and temperature, R is the universal gas

500　　constant, ρ_s is the density of the pyroclasts, ε is the volumetric fraction of a phase and the

501　　subscripts g and s refer to the gas and solids, respectively.

502　　　　Mixture density plots (Fig. 11) show a peak corresponding with the passage of the

503　　flow head. This peak decreases in magnitude with distance from source, which we interpret

504　　to indicate flow head dilution. However, at later times (e.g., 100 s), the PDC mean density is

505　　controlled by the competing effects of intra-current sedimentation of particles and elutriation

506　　via a buoyant gas stream. For A-2D, peak densities of ~57, 19, and 18 kg m^{-3} occurred at the

507　　three sampling positions at times ~50, 70, and 100 s. For C-2D, very similar values are

508　　reached about 10 s earlier. In contrast, B-2D produced peak densities of ~118, 38, and 30 kg

509　　m^{-3} at the same locations, roughly double the values of the other two runs. Nevertheless, it is

510　　worth noting that the exact values of the density in the basal cells can be affected

511　　significantly by the mesh resolution. The sedimentation process is influenced by the vertical

512　　mesh size and deposition, as discussed above, and deposition is not explicitly treated by the

513　　model. The sensitivity of model results to grid resolution is discussed in detail in the

514　　appendix.

515　　　　Mixture velocity also decreases with the distance from the vent and after the passage

516　　of the flow head. Please notice that mixture velocity 10 m above the ground is generally

517　　much lower than the front velocity (compare Fig. 11 to Fig. 10b), due to flow stratification.

518　　For A-2D, maximum velocities of 46, 40, and 34 m s^{-1} occurred at 2, 3, and 4 km at times

519　　~35, 60, and 75 s, respectively. For C-2D, maximum velocities at 2, 3, and 4 km, 10 m above

520　　ground, are 72, 44, and 33 m s^{-1}, at 23, 50, and 60 s, respectively. Apart from higher speed at

521　　the 2 km position, the values are close to those of A-2D, but occur 10-15 s earlier. For B-2D,

522　　peak velocities were 66, 43, 40 m s^{-1}, at times of 26, 50, and 65 s. Peaks in velocity always

523　　occur earlier than peaks in density, indicating that the arrival of the dilute ash cloud precedes

524　　the arrival of the dense basal layer. The large oscillations after about 110 s reflect the

525　　development of convective co-PDC plumes.

526   For A-2D, dynamic pressure peaks of ~44, 13, and 7 kPa occurred at the sampling

527   positions at times of ~45, 65, and 90 s, about 15-20 s after the arrival of the PDC front.

528   Similar values for C-2D occur almost 10 s earlier, because of the larger initial velocity of the

529   burst phase. For B-2D, dynamic pressure peaks of ~75, 28, and 14 kPa, occurred at the

530   sampling positions at times ~48, 65, and 80 s, about 20 s after the arrival of the PDC front.

531   The A-2D and C-2D simulated peak dynamic pressure in the region of severe damage at St.

532   Patricks and Morris (at about 3.4 km from the source) were between 10 and 15 kPa, values

533   less than those estimated to explain the damage observed [Sparks et al., 2002; Baxter et al.,

534   2005]. On the contrary, for B-2D, simulated dynamic pressure in the same region was as

535   much as 25 kPa, consistent with the minimum value (>25 kPa) proposed by Sparks et al.

536   [2002] and Baxter et al. [2005] to explain the damage observed. The reader is cautioned that

537   these near-ground (~10 m) dynamic pressures could be significantly underestimated due to a

538   grid size effect (see Appendix, Fig. A2). Nevertheless, the general conclusion appears to be

539   sustained.

540   An interesting feature of these simulations is that velocities in the region of severe

541   damage between 3 and 4 km appear to be similar for A-2D, C-2D and B-2D, i.e. 33-43 m s^{-1},

542   whereas doubling the mass approximately doubled the peak mixture density, and doubled the

543   dynamic pressure. We therefore conclude that damage potential on Montserrat may be linked

544   more closely with high mixture densities than with unusually high current speeds.

545   Modeled mixture temperatures were also recorded at 2, 3, and 4 km positions, 10 m

546   above ground. For all runs, and in all cases, peak values are roughly ~800°C, close to the

547   initial temperature of the lava dome. These high peak values indicate that the basal layer of

548   the PDC can keep high temperatures despite the intense air entrainment in the overlaying ash

549   cloud. At 90 s convective plumes increase entrainment and plume temperatures drop to 200-

550   400°C. Erosion and entrainment of cold substrate material on Montserrat undoubtedly

551   contributed to temperature reduction, but are not treated in these simulations. Nevertheless,

552   high temperatures of the ash in the Boxing Day event caused rapid ignition of furniture and

553   combustibles, and was a major source of damage even at the periphery of the impacted area

554   [Baxter et al., 2005].

555   Fig. 12 shows the dynamic pressure at R = 3.4 km (the distance relevant for damage

556   observed at St. Patricks) at 10 m above ground. For A-2D, the onset of the jump in dynamic

557   pressure associated with the arrival of the PDC front at SPT seismic station (at R = ~3.4 km)

558   occurred at ~60 s, whereas the peak dynamic pressure occurred at ~70 s. For B-2D the flow

559   front arrived at ~50 s with a peak at ~70 s. For C-2D the flow front arrival and peak dynamic

560 pressure roughly coincide at ~50-55 s. Given that the initial dome radius is 230 m, the
561 average velocity for A-2D was (3400-230 m)/60 s = 53 m s^{-1}, whereas for B-2D and C-2D,
562 the velocity was approximately 63 m s^{-1}. These values are close to the average velocities of
563 38-56 m s^{-1} inferred from the timing of the first seismic pulse, but <50% of the velocity
564 inferred from the second seismic pulse (113 m s^{-1}). Our models therefore support the
565 hypothesis that the first pulse destroyed the station, although we must emphasize that average
566 velocities fail to capture the complex velocity vs. distance estimates discussed in previous
567 sections. The main 2D simulation results are summarized in Table 2.
568
569 **5. 3D simulation results**

570 Guided by the 2D parametric runs, the 3D PDAC code was applied over a Digital
571 Elevation Model (DEM) with a 20-m grid. The DEM represents conditions just before the
572 blast, with topography from a debris avalanche deposit filling much of the original White
573 River valley. The 3D computational domain is extended 9 km in longitude (from X=76160 to
574 X=85060 on the UTM map), 9 km in latitude (from Y=41560 to Y=50460) and 6 km
575 vertically. The horizontal mesh resolution varies, very gradually, from 20 m near the source
576 up to 200 m on the lateral boundaries. The vertical resolution varies from 20 m over the first
577 800 m, and gradually increases to 200 m at the top of the domain. The non-uniform mesh
578 allowed us to increase the resolution in the regions near the source and the ground, where we
579 observe the largest gradients in the flow variables. The initial dome is represented by a
580 hemisphere centered at coordinates [X=80690m; Y=46550m; Z=710m] on the summit flank,
581 sloping to the south [see topography Figure 13]. Two 3D simulations are presented here, A-
582 3D (V_{DRE} = 5 × 10^6 m^3), and B-3D (V_{DRE} = 11 × 10^6 m^3). For both cases, K=10^{-12} m^2. We
583 compared the simulation results against one another, and against maps of deposits and
584 destruction and observational data [Sparks et al., 2002; Ritchie et al., 2002; Baxter et al.,
585 2005].
586
587 **5.1. Large-scale features**

588 The results of the 3D runs are shown in Figure 13 and 14. Fig. 13 (vertical slice
589 through the dome center, parallel to PDC propagation direction) shows the initial *burst* phase
590 for simulations A-3D (a) and B-3D (b). The simulation is characterized, as in the 2D cases,
591 by an initial expansion phase at t < 5s, when the pyroclastic mixture expands into the
592 atmosphere forming a quasi-spherical shell. The subsequent collapse of the cloud at t ~10 s
593 produces a PDC which travels down slope. The asymmetry of the collapse is due, in 3D, to

594   the source topography that provides an initial tilted flank on which the source rests, and an

595   impediment to the propagation toward the Northern sector. The blast phase is very similar for

596   A-3D and B-3D since the initial specific energy is nearly identical (Table 1).

597   Fig. 14a shows simulations A-3D propagating over a 20-m DEM of southern

598   Montserrat viewed to the north. The evolution of the blast and blast-generated PDC is

599   illustrated by color contours that represent total volume particle fraction, decreasing from

600   dark (10^{-2}) to light (10^{-6}). The figure illustrates important effects associated with local

601   topography, including accelerations affected by steep slopes, non-radial motions caused by

602   obliquely-oriented topographic elements, particle-size segregation better developed in

603   channels than on interfluves, and topography-influenced formation of buoyant plumes near

604   the source and above the PDCs. At 10 s (not shown) early gravitational collapse feeds the

605   PDC, followed by topographic segregation into two distinct PDC lobes. By 30 s the PDC is

606   spreading over a broad sector of the landscape, with its main axis directed through St Patricks

607   village, and segregation into local channels is shown by the development of several lobes.

608   There is a weak rise of near-source buoyant plumes. Just after 60 s only one lobe exists, in the

609   White River valley. By 90 s, multiple buoyant plumes are evolving above the source region,

610   while the densest portion of the main lobe verges on St Patricks village, and the more dilute

611   front extends over a 70° sector and to nearly 2 km offshore.

612   The second 3D simulation, B-3D (Fig. 14b), is representative of the higher-volume

613   destructional/erosional pulses. The PDC flow features are generally similar to, but more

614   strongly developed than, the previous run of Fig. 14a. At 10 s (not shown), early gravitational

615   collapse feeds the PDC, followed by topographic segregation. By 30 seconds the PDC has

616   spread over a 60° sector, centered about a main axis aligned to the southwest. Two lobes have

617   developed, concentrating most of the mass in the White River channel; the current also

618   moves in places over interfluves, aided in some cases by runup at channel bends. The densest

619   portions of the two lobes remain beyond 60 s. By 90 s, the densest portion of the PDC occurs

620   as a single lobe, and the PDC front has bypassed St Patricks and extends 3 km offshore, while

621   multiple co-PDC plumes are rising above the source region.

622   Further details of the 3D simulations are illustrated by contours log of the particle

623   volume fraction 10 m above the topographic surface and along a longitudinal (LL') and a

624   transverse (PP') section (Figure 15). The particle maps (Fig. 15a,d) show, in both cases, a

625   channelized flow to the east, in Dry Ghaut, recognized also in the field [Fig. 2; Druitt et al.,

626   2002]. The model blast-affected sector is roughly 70° in both simulations and compares well

627   with the mapped distribution (Fig. 2 and bold line in Fig. 15a,d).   In both A-3D and B-3D,

628 particles concentrate near the base of the flow whereas co-PDC plumes generally develop at

629 slope breaks and are significantly more dilute (Fig. 15b,c,e,f). The highest particle

630 concentration occurs in channels and decreases with height above the surface (Fig. 15b,c,e,f),

631 and laterally away from the centerline of the deepest channels (Figs. 15c,e). In general,

632 current velocities are greater in the 3D simulations due to channeling effects, but some

633 general trends are similar to the 2D runs. For example, doubling the dome mass (Simulation

634 B-3D) also increases the PDC density, dynamic pressure and velocity, and decreases the

635 elutriation rate (as in 2D).

636 Field studies of the SHV deposits provide evidence that mobile dense basal flows

637 drained into channels which did not directly connect with the primary source area (secondary

638 flows), including ravines west of St Patricks and Dry Ghaut to the east of the vent. They

639 were immediately recognized as representing an important, but puzzling and hitherto

640 underestimated hazard around active lava domes [Druitt et al., 2002]. The 3D simulations

641 presented here strongly suggest that this type of hazardous flow can form in blast-type

642 eruptions by PDCs which cross interfluves. Particle velocity vector maps (Fig. 16) augment

643 the maps of particle distributions and compare well to blowdown features in the blast-

644 affected area [Sparks et al., 2002; Baxter et al., 2005], as well as illustrate development of

645 these secondary flows (originating near the summit, flowing to the East in Dry Ghaut). On

646 the other hand, simulation B-3D produced a northward directed PDC lobe, which was able to

647 overtop the summit. This type of PDC was not observed in the natural event, and we

648 attribute the inconsistency mainly to the weak constraint to northerly motion provided by the

649 modeled source topography. Animated results from three oblique views of both 3D models

650 runs display the dynamic evolution of the phenomena mentioned above, and can be viewed

651 on on-line auxiliary material (Movies S4 to S6).

652 In both 3D models (map not shown) high temperatures in the basal part of the currents

653 extended even to the periphery of the PDC, where dynamic pressures were low. This is

654 consistent with field observations that temperatures were high and rapid ignition was a

655 primary source of building damage along the periphery of the affected zone [Baxter et al.,

656 2005].

657

658 **5.2 PDC dynamics**

659 The dynamic pressure, mixture density and mixture velocity at fixed probe locations

660 (shown by dots in Fig. 16) through time show that the dynamic pressure decreases with total

661 mass erupted as in 2D (Fig. 17). For example, consider the dynamic pressure along the flow

662   axis for the two runs at 2.2 km from source (Fig. 17, top two panels, solid lines). Doubling

663   the dome mass more than doubles the dynamic pressure, which can be attributed largely to an

664   increase in PDC density (Fig. 17, middle two panels), and, to a much lesser degree, to

665   changes in PDC velocity (Fig. 17, bottom two panels). This comparison agrees with the 2D

666   calculations which suggest that the dynamic pressure is roughly proportional to the erupted

667   mass and increases largely due to an increase in flow density, rather than to an increase in

668   flow velocity. Dynamic pressure also decreases significantly with distance from source and

669   with distance from the PDC axis towards the flow periphery, again with changes in flow

670   density causing the bulk of the changes in P_{dyn} (Fig. 17). For instance, the dynamic pressure

671   of A-3D at 2.2 km from source along the flow axis is nearly six times the dynamic pressure

672   along the flow periphery at the same distance from source, and is roughly three times the

673   dynamic pressure along the flow axis at 3.2 km (Fig. 17, top left panel).

674   The maximum dynamic pressure recorded at 10 m above the ground, 90 s into

675   simulation A-3D, is mapped in Fig. 18a. The map further illustrates that maximum dynamic

676   pressure decreases steeply with distance from source and with distance from the main and

677   secondary flow axes. The longitudinal (Fig. 18b) and transverse (Fig. 18c) sections show the

678   steep decay in more detail. The maximum dynamic pressure calculated by A-3D near St.

679   Patricks is about ~7 kPa, compared to estimates of >25 kPa required for the complete

680   destruction at this axial locality [Sparks et al., 2002; Baxter et al., 2005]. And, for A-3D,

681   peripheral areas experienced slowly-building peak pressures <5 kPa. Therefore, simulation

682   A-3D suggests that dynamic pressures resulting from a collapse of ≤ 5 million cubic meters

683   are probably too small to explain the most severe damage observed. Although these simulated

684   near-ground dynamic pressures could be underestimated by a factor of about two because of

685   the grid size effect (Appendix, Fig. A2), the general conclusion appears to be robust.

686   The maximum dynamic pressure achieved by B-3D near St. Patricks is about 16 kPa

687   (Fig. 18d,e,f). This value underestimates the actual dynamic pressure by a factor of about

688   two because of the grid size effect (Fig. A2), so we conclude that this result is roughly

689   consistent with estimates of >25 kPa based on field observations [Sparks et al., 2002; Baxter

690   et al., 2005]. The much lower dynamic pressures in peripheral areas are also consistent with

691   field-based estimates from damage. Therefore the dynamic pressures calculated for the B-3D

692   case can account for the destruction observed both along the main axis and peripheral areas.

693   A further aspect of dynamic pressure is related to the ability of a PDC to pick up and

694   entrain large rocks, trees, concrete slabs, etc., with these "missiles" themselves having the

695   capability to cause severe damage [Esposti Ongaro et al., 2002; Sparks et al., 2002; Baxter et

696 al., 2005]. Following the analysis by Wills et al. [2002], dealing with missiles transported by

697 heavy winds, in a steadily increasing current the condition for flight of a loose object is,

698 $\quad P_d\, C_D > \rho_s\, L\, g,$

699 Where P_d is dynamic pressure, C_D is the drag coefficient, ρ_s is density of the object, L is the

700 characteristic dimension of the object, and g is gravitational acceleration. The maximum size

701 of the object is thus proportional to the dynamic pressure and inversely proportional to

702 density of the object.

703 Applying this relation to the PDC dynamics at St. Patricks, we calculate maximum

704 size L of a loose lava block borne by the PDC. Assuming C_D is approximately one for a bluff

705 body, $P_d = 25$ kPa, and $\rho_s = 2000$ kg m^{-3}, yields a maximum block dimension $L = 1.3$ m,

706 which is consistent with the meter-sized blocks observed embedded in heavily impacted

707 houses on Montserrat [Sparks et al., 2002, Fig. 16c].

708 Damage due to such objects can be related to their kinetic energy K, given by

709 $\quad K = \frac{1}{2}\, \rho_s V\, (\vartheta\, u)^2,$

710 where V = volume, ϑ = fraction of the current speed attained by an object before impact, u =

711 current speed. Assuming $V = L^3 = (1.3$ m$)^3 = 2.2$ m^3, $\vartheta = 0.36$ (based on wind-tunnel tests for

712 cubes [Wills et al., 2002]), and $u = 45$ m s^{-1} (sampled at 10 m above ground, Fig. 16), the

713 kinetic energy is about 580,000 J. Since kinetic energies of a few tens of J are sufficient to

714 seriously damage building components [Minor, 1994], such missiles can be considered an

715 important hazard process related to PDC dynamics on Montserrat and elsewhere.

716 We finally note that dynamic pressures calculated for the 3D simulations represent a

717 lower bound for the given volumes, because not all energy was focused directly to the south.

718 For example, if the source boundary were changed to a quarter-sphere (with the same total

719 volume as the hemisphere), with an east-west trending vertical back-boundary, the burst

720 phase would be directed entirely to the south and would likely have been more damaging. We

721 will explore the specific effects of source geometry in a future study.

722

723 **6. Discussion**

724 In general terms, the modeling results presented here have led to several scientific

725 insights about the sudden decompression and subsequent destruction of a lava dome.

726 According to our model results, the directed volcanic blast can reasonably be described by

727 three main phases; the *burst, collapse* and *PDC* phases. It appears that dome permeability

728 and source pressure distribution can influence blast characteristics, mostly affecting the burst

729   phase and co-PDC plume development, and asserting lesser influence on asymmetric collapse

730   characteristics and PDC velocity, density, dynamic pressure, and runout distance. On the

731   other hand, total dome mass appears to exert the greatest control on PDC runout and dynamic

732   pressure, which largely determine whether or not an event will be highly destructive.

733   Comparison between 2D and 3D results indicates that topography strongly influences the

734   dynamics of the PDC. For example the 3D results capture the evolution of enigmatic high-

735   concentration mobile dense basal flows in several channels not directly connected with the

736   primary source area [Druitt et al., 2002] and simulate the steep decline in dynamic pressure

737   with lateral distance from PDC axes. From these comparisons, we conclude that 3D

738   modeling with topography is essential for full analysis of directed volcanic blasts, especially

739   for exploring the effects of channeling on the distribution of pyroclastic deposits.

740   Given that the observed damage and deposit characteristics are the primary evidence

741   of the Boxing Day blast characteristics and dynamics, we made broad comparisons between

742   model results and estimates made from field analysis. From these comparisons, we suggest

743   several conclusions specific to the 1997 Boxing Day event at SHV. The 3D simulations

744   generally capture the geometry of the mapped sector of the Boxing Day event, as well as

745   numerous other basic characteristics of the distribution of the eruptive products, including the

746   development of multiple PDC lobes with the highest concentrations occurring along channel

747   axes, and the formation of secondary pyroclastic flows in lateral channels. High-volume

748   simulations (in both 2D and 3D) calculate PDC dynamic pressures consistent with field

749   observations of structural damage, while dynamic pressures associated with low-volume

750   simulations appeared insufficient to explain observations, providing evidence that the

751   observed severe damage was likely caused by high-volume pulses, rather than low-volume

752   pulses. A systematic decrease in peak PDC dynamic pressure with distance from source and

753   from lobe axes was also reproduced, in accordance with the observed damage. Modeled

754   temperatures are high over the extended region of the PDC even at the periphery where

755   dynamic pressures were low, consistent with ignition being the major source of observed

756   damage in those areas [Baxter et al., 2005]. The relatively sharp rise in dynamic pressure at

757   St Patricks (R = ~3.4 km; t = ~50 s) suggests average 2D model speeds of 53-63 m s^{-1}. These

758   average speeds are reasonably consistent with estimates of 38-56 m s^{-1} inferred by assuming

759   that the first seismic pulse destroyed seismic station MSPT, but are roughly half of the

760   velocity estimated by assuming that the second seismic pulse destroyed the station,

761   supporting the hypothesis that the first pulse destroyed the station. These comparisons

762   suggest that the model presented here, along with its simplifying assumptions, captured the

763 essence of the large-scale dynamics of the lateral blast at SHV, and could be useful for
764 understanding hazards associated with blasts in general.

765   For the 1980 Mount St Helens blast, Kieffer [1981, 1984] developed the hypothesis
766 that the most severe zone of damage could be explained by supersonic flow (Mach number
767 >3) within a shock wave-constrained flow field. Kieffer also proposed that the boundary
768 between the 'direct blast zone' and the 'channelized blast zone' north of the vent
769 corresponded to a transition from supersonic to subsonic flow marked by a Mach disk shock
770 at ~11 km from source. Wohletz [1998], for the MSH blast specifically, calculated leading
771 shock wave overpressures of 40 kPa and dynamic pressures of 1 kPa at 10 km using the full
772 thermal energy (7 Mt) released during lateral propagation of the blast, and assuming that the
773 energy release time and empirical relations were similar to surges driven by a surface nuclear
774 explosion [Glasstone and Dolan, 1977]. We discuss supersonic flow and shock waves below
775 within the context of the Boxing Day event on Montserrat.

776   Under the assumption of mechanical equilibrium between the phases, no heat transfer
777 between them, and no compressibility effects in the solid phases, the sound speed in a
778 multiphase gas-particle mixture can be computed by the formula:

779
$$c = \left(\frac{\gamma_g R T_g}{Y} \right)^{\frac{1}{2}} \left(Y + (1-Y)\frac{\rho_g}{\rho_s} \right)$$

780 where Y is the mass fraction of gas in the multiphase mixture, ρ_g and ρ_s are the gas and solid

781 densities, T_g is the gas temperature, γ_g is the ratio of specific heats for the gas phase, and R is
782 the perfect gas constant [Wallis, 1969; Dobran et al., 1993, Gidaspow, 1994]. Depending on
783 the transformation, γ_g can be equal to 1.4 (adiabatic expansion of gas) or 1 (isothermal
784 expansion). Due to the multiparticle nature of the mixture and therefore to the different
785 degrees of equilibrium between gas and particles we tested both adiabatic and isothermal
786 conditions. Nevertheless, the large exchange area between gas and particles, together with
787 the high concentration of solids at the base of the PDC, favor (as shown by simulation
788 results) an isothermal expansion. Therefore we prefer the value $\gamma_g = 1$. Moreover, as a first-
789 order estimate, we did not include a slip velocity correction due to its relatively small value
790 compared to the horizontal flow speed. The above equation has been validated by Gidaspow
791 and Driscoll [2007] by showing it appropriately describes the propagation of pressure waves
792 through a fluidized bed over a wide range of void fractions. According to it, the sound speed
793 of the mixture decreases with increasing particle volume fraction until a minimum is reached

794   at a void fraction of 0.5. Similar estimates of the sound speed of the eruptive mixture can be

795   obtained by using the pseudogas approximation; for instance Kieffer [1981] assumed γ_{mix} =

796   1.04 and obtains soundspeed values within a difference of few percent of our values. The

797   associated Mach number is defined as $M = \dfrac{\sqrt{u_m^2 + v_m^2}}{c}$, where u_m and v_m are the mixture

798   horizontal and vertical velocity components, respectively. Because the sound speed can be

799   quite low in our gas-particle mixtures, we now explore the Mach numbers in C-2D and B-2D,

800   the simulations most likely to exhibit supersonic flow. Simulation C-2D has the highest burst

801   velocities, whereas B-2D exhibits the highest PDC velocities and has the lowest mixture

802   sound speeds due to high particle concentration. Figures 19 shows Mach number contours for

803   these two simulations.

804   For B-2D, the transformation from the burst phase to collapsing stream occurs in the

805   first few seconds and the transformation from collapse phase to PDC phase is largely

806   complete by 10 s (Fig. 19a). The PDC displays a local supersonic basal region, enhanced by

807   topography. For instance at 30 s (Fig. 19b), isolated regions with M > 1.6 occur in front of

808   local steep areas that promoted acceleration. By 50 s (Fig. 19c), M > 1 occurs in a thin basal

809   zone limited to 1.6 - 2.3 km from source, whereas the PDC has spread to 3.6 km, and

810   dynamic pressures >15 kPa (and rising) already occur in the subsonic region at 3 km (see Fig.

811   11 above).

812   C-2D shows the development of a concentric region of supersonic flow at 1 s in the

813   burst phase (not shown), grading to a broader and gradually less concentric region of

814   supersonic flow (with M >2) in the laterally-directed collapsing stream (Fig. 19d at 10s). By

815   30 s the flow is subsonic nearly everywhere, except a very narrow region (R~1 km) where M

816   >1 in the PDC body (Fig. 19e). At later stages the flow Mach number decreases due to

817   deceleration. At 50s (Fig. 19f) the maximum Mach number is roughly 0.8 at 3-4 km from the

818   source.

819   The distribution of the mixture Mach number (over the dispersal sector at 10 m above

820   the ground) is shown for simulation B-3D at 50s (Figure 20). The mixture sound speed is

821   computed from the same relation used above, and ranges from 40 m s^{-1} at the base of the

822   PDC (where the particle concentration is the highest) to about 400 m s^{-1} in the dilute ash-

823   cloud, where the ash concentration is low but the temperature is still high. Maximum Mach

824   number of approximately 1.0 occurs in a small patch along the main channel, where the

825   velocity and the flow density are the highest, but apart from this the PDC is internally

826   subsonic. Along longitudinal (Fig. 20b) and transverse sections (Fig. 20c), the distribution of

827   the Mach number is very similar to that observed in 2D, with the highest values occurring in

828   the basal layer of the PDC. The Mach numbers in run A-3D (not shown) are everywhere

829   subsonic, suggesting that in the simulated events, supersonic effects are of very local

830   occurrence and of minor importance. To summarize, our model results suggest that the flow

831   is only locally supersonic (in correspondence with the regions with high particle

832   concentrations) and strongly transient, so that we can reasonably exclude any important effect

833   due to strong, persistent internal shock waves, beyond the burst phase and region (up to 2 s

834   after onset and distances < 1 km).

835   For the 1980 Mount St. Helens blast, it was hypothesized that an overpressured jet

836   horizontally emanated from a vent, resulting in a strong (Mach disc) shock normal to the blast

837   direction [Kieffer, 1981]. In such an underexpanded jet, the flow accelerates due to the

838   decompression and is supersonic in an extended region between the vent and the shock.

839   Based on our Montserrat simulations, we cannot exclude the possibility that increasing the

840   scale (total mass and energy) of the eruption to the size of the MSH blast could lead to the

841   formation of a short-lived overpressured jet. Nevertheless, according to the simulations

842   presented here, the strongly transient behavior of a blast and the generally low Mach numbers

843   in the corresponding PDC make us skeptical that a supersonic, underexpanded quasi-steady

844   horizontal jet of wide extent existed during the Boxing Day event.

845   The severe damage at St. Patricks appears to have been caused by the high dynamic

846   pressure of subsonic PDCs (>25 kPa), and impacts of large missiles (also related to dynamic

847   pressure), rather than by shock waves associated with supersonic flow, given that calculated

848   Mach number never exceeds unity in the region of damage. The existence of local regions of

849    $M > 1$ implies that perturbations of the flow pressure (e.g., due to sudden changes in the

850   topographic profile) can generate internal shock waves. Nevertheless, no discontinuities

851   were calculated in these model runs at the mesh scale (a recent application of the PDAC code

852   to the simulation of the shock wave propagation in supersonic volcanic jets [Esposti Ongaro

853   et al., 2006] has demonstrated that the code is able to accurately capture the flow

854   discontinuities in the compressible regimes even using a relatively coarse mesh of more than

855   10 m). This conclusion, however, does not exclude the possibility of localized generation of

856   internal shock waves in isolated regions, or of damage by supersonic flow in the very

857   proximal area. We also note that with some alternative source conditions, the burst phase

858   could be more focused to the south.

859

7. Conclusions

Based on our model simulations we are able to separate the transient directed-blast at SHV into three main parts, the *burst phase*, the *collapse phase*, and the *PDC phase*. In the burst phase, the pressurized mixture is driven by kinetic energy of the gas phase, expanding rapidly into the atmosphere, with much of the expansion having an initial lateral component because of the geometry of the pressure release surface. The erupted material fails to mix with sufficient air to form a buoyant column and thus, in the collapse phase, falls beyond the source as a stream of gas and pyroclasts. The material then moves parallel to the ground surface as a density current in the mainly subsonic PDC phase. Local supersonic flow is possible in the PDC phase, but it likely results from high mixture density, rather than extremely high velocities. This idealization of directed blasts contrasts with some previous models (Kieffer, 1981, 1984; Wohletz, 1998].

Our modeling results also indicate that the total mass in the PDC has great control on inertia and runout, and can largely determine whether or not an event will be highly destructive. Further, source permeability and source pressure distribution can strongly influence burst-phase characteristics and co-PDC plume development, but affects only minor control over asymmetric fountain characteristics and PDC propagation. Topography strongly influences the dynamics of PDC evolution, and only 3D models incorporating 3D topography can capture the effects of channeling on the distribution of PDC deposits. Despite the complexity of the phenomena, our simulation results were consistent with field observations of depositional features, structural damage, and damage due to fires ignited by the pyroclastic event. In particular our calculations suggest that the severe damage observed in the St Patricks area on Montserrat can reasonably be explained by high dynamic pressures and missile impact loading within subsonic PDCs generated by high-volume pulses.

Appendix
Numerical resolution on rectilinear meshes

The PDAC code solves the multiphase transport equations on a rectilinear mesh in 2D (cylindrical or Cartesian) and 3D (Cartesian) [Esposti Ongaro et al., 2007; Neri et al., 2007]. The discretization schemes adopted in the PDAC code are accurate to the second order in a Taylor expansion on a uniform mesh. In the simulations performed we adopted non-uniform meshes in order to reduce the number of cells and, consequently, the execution time of each run. The use of a non-uniform mesh allowed us to increase the resolution in the regions near

894   the source and the ground, i.e. in the regions where we observe the largest gradients in the

895   flow variables. In 2D, the computational domain extended 10 km horizontally and 8 km

896   vertically and was discretized into 400×200 computational elements. The horizontal mesh

897   size was uniform in the first 600 m with a resolution of 20 m, then increased radially up to

898   100 m at 6 km and then was left constant at 100 m up to 10 km. Vertically, the mesh size was

899   uniform in the first 1500 m with a resolution of 10 m, then was increased gradually up to 60

900   m. In 3D, the computational domain was extended over a 9 km × 9 km area and up to 6 km

901   vertically and was discretized into 128×128×100 cells. In this case, we adopted a horizontal

902   resolution of 20 m, in a box of 500 m enclosing the source, and increased this gradually to

903   100 m beyond the 500-m boundaries. The vertical mesh resolution was uniform at 20 m for

904   the first 800 m, and then increased up to 200 m. To reduce the numerical error, in both 2D

905   and 3D, we limited the radial cell-size increase rate to 1.05, as is the common practice in

906   numerical modeling. The numerical error strongly depends on the diffusion properties of the

907   numerical scheme adopted and also on the flow Reynolds number. We therefore performed

908   several sensitivity tests to evaluate the effects of the horizontal mesh non-uniformity and

909   vertical mesh resolution on the numerical solutions.

910   Figure A1 presents the isocontours from -8 to -1 of the $\log_{10}$ of the total particle

911   volumetric fraction in the atmosphere at 90 and 180 s for simulation A-2D and for various

912   computational meshes, both uniform and non-uniform. The results show a minor effect of the

913   mesh features on the large-scale dynamics of the PDC propagation. In particular, the effect of

914   the horizontal cell stretching is negligible at 90 s (Figure A1, a and b), when the flow is

915   almost entirely in the uniform region of the computational domain. At 180 s (Figure A1, e

916   and f) some difference in the PDC runout can be observed, due to the different horizontal

917   resolution (20 m vs. 100 m). The effect of the vertical resolution on the large-scale

918   propagation of PDCs is also quite limited, as demonstrated by comparing the runout of PDCs

919   at 90 s with a mesh of 6, 10, and 20 m (Figure A1, c, b, and d). At 180 s the difference is

920   slightly more pronounced but still within a 10% tolerance. Similar results were obtained and

921   discussed by Dobran et al. [1993] and Neri et al. [2003]. Similarly, in 3D, the comparison

922   between maps of the total particle volumetric concentration at 90 s obtained with a uniform

923   (50 m) and non-uniform (20-100 m) horizontal discretization (not shown) confirms the

924   relatively minor effect of cell stretching on the solutions of explosion dynamics.

925   Because PDCs show strong vertical density and velocity gradients close to the

926   ground, the influence of the vertical mesh resolution on dynamic pressure is more significant

927   at the base of the flow. As a consequence, flow sedimentation and stratification computed by

928   the model significantly depends on grid size, as already noted in multiparticle simulations by

929   Neri et al. [2003]. For example, Figure A2 shows the influence of mesh size on vertical

930   profiles of mixture density, velocity, and dynamic pressure for the PDC of simulation A-2D.

931   From the plots one can see that the solutions begin to converge on a single solution as vertical

932   grid size decreases (compare the change from the 20 m to 10 m grid to the change from the

933   10 m to 6 m grid). Generally speaking the smallest grid spacing, in this case 6 m, produces

934   the most accurate solution. Results obtained with the 6 and 10 m meshes produce similar

935   solutions and flow gradients. In detail, they produce similar velocity profiles with maxima

936   about 50-60 m above the ground (Fig. A2, b and e), and nearly identical density profiles (Fig.

937   A2, a and d). The resulting peak in dynamic pressure is approximately 20-30 m above the

938   ground (Fig. A2 c and f). The similarity between the solutions on the 6 m and 10 m grids

939   suggests that a resolution of 10 m is adequate to quantitatively describe the primary flow

940   features. On the other hand, the solutions on the 20 m mesh significantly underestimate the

941   maximum value of dynamic pressure (relative to the 6 m grid) and do not capture patterns

942   close to the ground. Unfortunately, a 10 m mesh resolution is difficult to achieve in 3D

943   simulations, because of the substantial increase in the total number of computational elements

944   and associated computing time, and therefore a 20 m minimum grid size was adopted in our

945   main 3D simulations. This choice does not significantly affect the large-scale dynamics of the

946   explosion and PDC propagation (see Figure A1 above and similar analyses reported in Neri et

947   al., 2003), but likely underestimates the PDC dynamic pressure by roughly a factor of two

948   (Fig. A2c,f). Our results show that the dynamic pressure profile of the PDC is characterized,

949   at least under the conditions considered in our simulations, by a sharp gradient from the

950   ground to its maximum value at approximately 20-30 m above the surface. As a consequence,

951   the estimate of dynamic pressure at 10 m above ground or lower may be subject to

952   considerable uncertainty, due to the grid size effect and also the complex effect of the ground

953   boundary condition on the flow behavior [Dufek and Bergantz, 2007].

954   Finally, it should be noted that mesh resolution also affects the accuracy of the

955   topographic description. To reduce errors associated with inaccurate descriptions of

956   topography we adopted a new immersed-boundary technique [De' Michieli Vitturi et al.,

957   2007] suited to compressible multiphase flows in order to accurately describe, even with the

958   relatively coarse mesh adopted, the no-slip condition at the interface between the fluid and

959   the irregular 2D and 3D topography.

960

961 The computational grids used to date included up to 300 thousand cells in 2D and 2.5 million
962 cells in 3D and required the challenging solution of several billions of algebraic equations.
963 The parallelization strategy that allowed such an accomplishment was based on the
964 decomposition of the domain among the computational processors by adapting the numerical
965 solution algorithm to the parallel environment [Esposti Ongaro et al. 2007]. A parallel
966 communications layer based on the Message Passing Interface (MPI) protocol and a friendly
967 input/output interface make the new PDAC code portable on most parallel (shared- and
968 distributed-memory) architectures and transparent to the programmers and the users. The new
969 code is thus able to exploit the peak performance of large supercomputers and workstation
970 clusters. In detail the code was run on a Linux cluster with 66 AMD Opteron CPUs at 1 GHz
971 and 52 GB RAM, interconnected with a low-latency Myrinet network. On this machine, 3D
972 runs took about 2500 total CPU hours.

973

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Table captions

Table 1. List of the main parameters used in 2D and 3D simulations. κ is the porous dome permeability, V_{DRE} is the Dense Rock Equivalent volume of the dome, R_d is the resulting dome radius, M is the solid mass in the dome, α the porosity (void fraction) and E is the expansion energy per unit mass assuming an adiabatic or isothermal expansion (see text). The total mass in the 2D runs is multiplied by a factor accounting for the asymmetric distribution of the deposit over a sector of 70°.

Table 2. List of the main simulation outputs from 2D simulations. H_b is the maximum burst height above the dome (see Figs. 3, 5, 7), $U_{b,g}$ is the gas *burst* velocity, $U_{b,p}$ is the three particles *burst* velocity, U_f is the average velocity of the PDC after collapse, T_p is the time at which the phoenix cloud form from the PDC front, E is the percentage of pyroclasts elutriated at the final simulation time, Rm_{max}, Um_{max}, Pd_{max} are the maximum mixture density, velocity and dynamic pressure at 10m and 2, 3 and 4 km from the vent (see Fig. 11), Pd_{SP} is the maximum dynamic pressure at St. Patrick village (R=3.4 km, see Fig. 12).

Figure captions

Figure 1. The area affected by the 1997 Boxing Day lateral blast on Montserrat, view from south. a) before: foreground, St. Patricks village (left) and White River valley; background, SHV. b) after, showing debris avalanche deposit in and near the valley, and widespread blanket of PDC deposits over 70° sector. St. Patricks at lower left is completely destroyed.

Figure 2. Distribution of 1997 Boxing Day deposits (from Sparks et al., 2002). A-A' marks the profile used in 2D runs A, B & C.

Figure 3. a) Initial expansion of 2D simulation A-2D ($V_{DRE} = 5$ x 10^6 m^3, K $= 10^{-12}$ m^2). Contours are $\log_{10}$ of particle volume fraction. Initial condition, 2 s, 5 s and 12 s into simulation. By 12s the plume exhibits the collapse phase. b) Trajectories of fluid particles from 0 to 15s defining the burst phase and collapse phase of eruption.

Figure 4. Simulation A-2D ($V_{DRE} = 5$ x 10^6 m^3, K $= 10^{-12}$ m^2). Contours are $\log_{10}$ of particle volume fraction (color map as in Fig. 3a). At 10s the burst phase has ceased and the PDC moves along the volcanic slope. At 20s the PDC head forms by the effect of the air entrainment at 1.5 km. At 40s in the PDC phase, the leading edge has thickened and most of the solid mass has entered the PDC. By 90s the PDC has progressed beyond the shoreline and further thickening of the leading edge is evident. By 180 s the PDC has reached 8 km and segregated fines are forming a co-PDC plume, with minor plumes at the trailing edge. At 240s, co-PDC plumes are well-developed and vertical motion dominates. Animated contours can be viewed on Movie S1 in the on-line auxiliary material.

Fig 5. a) Initial expansion of simulation B-2D ($V_{DRE} = 10$ x 10^6 m^3 , K $= 10^{-12}$ m^2). Contours are $\log_{10}$ of particle volume fraction. Initial condition, 2 s, 5 s and 12 s into simulation. By 12s the plume exhibits the collapse phase. b) Trajectories of the fluid particles from 0 to 15s, defining the burst phase and collapse phase of eruption. The initial phase is not greatly affected by total mass (compare to Fig. 3a and 3b).

Figure 6. Results of B-2D ($V_{DRE} = 10$ x 10^6 m^3 , K $= 10^{-12}$ m^2). Contours are $\log_{10}$ of particle volume fraction (color map as in Fig. 5a). From 0 to 40s the dynamics is similar to A-2D, but the PDC front is more advanced. At 40s in the PDC phase, the leading edge has thickened. By 90 s the

PDC has progressed well beyond the shoreline with further thickening and broadening of the leading front. At 180s the increased dome mass and inertia results in high-speed runout beyond the computational limit of 8 km (PDC motion continues). Deposition is offshore. Buoyant co-PDC plumes are in the early stages of development. Animated contours can be viewed on Movie S2 in the on-line auxiliary material.

Figure7. a) Initial expansion of 2D simulation C-2D ($V_{DRE} = 5 \times 10^6$ m^3 , K = 10^{-14} m^2). Contours are $\log_{10}$ of particle volume fraction . Initial condition, 2 s, 5 s and 12 s into simulation. The initial phase is strongly affected by initial total specific gas energy (compare Fig. 3). b) Trajectories of fluid particles from 0 to 10s, defining the burst phase and collapse phase of eruption (please notice the change in the axis scale with respect to Figs. 3b) and 5b).

Figure 8. Pressure perturbation at ground level and different radial distances (from 1 to 3.5 km) produced by the exploding dome in simulation C-2D.

Figure 9. Results of C-2D ($V_{DRE} = 5 \times 10^6$ m^3 , K = 10^{-14} m^2). Contours are $\log_{10}$ of particle volume fraction (color map as in Fig. 5a). At 10s the pyroclastic material is expanding in the atmosphere (burst phase) by the effect of the high initial gas overpressure. At 20s the erupting material is collapsing to the ground forming a PDC. At 40s in the PDC phase, the leading edge has thickened. By 90 s the PDC has progressed past the shoreline with further thickening and broadening of the leading front. By 180 s the PDC has passed 6 km but has stalled and segregated fines are forming a co-PDC plume, with minor plumes at the trailing edge. At 240s, co-PDC plumes are well-developed onshore and vertical motion dominates. Animated contours can be viewed on Movie S3 in the on-line auxiliary material.

Figure 10. a) Front position versus time, and b) Front velocity versus position of simulations A-2D (solid line), B-2D (dashed) and C-2D (dotted). The front is tracked by following the most advanced part of the flow, irrespective of its shape (expanded flow head or thin basal flow).

Figure 11. Time-wise variation of the mixture density (top), mixture velocity (middle) and flow dynamic pressure (bottom) at 2 km (red), 3 km (green) and 4 km (blue) from the source. Values are sampled 10m above the ground level. Plots on the left are results from an erupted mass of $V_{DRE} = 5$

x 10^6 m^3 and different dome permeabilities (A-2D:10^{-12} m^2 - solid line; C-2D: 10^{-14} m^2 - dashed line). Plots on right are results from a higher erupted mass: B-2D (V$_{DRE}$ = 10 x 10^6 m^3) and high dome permeability (10^{-12} m^2).

Figure 12. Flow dynamic properties at St Patricks, 3.4 km from source, resulting from simulations A-2D (solid line), B-2D (dashed) and C-2D (dotted). a) Time-wise variation of the flow dynamic pressure. Values are sampled 10m above the ground level. b) Vertical flow profile at the time of maximum dynamic pressure reported in the legend.

Figure 13. Isocontours [-8:0:-1] of the Log$_{10}$ of the total particle fraction at t=0s, t=5s and t=10s across a vertical section parallel to the Y axis in 3D simulations [X=80700]. The dark solid contour indicates the initial volume of the exploding dome at [X=80690m; Y=46550m; Z=710m]. A) Simulation A-3D (V$_{DRE}$ = 5 x 10^6 m^3, K = 10^{-12} m^2); B) B-3D (V$_{DRE}$ = 11 x 10^6 m^3, K = 10^{-12} m^2). The sequences can be compared with those in 2D in Fig. 3 and 5 (but the initial position of the dome is somewhat different; see text).

Figure 14. Temporal evolution of 3D pyroclastic dispersal process at 30, 60 and 90s. View from South on 20-m grid DEM. The isosurfaces correspond to the total particle concentrations of 10^{-6} (outer, light brown) and 10^{-2} (inner dark) a) Simulation A-3D (V$_{DRE}$ = 5 x 10^6 m^3, K = 10^{-12} m^2); b) Simulation B-3D (V$_{DRE}$ = 11 x 10^6 m^3, K = 10^{-12} m^2). Animated contours can be viewed on Movie S4 to S6 in the on-line auxiliary material.

Figure 15. Left panels: Simulation A-3D (V$_{DRE}$ = 5 x 10^6 m^3, K = 10^{-12} m^2); Right panels: Simulation B-3D (V$_{DRE}$ = 11 x 10^6 m^3, K = 10^{-12} m^2). a,d) Map of the log$_{10}$ of total particle concentration at 10m above ground (the basal cell) at 90 s. Note channelized flow to the east, in Dry Ghaut, which was also recognized in the field. The bold line indicates the boundary of the debris avalanche and blast deposits. b,e) Longitudinal LL' section of the log$_{10}$ of total particle concentration along the flow direction (seen from NW). c-f) Transversal PP' section (seen from NE).

Contours are log$_{10}$ of particle volume fraction. Please note that the color scale is different in the maps from the sections to highlight the weaker variations in the spatial distribution of pyroclasts.

Figure 16 Maps of particle velocity vectors at 90s for simulations A-3D (a) and B-3D (b).

Values are sampled at 10 m above ground level (the basal cell). Points p1-p4 indicates the probe positions for the sampling of Fig. 20 and correspond to central (p1,p3) and peripheral (p2,p4) locations.

Figure 17. Dynamic pressure, mixture density and mixture velocity at 10m above the ground surface at selected locations marked by the dots in Fig. 18. Left) A-3D, Right) B-3D. The value of the maximum dynamic pressure (corresponding to the passage of the PDC head) drastically decreases in moving away from the source, and also from the flow axial region to the flow periphery.

Figure 18. Comparison between the *maximum* dynamic pressure of simulation A-3D (left plots) and B-3D (right plots). a-d) Map view at 10 m above ground surface in the basal cell at 90 s (dome positioned at [X=80690m;Y=46550m;Z=710m]). Solid lines mark longitudinal and transverse sections; b-e) Longitudinal section topography (green) and corresponding simulated maximum dynamic pressure (blue). Please notice that the longitudinal section does NOT correspond to the flow direction or to the steepest slope (see the map). The maximum value of the dynamic pressure drastically decreases with the distance from the source; c-f) Transverse section topography (green) and corresponding simulated maximum dynamic pressure (blue). Peaks in maximum dynamic pressure correspond to deep valleys where particles tend to concentrate, providing evidence that lateral peaks in maximum dynamic pressure are controlled by flow density, rather than flow velocity. The maximum value of the flow dynamic pressure in B-3D is almost double with respect to A-3D due to the increase of the erupting mass.

Figure 19. Mach number distributions for 2D simulations of volcanic blast at Soufrière Hills volcano; Isocontours are traced every 0.2. Maximum values are saturated in red above M=2.0, so that the green color corresponds to M~1 (sonic velocity, white isoline). a-b-c) Simulation B-2D (V_{DRE} =10 x 10^6 m^3, K=$10^{-12}m^2$). The collapse phase (t=10s) is characterized by relatively high Mach number (M>2) in a proximal region (R = 500-800 m). High values of the Mach number at 30s correspond to regions at high particle concentration, rather than high velocity. The region affected by locally supersonic flow is limited to R<2.5 km and t = 50s.
d-e-f) Simulation C-2D (V_{DRE} = 5 x 10^6 m^3, K=$10^{-14}m^2$). Collapse phase shown at 10 s, with transformation to PDC phase nearly complete by 20 s (not shown). Further movement shows thickening and distortion of PDC front edge by air drag. By 30 s, the region for M>1 is limited to a

thin basal patch ~1.5 km from source. By 50 s, with the plume front at the site of destroyed houses (3.4 km), the basal zone of the PDC displays M<0.8, but with high dynamic pressure.

Figure 20. a) Map of the distribution of mixture Mach number at 50s, and at 10m above the ground level, for simulation B-3D ($V_{DRE} = 11 \times 10^6$ m^3, $K = 10^{-12}$ m^2). b) Longitudinal section LL' and c) transversal section PP' of the Mach number distribution. Isocontours are shown for every 0.2 change. Maximum value observed is about M~1.0, comparable with that observed in 2D (Fig. 19).

Figure A1. Influence of the mesh size and stretching on the large-scale PDC dynamics at 90s (left plots) and 180s (right plots). Isolines represent the $\log_{10}$ of the total particle volumetric fraction from -8 to -1. a,e) Reference simulation A-2D: dx varies from 20 to 100m, vertical minimum size is dz=10m (total number of cells N_t= 8×10^4). b,f) Uniform horizontal resolution of 20m, vertical minimum size is dz=10m (N_t= 2×10^5). c,g) Uniform horizontal resolution of 20m, vertical minimum size is dz=6m (N_t= 3×10^5). d,h) Uniform horizontal resolution of 20m, vertical minimum size is dz=20m (N_t= 1.5×10^5).

Figure A2. Influence of the vertical mesh size on the PDC density (a,d), velocity (b,e) and dynamic pressure (c,f) profiles. a, b, and c is at 90 s and 3 km from source; d, e and f is at 90s and 4 km from source. The vertical resolution plotted are 6 m (solid line), 10 m (dashed line), and 20 m (dotted line), with a uniform horizontal resolution of 20 m. The ordinates report the height above the topography in meters (the ground elevation is 161 m at 3 km and 0 m at 4 km).
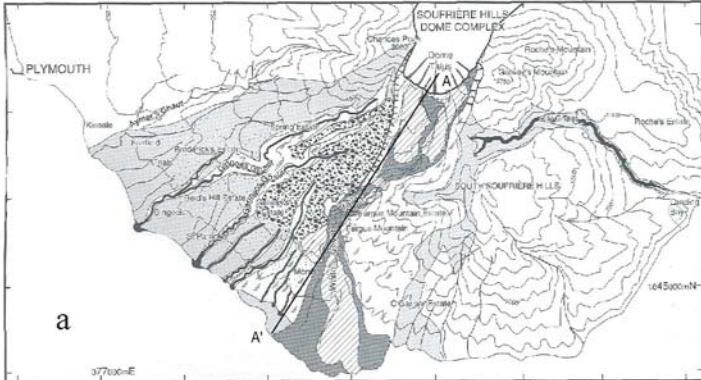
Extent of the Deposits | LEGEND | Topographic Features:

Valley-confined Facies:
- Block-poor deposits (Surge-derived pyroclastic flow)
- Block-rich deposits

Unconfined Facies:
- Unit I: Layers 1 & 2 (1st pulse)
- Unit II: Layers 1 & 2 (2nd pulse) (dots represent presence of layer 1 only)
- Debris avalanche deposits

Topographic Features:
- Steep valley sides
- Scouring
- Dome talus slope
- Contours and heights in feet (0.3048 m)
- River

0   1 km

Labels on map: PLYMOUTH, SOUFRIÈRE HILLS DOME COMPLEX, Chances Peak, Dome, Gages Mtn., Rochers Mountain, Stanley's Mountain, Roche's Estate, Amersham, Kinsale, Fort d..., Ruins..., Devil's Hill Estate, Lee's..., St Pa... Hill, Dagenham, Parque Mountain Reservoir, Gargos Mountain, SOUTH SOUFRIÈRE HILLS, Germans River, Langley River

A — A'

a

377000=E   1645000=N

a)

b) t=15s

a) Contour plot showing R [m] on the horizontal axis (0 to 1400) and Z [m] on the vertical axis (500 to 1700), with time contours labeled t=0, t=2s, t=5s, and t=12s. Color scale ranges from -1 to -8.

b) Trajectory plot at t=10s, with horizontal axis from 0 to 1000 and vertical axis from 600 to 1600.

Front position / Front velocity

Dynamic Pressure @ St. Patrick
R = 3.4 Km, z = 10 m
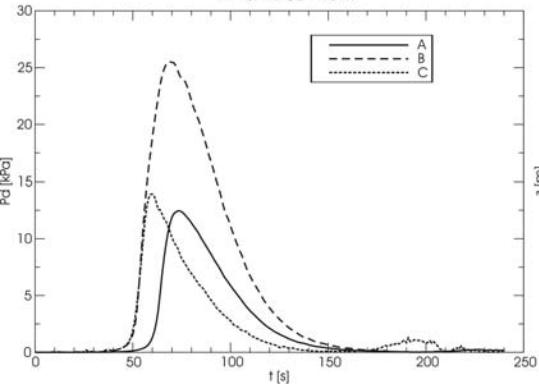
Mixture velocity modulus @ St. Patrick
R = 3.4Km

a)

b)

t=30s

t=60s

t=90s

a) P   L

M = 1.0

L'   P'

t = 50 s

b) L   M = 1.0   L'

c) P'   M = 1.0   P

0.0   1.0   2.0
Mach
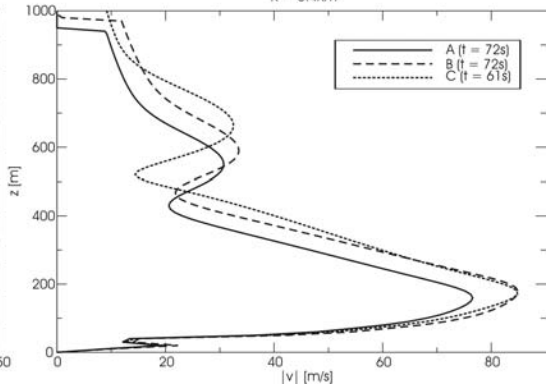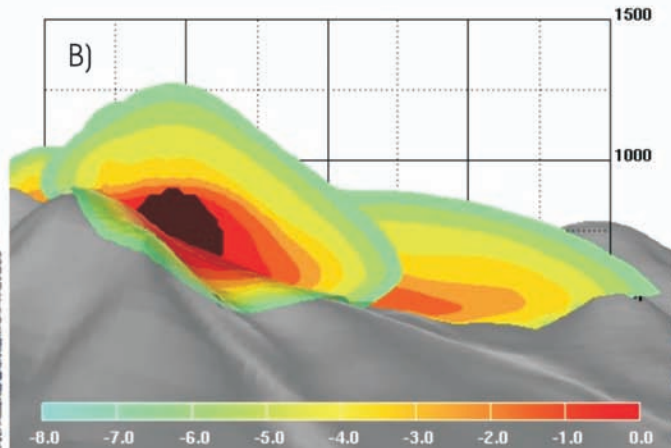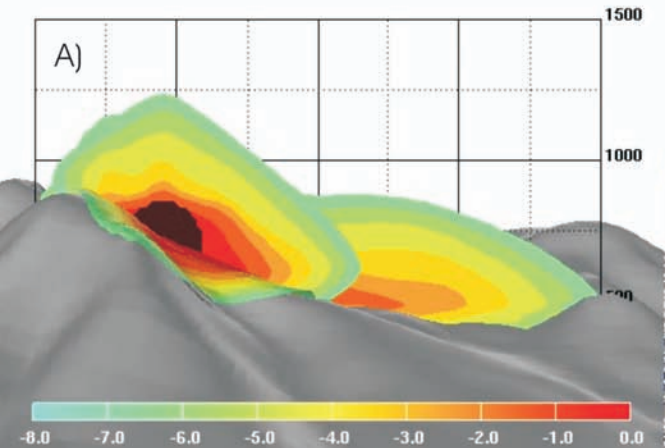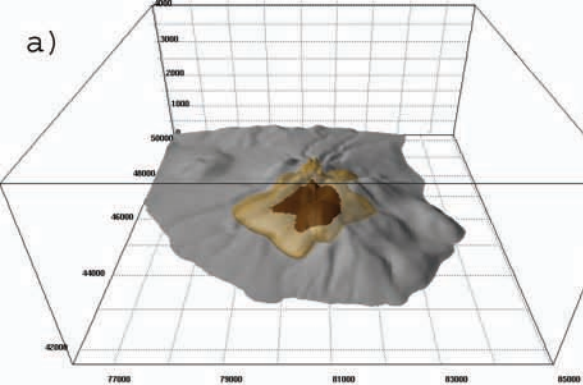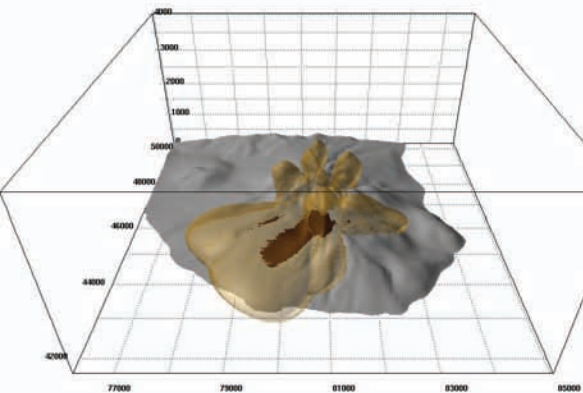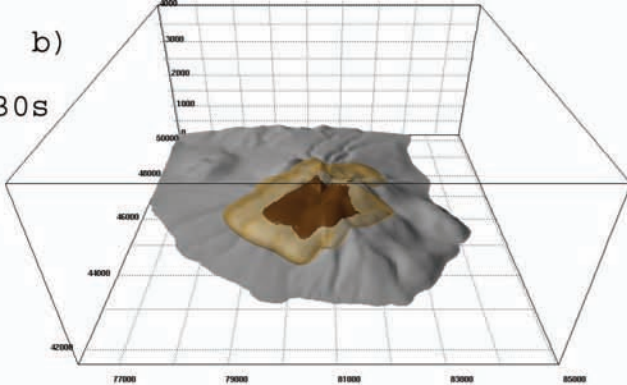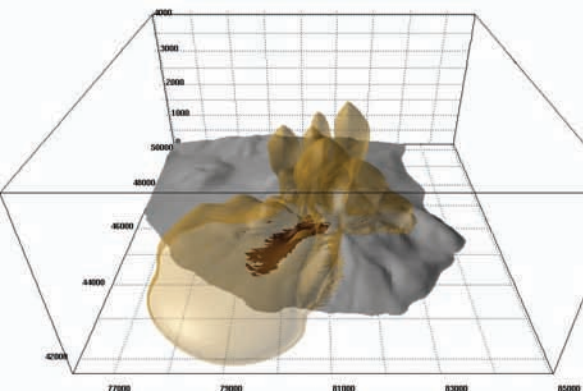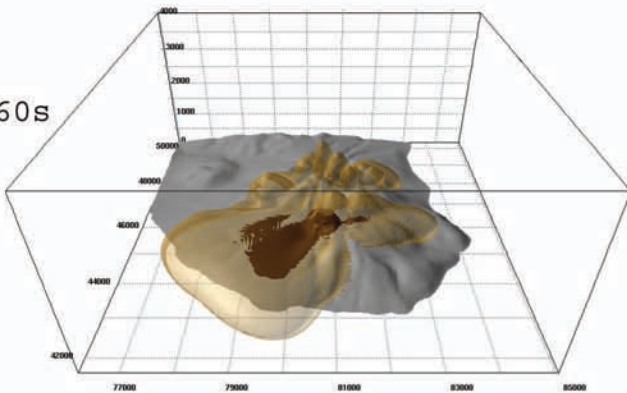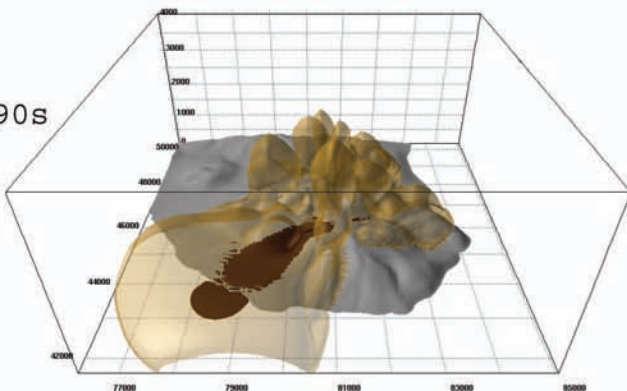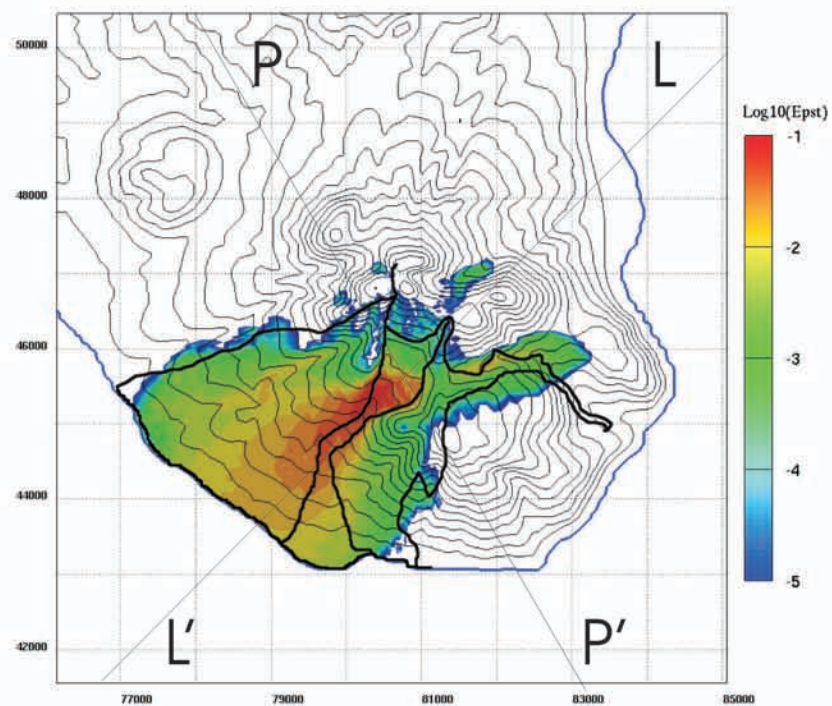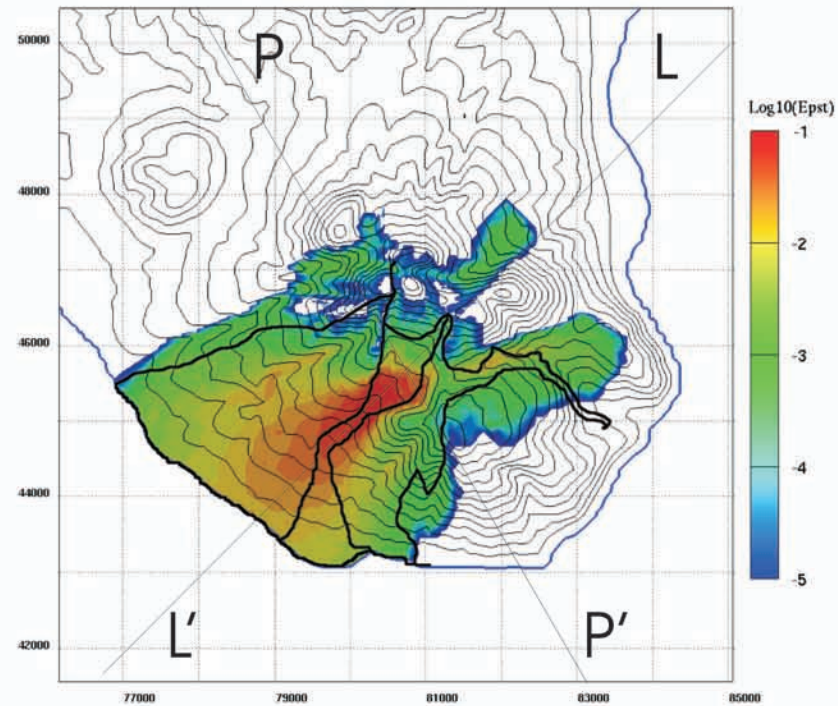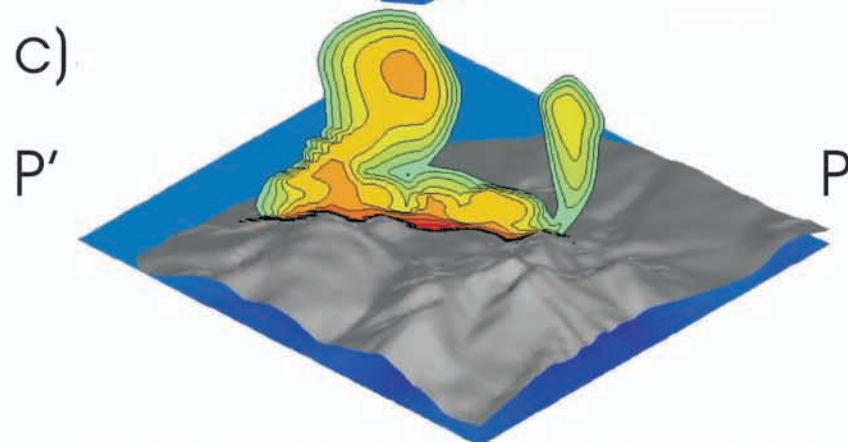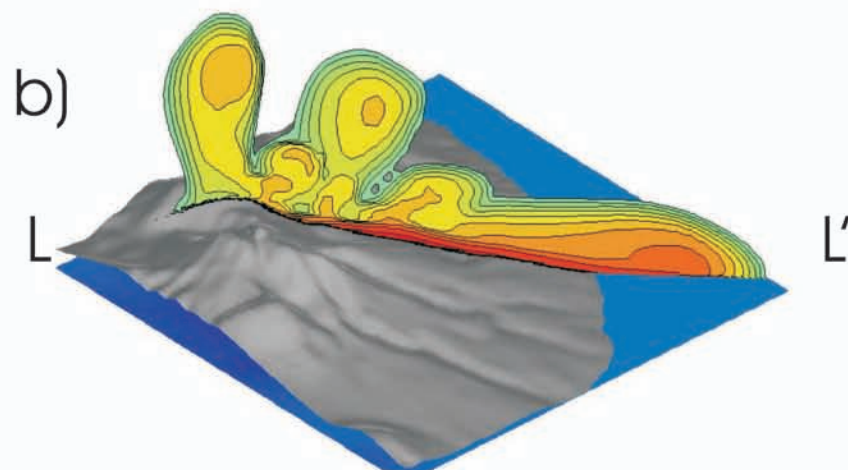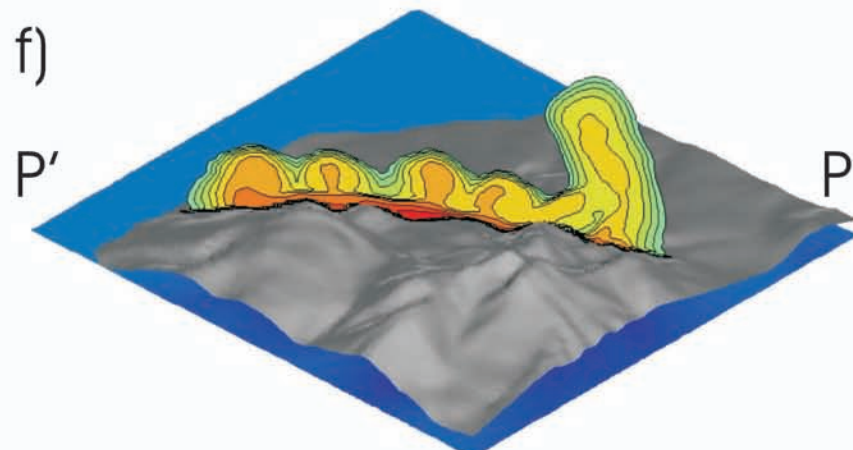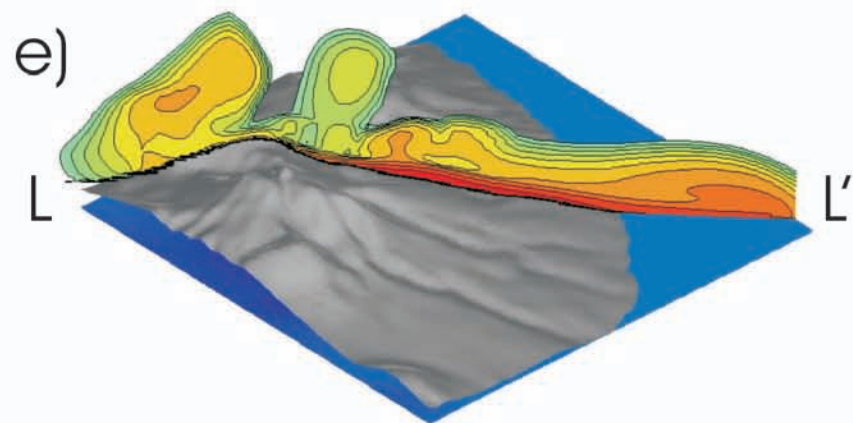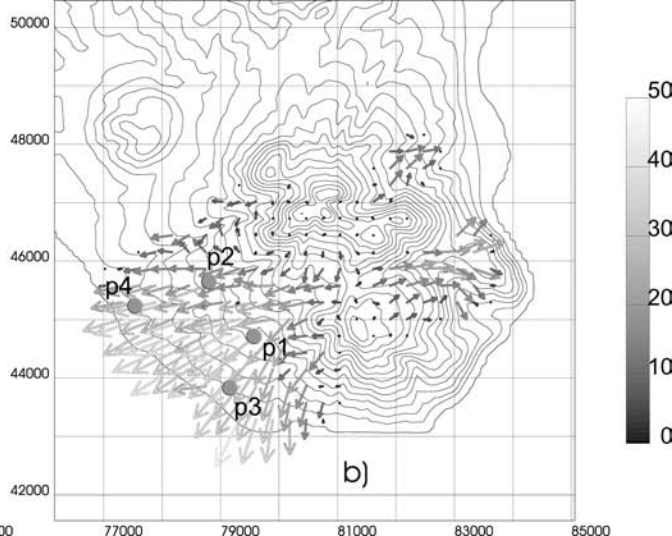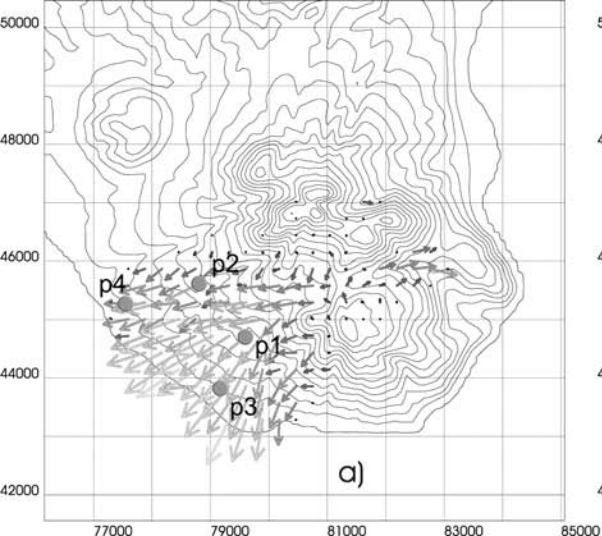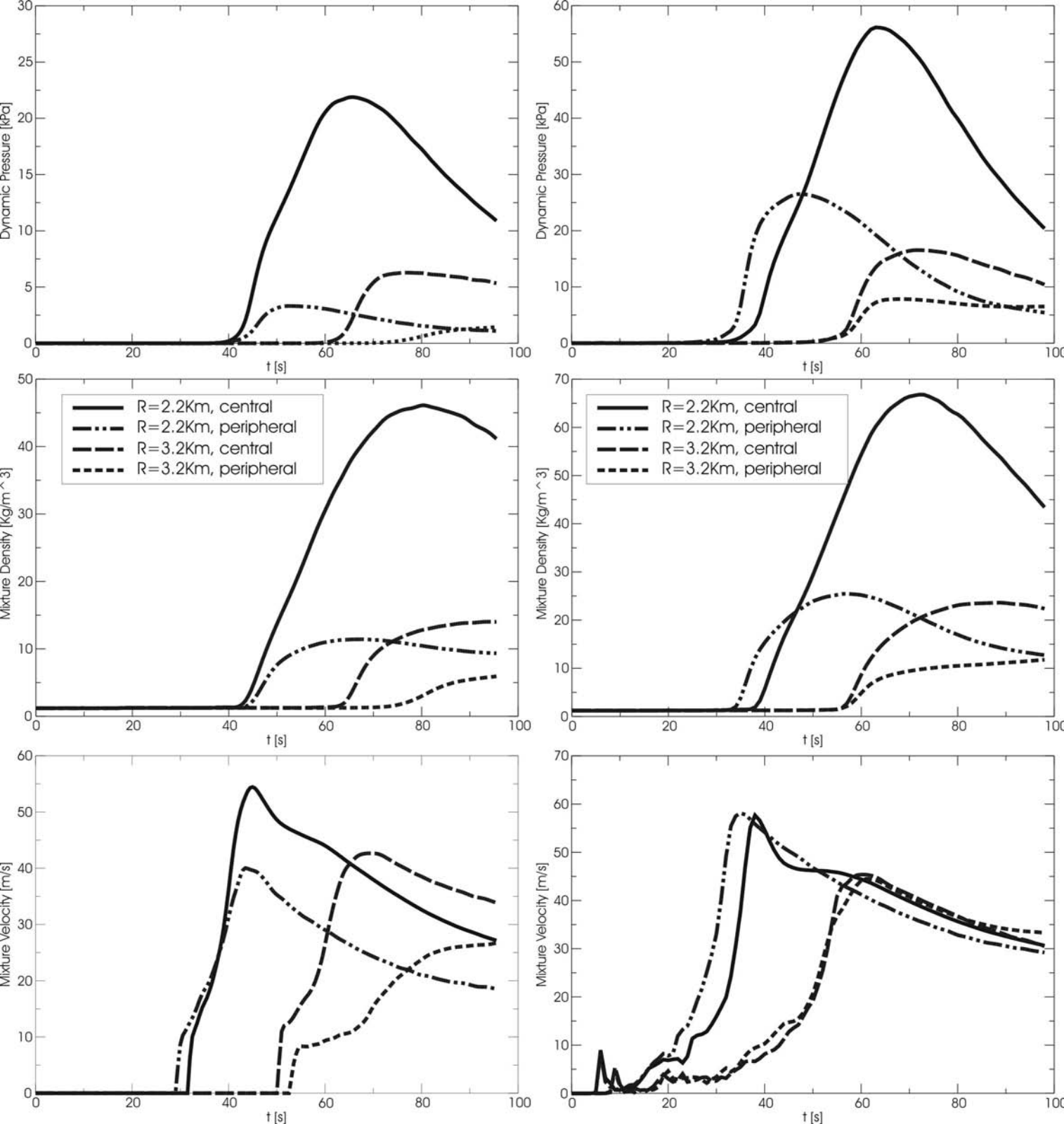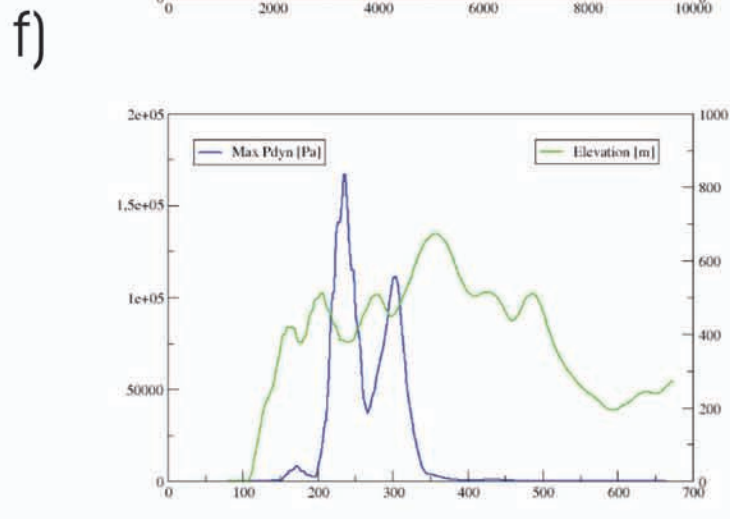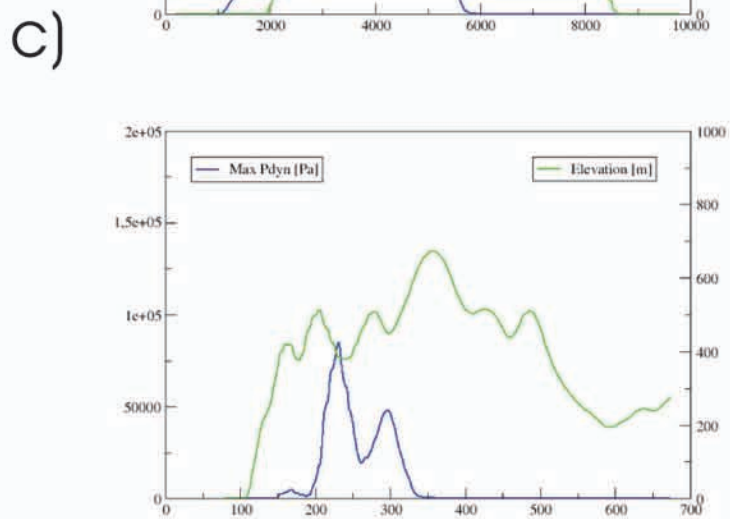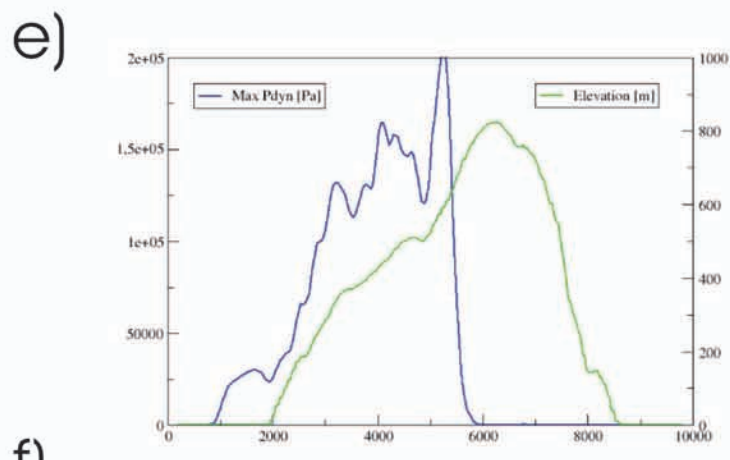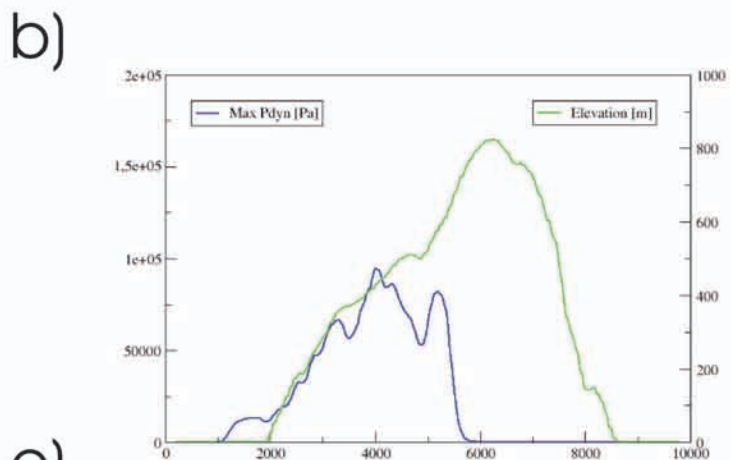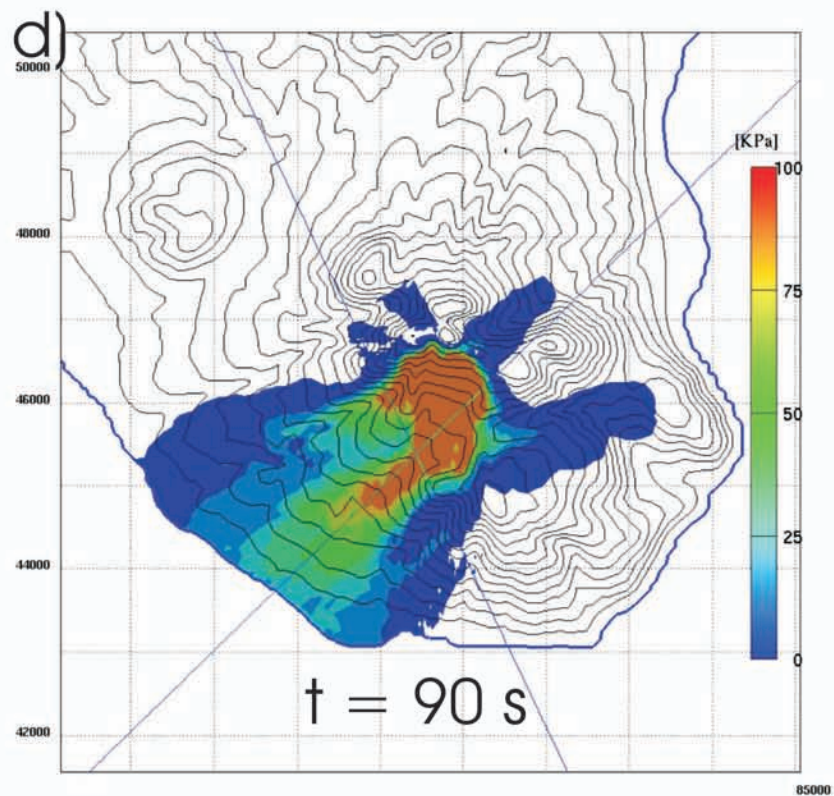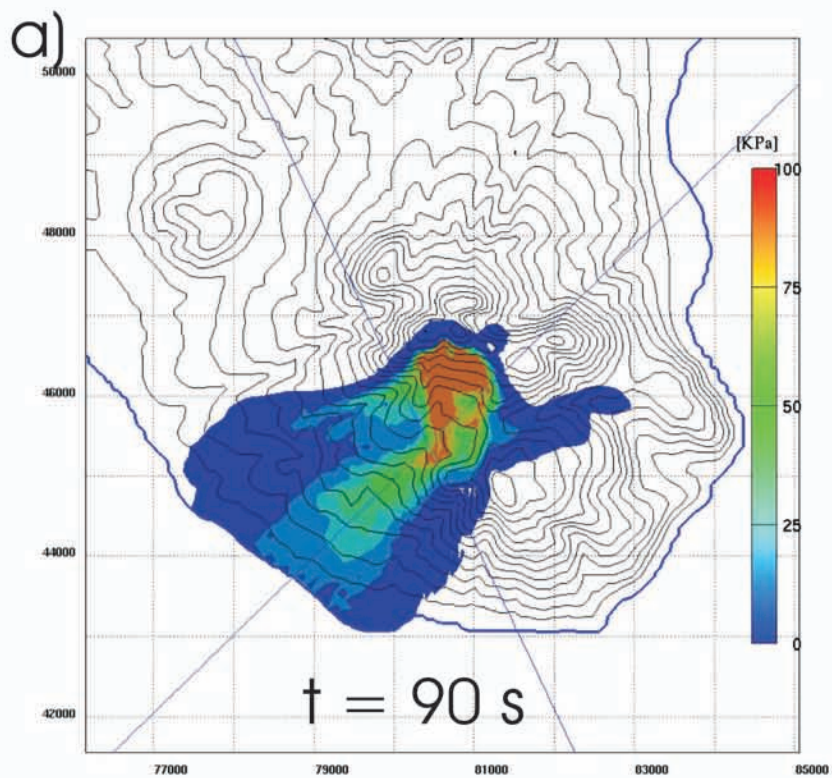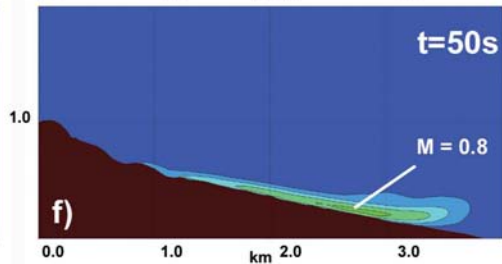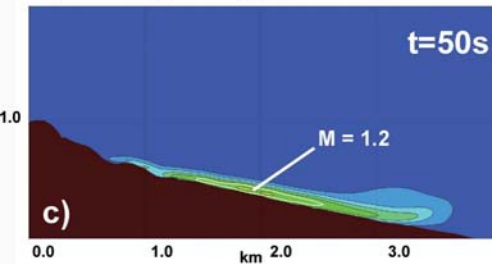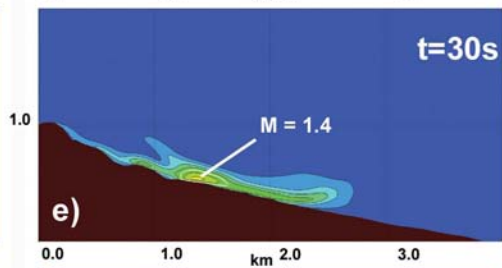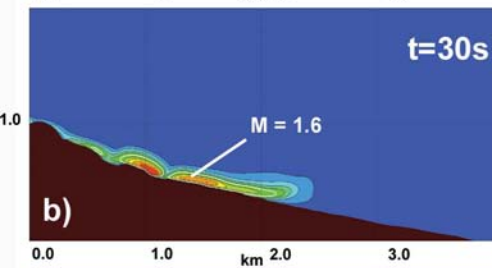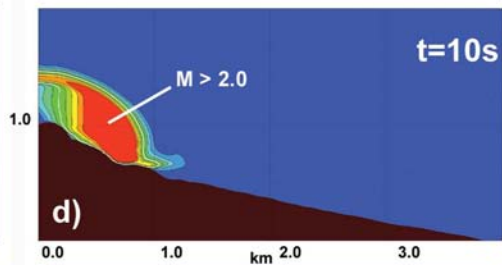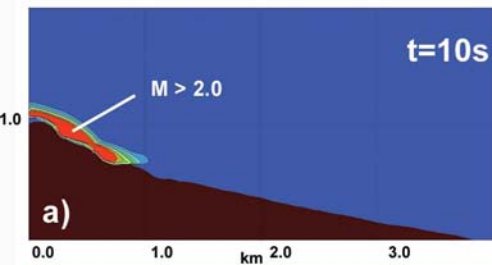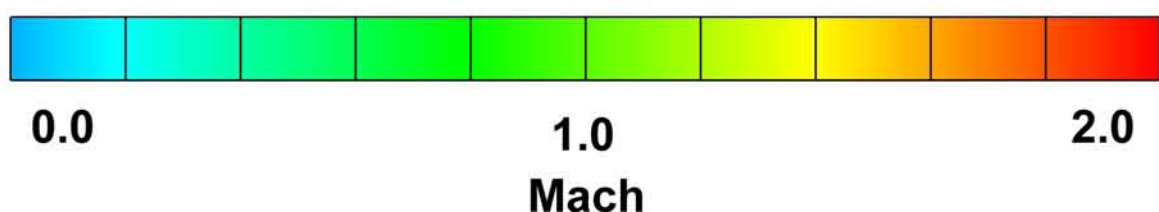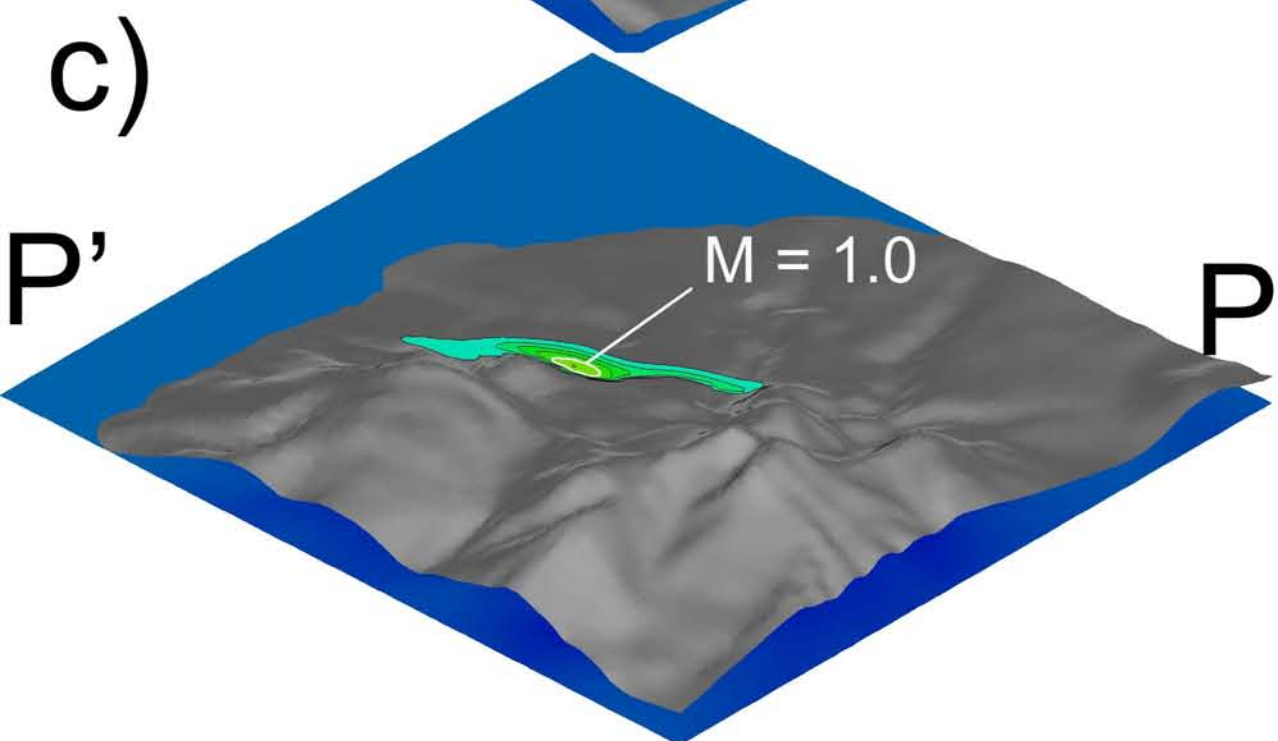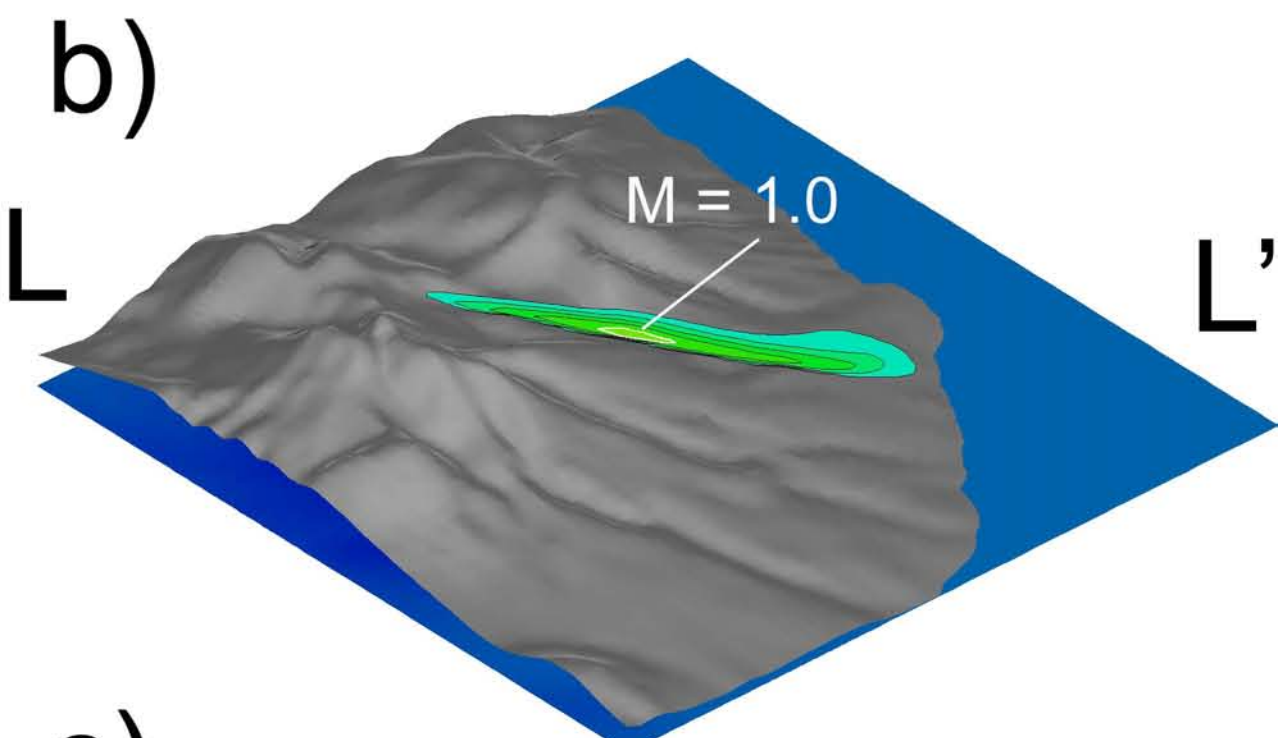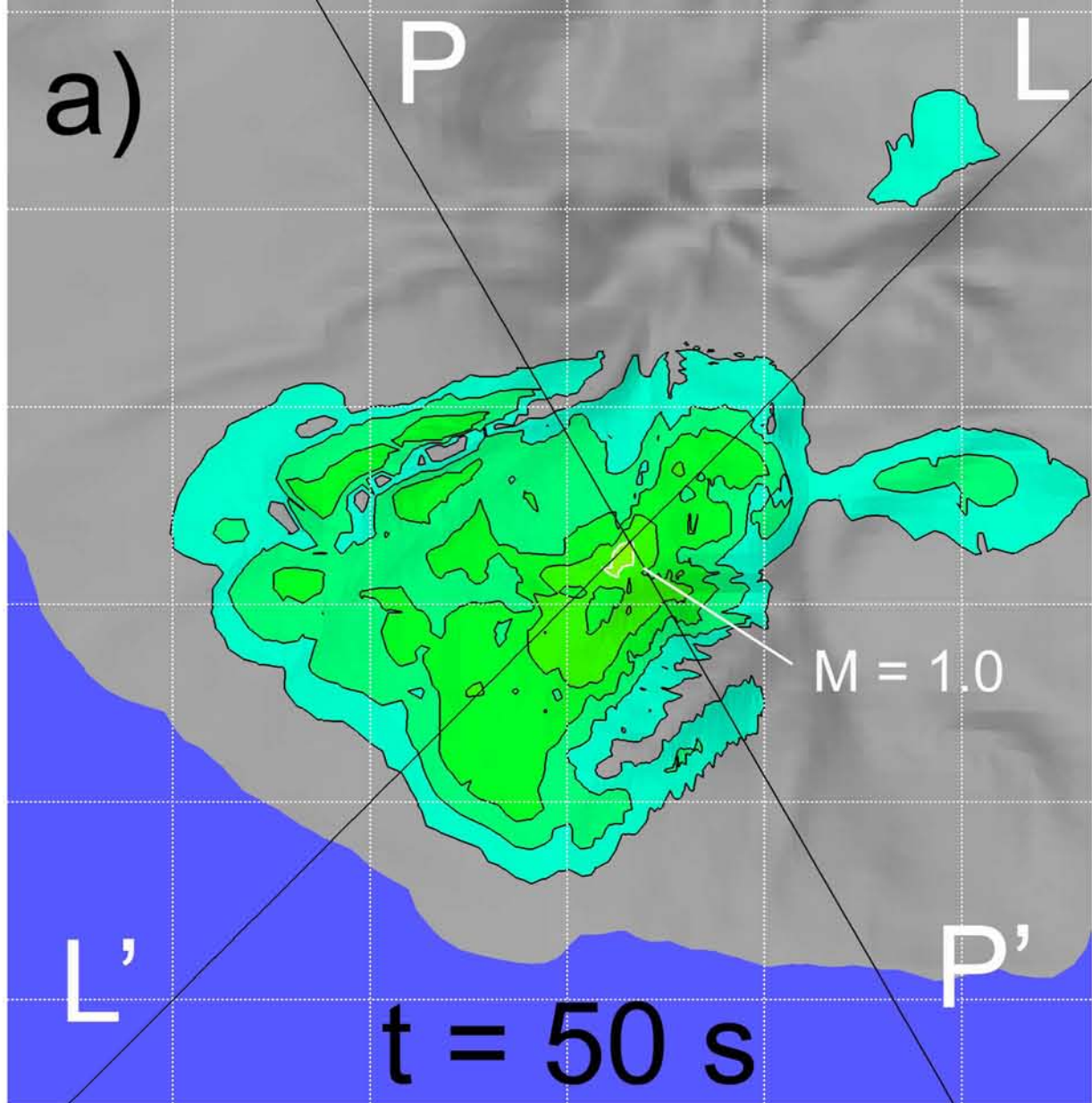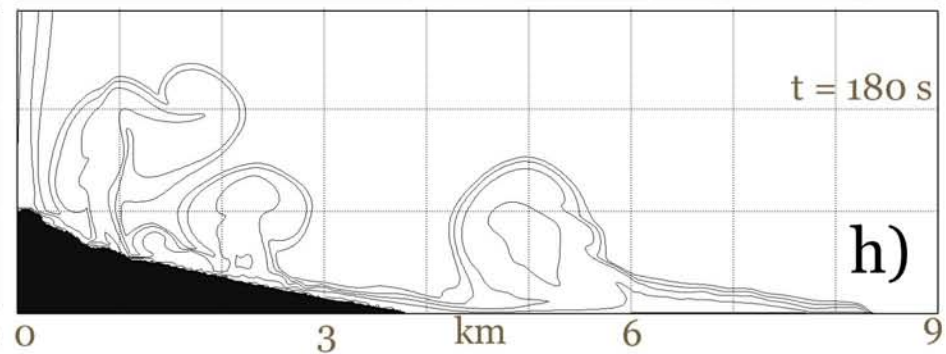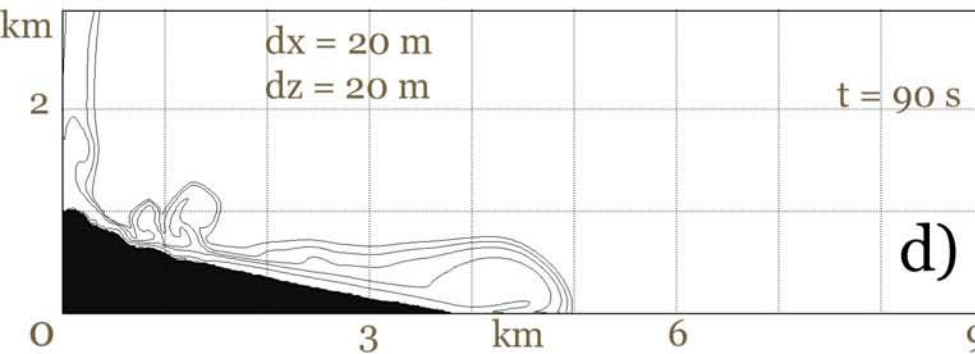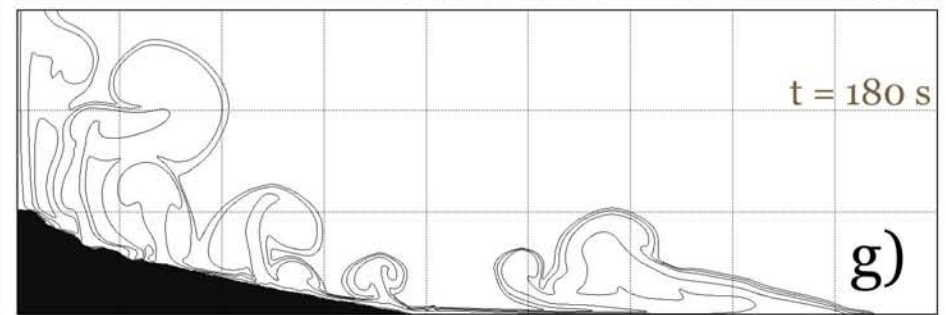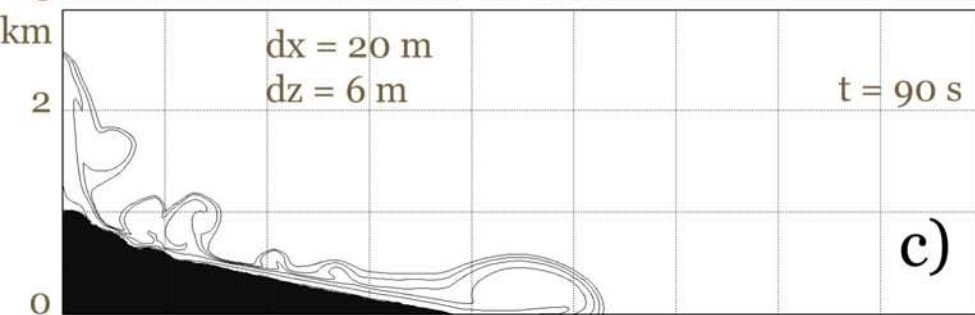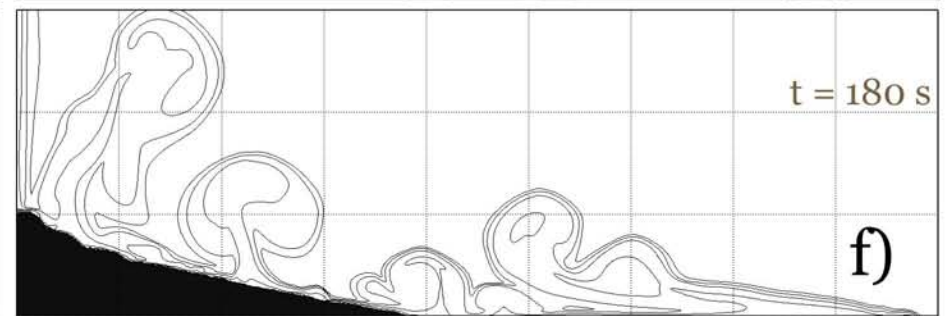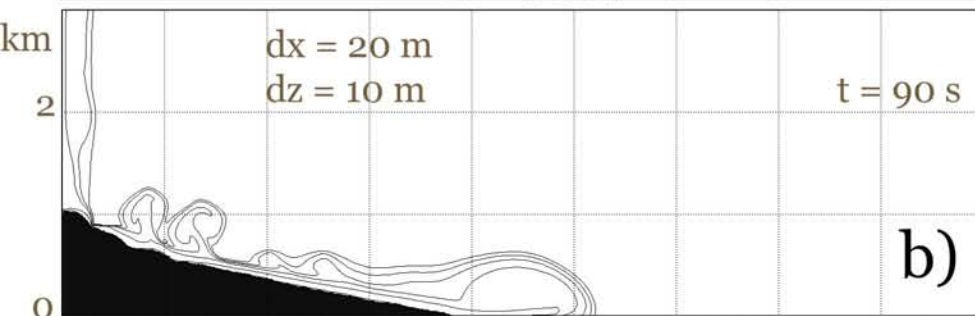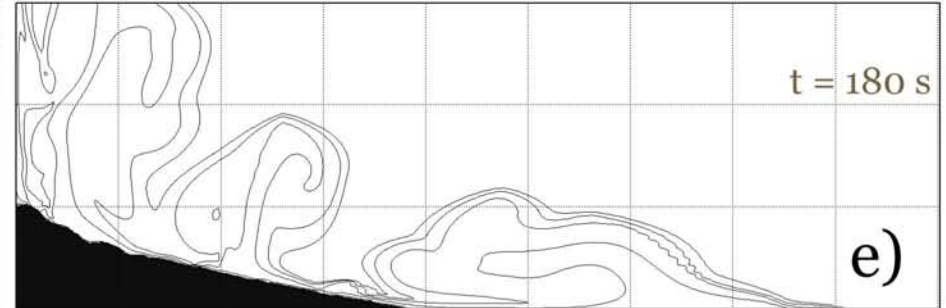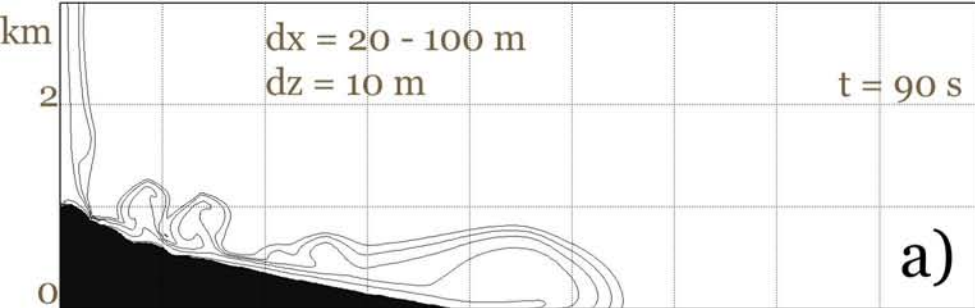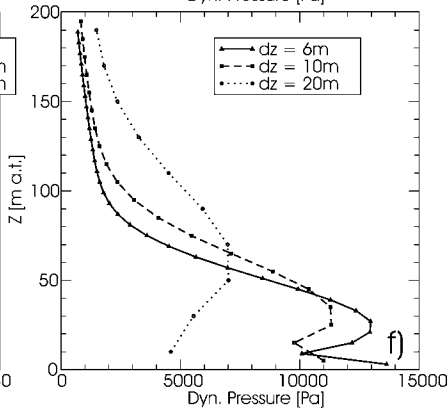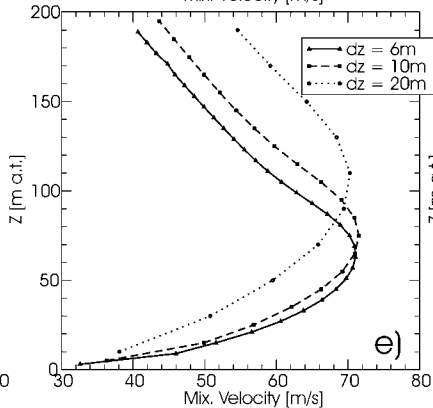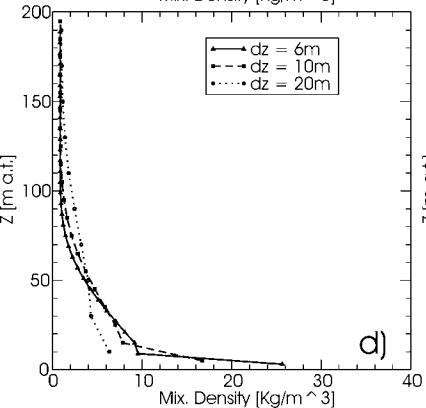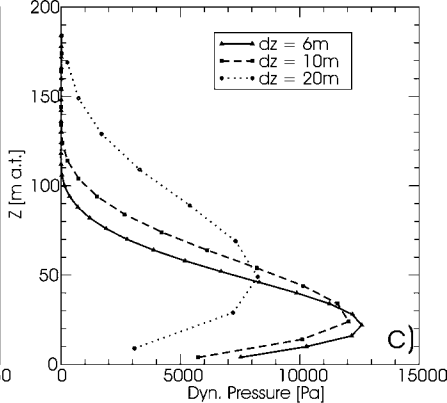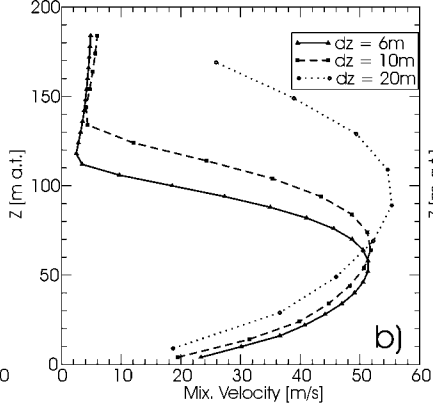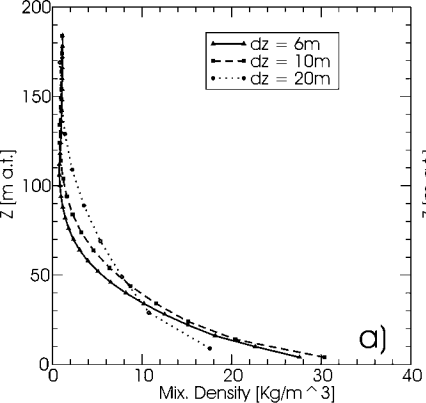
Run	$\kappa(m^2)$	V_{DRE} (m^3)	R_d (m)	Mass (kg)	α	E [J/kg]
A-2D	10^{-12}	5.0×10^6 $\times (360/70)$	227	60×10^9	0.1	320-490
B-2D	10^{-12}	10.0×10^6 $\times (360/70)$	280	120×10^9	0.1	390-610
C-2D	10^{-14}	5.0×10^6 $\times (360/70)$	227	60×10^9	0.1	1880-3380
A-3D	10^{-12}	5.0×10^6	142	12×10^9	0.1	320-480
B-3D	10^{-12}	10.0×10^6	180	24×10^9	0.1	340-520

Table 1

Run	H_b (m)	$U_{b,g}$ (m s^{-1})	$U_{b,p}$ (m s^{-1}) (5000, 500, 50μm)	U_f (m s^{-1})	T_p (s)	E (%) (5000, 500, 50 μm)	Rm_{max} (kg m^{-3}) (at 2,3,4 km)	Um_{max} (m s^{-1}) (at 2,3,4 km)	Pd_{max} (kPa) (at 2,3,4 km)	Pd_{SP} (kPa)
A-2D	250	160	75,125, 155	70	160	50, 20, ~0	57, 19, 18	46, 40, 34	44, 13, 7	>12.5
B-2D	300	160	75,125, 155	80	>180	0	54, 16, 17	72, 44, 33	46, 16, 6	>26
C-2D	500	175	85,145, 175	90	150	65, 30, <5	118, 38, 30	66, 43, 40	75, 28, 14	>14

Table2