

22 comparison of the MFIX boundary conditions with the ones obtained from experiments is
23 presented, showing good agreement between the simulated and predicted flow-front velocities.

24

25 **Keywords**

26 Granular flows, Numerical simulations, MFIX, Boundary conditions

27

28 **1. Introduction**

29 Granular flows are mixtures of discrete solid particles dominated by grain contacts where the
30 contribution of any interstitial fluid to the flow dynamics is negligible. Those mixtures belong to the
31 family of multiphase flows, which have been extensively studied in a wide range of industrial
32 (fluidised beds, pneumatic transport, etc.) and geophysical (e.g., dry volcanic granular flows, debris
33 avalanches, etc.) applications. Such mixtures, which can be characterised by a wide range of particle
34 sizes, concentrations and materials (Sulpizio et al., 2010; Syamlal et al., 1993), are greatly dissipative
35 due to frictional and inelastic collisions (Boyle and Massoudi, 1989; Dartevelle, 2004; Jaeger et al.,
36 1996).

37 Specifically, dry volcanic granular flows are generated in different ways and from various sources,
38 such as the collapse of eruptive columns and volcanic domes (Iverson and Vallance, 2001; Sulpizio
39 et al., 2016, 2010). The former are injection into the atmosphere of gas-particles flows (Branney and
40 Kokelaar, 2002) , while the latter consist of magma extruded from a vent that piles up because of
41 its viscosity (Harnett et al., 2018). These types of flows occur frequently in nature and can be
42 hazardous and enormously destructive (e.g. Branney and Kokelaar 2002, Iverson 1997, Louge et al.
43 2012, Zanchetta et al. 2004); improving the knowledge of their key features would greatly enhance

44 hazard assessment and planning strategies for minimising the impact of these events on the
45 environment.

46 In recent years, several authors have employed multiphase computational fluid dynamics (CFD)
47 techniques to investigate a variety of processes characterising volcanic flows such like impinging jets
48 (e.g. Valentine and Sweeney 2018), dense granular flows (e.g. Breard et al. 2019, Lube et al. 2019)
49 and collapsing phenomenon (e.g. Valentine 2020). The physical laws governing the flow-wall
50 dynamics implemented in the used CFD models and their effects on the behaviour of the simulated
51 volcanic flows were not investigated. The crucial importance of the boundary conditions to
52 quantitatively predict the granular flow parameters was amply demonstrated by several
53 experiments on the rapid shearing of glass or polymer spheres where granular mixtures with the
54 same density and at the same shear rate, sliding on channel surfaces with different roughness,
55 recorded different shear stresses, velocities and flow rates (Hanes and Inman, 1985; Jop et al., 2005;
56 Sarno et al., 2018a; Savage and Sayed, 1984). Consequently, to investigate the dynamics influencing
57 the flow-wall interaction, we have simulated dense granular flows employing a multiphase CFD
58 solver to understand the role of the implemented boundary conditions.

59 The multiphase CFD simulation tool used, MFIX (<http://mfix.netl.doe.gov/>) (Syamlal et al., 1993),
60 provides a suite of models that allows for the simulation of multiphase flows using different
61 approaches, such like the Discrete Element Method (DEM)(Cundall and Strack, 1979; Garg et al.,
62 2012; Li et al., 2012) and the Two-Fluid Model (TFM)(Campbell, 1990; Lun et al., 1984). In DEM the
63 motion of solid particles is simulated by coupling the particles to the fluid flow field using Newton's
64 laws and taking particle-particle and particle-wall interactions into account. In TFM, the solid phase
65 is treated as a fluid whose motion is governed by the Navier-Stokes Equation, with additional models
66 accounting for the rheology of the solid phase, the momentum coupling between the solid and the
67 fluid phase, and the solid-wall interaction. The DEM approach is simpler than the TFM (which relies

68 on a continuum approach), however, storing information for each single particle is computationally
69 expensive and DEM's application is still limited to the analysis of granular material composed of
70 several hundred thousand particles (Ge et al., 2015) –a number which is very small to represent real
71 systems. The heavy computational demand strongly limits the applicability of the DEM to volcanic
72 granular flows, which involve several million of particles with different sizes (from microns to
73 meters), densities (from hundreds to few thousand of kg m^{-3}) and shapes (from almost spherical to
74 highly irregular) (Neglia et al., 2020). To date the TFM approach remains the more feasible one for
75 these kinds of flows.

76 In the present work, we first explore the existing relationships implemented in TFM MFIX by focusing
77 on the boundary conditions for the solid phase. We investigate these boundary conditions
78 describing the dynamic interaction between the solid phase and a rigid wall. We then undertake a
79 sensitivity analysis focusing on the parameters appearing in the solid-wall boundary conditions.
80 Finally, we apply MFIX to replicate a large-scale experiment on volcanic dry granular mixture flowing
81 in an inclined channel; by using the knowledge carried out by the sensitivity analysis, we set-up the
82 optimum MFIX simulations configuration.

83

84 **2. From theory to an optimal MFIX configuration: sensitivity analyses of wall** 85 **boundary conditions**

86 In this section we introduce 1) the TFM implemented in MFIX and 2) the boundary conditions (BC)
87 controlling the interaction between the solid phase and a wall.

88

89 **2.1. Two-Fluid Model governing equations**

90 The TFM treats the gas and solid phase as interpenetrating continua, whose motion is solved using
 91 the Eulerian-Eulerian approach. Flow variables are volume-averaged over a region (named control
 92 volume -CV) that is large when compared to the particle size but small compared to the scale of
 93 macroscopic variations inside the flow domain (Anderson and Jackson, 1967). In the TFM, the
 94 Navier-Stokes equations for the conservation of mass, momentum and energy for each phase are
 95 solved, with constitutive equations accounting for the interphase interactions. In the following we
 96 do not report the energy conservation equations since in this study we consider the flow isothermal.
 97 The mass conservation equations for gas and m^{th} solid phase are:

$$99 \quad \frac{\partial(\varepsilon_g \rho_g)}{\partial t} + \nabla \cdot (\varepsilon_g \rho_g \mathbf{U}_g) = 0 \quad 1$$

$$100 \quad \frac{\partial(\varepsilon_{sm} \rho_{sm})}{\partial t} + \nabla \cdot (\varepsilon_{sm} \rho_{sm} \mathbf{U}_{sm}) = 0 \quad 2$$

101

102 where ρ is the density, ε is the volume concentration, U is the velocity and the subscripts s and g
 103 denote the solid and fluid phase, respectively. All symbols are listed in Table 1. The first term on the
 104 left-hand side accounts for the rate of mass change per unit volume, and the second one is the
 105 convective mass flux. Potential sources and sinks due to phase changes and chemical reactions are
 106 neglected.

107 The momentum equations for the gas and solid phase are:

108

$$109 \quad \frac{\partial(\varepsilon_g \rho_g \mathbf{U}_g)}{\partial t} + \nabla \cdot (\varepsilon_g \rho_g \mathbf{U}_g \mathbf{U}_g) = \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \mathbf{g} - \sum_{m=1}^M \mathbf{I}_{gm} \quad 3$$

$$110 \quad \frac{\partial(\varepsilon_{sm} \rho_{sm} \mathbf{U}_{sm})}{\partial t} + \nabla \cdot (\varepsilon_{sm} \rho_{sm} \mathbf{U}_{sm} \mathbf{U}_{sm}) = \nabla \cdot \boldsymbol{\tau}_{sm} + \varepsilon_{sm} \rho_{sm} \mathbf{g} + \mathbf{I}_{gm} + \sum_{\substack{l=1 \\ l \neq m}}^M \mathbf{I}_{ml} \quad 4$$

111

112 here $\boldsymbol{\tau}_g$ and $\boldsymbol{\tau}_{sm}$ are the fluid and solid phase stress tensor, respectively, \boldsymbol{g} is the gravitational
113 acceleration, \boldsymbol{I}_{gm} represents the transferred momentum between the gas phase and the m^{th} solids
114 phase and \boldsymbol{I}_{ml} is the interaction force between the m^{th} and l^{th} solid phase. The first and the second
115 term on the left-hand side (Eq. 3 and 4) represent the net rate of momentum change and the net
116 rate of momentum transferred by convection, respectively, and the first and second term on the
117 right-hand side (Eq. 3 and 4) represent the internal stress and the body forces, respectively.

118 Johnson and Jackson (Johnson and Jackson, 1987) proposed a model to describe the kinetic and
119 frictional stresses that contribute to the solid stress tensor $\boldsymbol{\tau}_{sm}$, where the kinetic contribution is
120 calculated applying the kinetic theory to the granular material (Boyle and Massoudi, 1989) and the
121 frictional contribution is computed by means of the rigid-plastic rheological model proposed by
122 Schaeffer (Schaeffer, 1987). MFIK combines the two theories by considering a “switch” value
123 represented by the void fraction at maximum packing ε_g^* (Syamlal et al., 1993):

124

$$125 \quad \boldsymbol{\tau}_{sm} = \begin{cases} -P_{sm}^f \boldsymbol{I} + 2\mu_{sm}^f \boldsymbol{S} & \varepsilon_g \leq \varepsilon_g^* \\ (-P_{sm}^k + \eta\mu_b \nabla \cdot \boldsymbol{v}_s) \boldsymbol{I} + 2\mu_{sm}^k \boldsymbol{S} & \varepsilon_g > \varepsilon_g^* \end{cases} \quad 5$$

126

127 where P_{sm}^f and P_{sm}^k are the solid pressure for the frictional and kinetic-collisional regime,
128 respectively, \boldsymbol{I} is the unit tensor, \boldsymbol{S} is the strain rate tensor, $\eta = (1 + e_p)/2$ with e_p being the
129 particle-particle coefficient of restitution, μ_{sm}^k and μ_{sm}^f are the kinetic and solid viscosity,
130 respectively, and μ_b is the bulk viscosity. The higher e_p , the lower the dissipation rate given by
131 inelastic collisions. Similar to e_p , there is a restitution coefficient for particle-wall collision (e_w).

132 The solid pressure P_{sm}^k originates from the particles' kinetic interactions and is modelled as:

133

$$134 \quad P_{sm}^k = \varepsilon_{sm} \rho_{sm} \theta_m \left(1 + 4\eta \sum_{n=1}^M \varepsilon_{sn} g_{0,mn} \right) \quad 6$$

135

136 where g_0 is the radial distribution function, which quantifies the probability of finding two particles
137 at that specific location (Boyle and Massoudi, 1989) and acts as a correcting factor when the
138 concentration is high enough to break the molecular chaos assumption (Darteville, 2004) and θ is
139 the granular temperature, which quantifies the agitation state of the particles. θ is proportional to
140 the mean quadratic fluctuating velocity due to the random motion of the particles:

141

$$142 \quad \frac{3}{2} \theta_m = \frac{1}{2} \langle c_m'^2 \rangle \quad 7$$

143

144 where c_m' is the fluctuating component of the instantaneous velocity C_m of the m^{th} solid phase
145 defined as $C_m = U_{sm} + c_m'$. The term on the right-hand side of Eq. 7 defines the granular energy of
146 the continuum.

147 The solid pressure P_s^f is calculated using the model proposed by Schaeffer (1987) for a plastic flow
148 of a granular medium occurring at critical state, i.e. when the solid volume concentration exceeds
149 the maximum packing. The Schaeffer model is based on plastic flow theory of Jenike (1987), who
150 used an arbitrary function to take into account a certain amount of compressibility in the solid phase
151 (Pritchett et al., 1978) and to prevent unphysically large solids volume concentration (Gera et al.,
152 2004). The Schaeffer model was implemented in MFIX by Syamlal et al. (1993) as:

153

$$154 \quad P_s^f = P^* = A(\varepsilon_g^* - \varepsilon_g)^{10} \quad 8$$

155

156 where A is a constant taken equals to 10^{24} Pa and P^* represents the solid pressure at the critical
157 state.

158 More recently, the Princeton model (Srivastava and Sundaresan, 2003) for solid pressure
159 calculation, was implemented in MFIx. The Princeton model starts from the quasi-static model
160 proposed by Schaeffer and modifies it to account for strain rate fluctuations associated with the
161 generation of shear layers that decrease the shear stress in the granular material (Savage, 1998). In
162 this way, numerical singularities are avoided in the region where $\mathbf{S} = 0$ as long as $\theta \neq 0$. The solid
163 pressure P_s^f can be expressed as:

164

$$165 \quad P_s^f = P^* \left(1 - \frac{\nabla \cdot \mathbf{U}_s}{N\sqrt{2} \sin \delta_{int} \sqrt{\left(\mathbf{S} : \mathbf{S} + \frac{\theta}{d^2}\right)}} \right)^{\frac{1}{N-1}} \quad 9$$

166

$$167 \quad P^* = \begin{cases} A(\varepsilon_g^* - \varepsilon_g)^{10} & \varepsilon_g < \varepsilon_g^* \\ Fr \frac{(\varepsilon_s - \varepsilon_s^{min})^B}{(\varepsilon_s^* - \varepsilon_s)^C} & \varepsilon_g^* \leq \varepsilon_g < (1 - \varepsilon_s^{min}) \\ 0 & \varepsilon_g \geq (1 - \varepsilon_s^{min}) \end{cases} \quad 10$$

168

169 where ε_s^{min} is equal to 0.5, δ_{int} is the internal friction angle, d is the particles diameter, Fr and the
170 exponents B and C are constants equal to 0.05 Pa, 2 and 5, respectively. The exponent N is equal

171 to $\sqrt{3}/2 \sin \delta_{int}$ in dilatation conditions ($\nabla \cdot \mathbf{U}_s \geq 0$) or equal to 0 in compaction conditions
 172 ($\nabla \cdot \mathbf{U}_s < 0$). The strain rate fluctuations are represented by the term θ/d^2 . If the granular material
 173 is compacted, the solid pressure will be equal to the critical pressure P^* . For all the simulations
 174 discussed in the present paper, the Princeton frictional model was selected because tests on the
 175 two frictional models conducted by Breard et al. (2019), showed that the Princeton model leads to
 176 a more gradual variation of P_s^f and to a better dissipation of the pore pressures compared to what
 177 obtained with the Schaeffer one.

178 The particles agitation state can be quantified by means of the granular temperature θ (Eq. 7). The
 179 conservation equation of the granular energy (right-hand side term of Eq. 7) is given by:

180

$$181 \quad \frac{3}{2} \rho_{sm} \left(\frac{\partial(\varepsilon_{sm} \theta_m)}{\partial t} + \nabla \cdot (\varepsilon_{sm} \theta_m \mathbf{U}_{sm}) \right) = -\nabla \cdot \mathbf{q}_m + \boldsymbol{\tau}_{sm} : \nabla \cdot \mathbf{U}_{sm} - \gamma_{\theta_m} + \varphi_{gm} + \sum_{l=1, l \neq m}^M \varphi_{lm} \quad 11$$

182

183 where \mathbf{q} is the diffusive flux of granular energy, γ_{θ} is the granular energy dissipation due to inelastic
 184 collisions, φ_{gm} represents the transferred granular energy between gas and the m^{th} solids phase
 185 and φ_{lm} accounts for the transferred granular energy between the m^{th} and l^{th} solid phases. The
 186 terms on the left-hand side are the rate of change and the advection of the granular temperature,
 187 respectively. The first term on the right-hand side (Eq. 11) is the diffusive transport of granular
 188 energy, the second term is the net rate of granular energy produced by shear and the last three
 189 terms represent dissipation of granular energy.

190

Symbol	Description	Dimension
--------	-------------	-----------

A	constant of Eq. 10	Pa
B	constant of Eq. 10	-
c_w	source term in Eq. 14 due to particle-wall slip	kg s^{-3}
C	constant of Eq. 10	-
C_m	instantaneous velocity	m s^{-1}
c'_m	fluctuating component of C_m	m s^{-1}
d	particle diameter	m
D	dissipation rate of granular energy due to inelastic collisions	kg s^{-3}
e_p	restitution coefficient for the particle-particle collision	-
e_w	restitution coefficient for the particle-wall collision	-
Fr	constant of Eq. 12	Pa
g	gravitational acceleration	m s^{-2}
h_w^u	wall velocity transfer coefficient	m^{-1}
h_w^θ	wall granular temperature transfer coefficient	$\text{kg m}^{-2} \text{s}^{-1}$
I	unit tensor	-
I_{gm}	momentum transfer from fluid phase to m^{th} solid phase	$\text{kg m}^{-2} \text{s}^{-1}$
I_{ml}	momentum transfer from m^{th} to l^{th} solid phase	$\text{kg m}^{-2} \text{s}^{-1}$
k	function of wall friction angle and restitution coefficient	-
$\overline{M_{t,w}}$	average tangential momentum transferred per collision	kg m s^{-1}

n	fluid-to-wall normal	-
n_1	wall-to-fluid normal	-
N	function of internal friction angle	-
P	pressure	Pa
q	diffusive flux of granular energy	kg s^{-3}
r	normalized slip velocity at the wall	-
S	strain rate tensor	s^{-1}
t	time	s
U	velocity	m s^{-1}
U_{mg}	solid velocity magnitude	m s^{-1}
U_{sl}	slip velocity	m s^{-1}

Greek symbol	Description	Dimension
γ_θ	granular energy dissipation due to inelastic collisions	kg s^{-3}
δ_{int}	internal friction angle of the granular material	$^\circ$ (degree)
δ_w	Wall friction angle of the granular material	$^\circ$ (degree)
ε	volume concentration	-
η	function of the inelastic collision	-
θ	granular temperature	$\text{m}^2 \text{s}^{-2}$
μ	viscosity	Pa s

μ_b	bulk viscosity	Pa s
ρ	density	kg m ⁻³
φ_{gm}	transferred granular energy between gas and m th solid phase	kg s ⁻³
φ_{lm}	transferred granular energy between m th and l th solid phase	kg s ⁻³
ϕ	specularity coefficient	-
ϕ_0	specularity coefficient when r goes to zero	-

Subscripts

g	fluid phase
m	solid phase m th
s	solid phase
w	wall

Superscript

f	frictional
min	minimum concentration referred to the Princeton model
k	kinetic
*	maximum packing

191 Table 1. List of symbols with description and physical dimension.

192

193 **2.2 Boundary conditions available in MFIX**

194 The following boundary conditions for the conservation equations of the gas and solid phases are
 195 considered in MFIX: no-slip (zero velocity at the wall), free-slip (velocity gradient vanishes at the
 196 wall) and partial-slip wall condition, which controls the trend of velocity for the gas and solid phases
 197 and of the granular temperature from the flow to the wall:

198

$$199 \quad \frac{dU}{dn} + h_w^u (U - U_w) = 0 \quad 12$$

200

$$201 \quad \frac{d\theta}{dn} + h_w^\theta (\theta - \theta_w) = c_w \quad 13$$

202

203 where c_w is the source term due to particle-wall slip, U_w and θ_w are the velocity and granular
 204 temperature at the wall, n is the fluid-to-wall normal, and h_w^θ and h_w^u are the transfer coefficients,
 205 which regulate the spatial rate with which U and θ approximate U_w and θ_w .

206 The parameters in the partial-slip boundary conditions can be defined in in two different ways: user-
 207 defined values that apply to all the walls in the whole computational domain or local flow-
 208 dependent values calculated for the solid phase by means of the Johnson and Jackson (1987) or
 209 Jenkins (1992) models.

210 Johnson and Jackson (1987) developed a condition for the slip velocity of particles relative to a wall
 211 by equating the tangential force per unit area exerted on the wall by the particles to the stress due
 212 to the granular assembly close to the boundary:

213

$$214 \quad \frac{U_{sl} \tau_{sm} n_1}{|U_{sl}|} + \frac{\phi \sqrt{3} \theta \pi \rho_s \varepsilon_s |U_{sl}|}{6 \varepsilon_s^* \left[1 - \left(\frac{\varepsilon_s}{\varepsilon_s^*} \right)^{\frac{1}{3}} \right]} + P_s^f \tan \delta_w = 0 \quad 14$$

215

216 where \mathbf{n}_1 is the boundary-to-flow unit normal vector, U_{sl} is the slip velocity relative to the wall and
 217 ϕ is the specularity coefficient, which varies between zero for perfectly specular collision and unity
 218 for perfectly diffuse collisions (Johnson and Jackson, 1987) and depends on the particle and wall
 219 properties (including the surface roughness) (Li et al., 2010b). Specular and diffuse collisions
 220 correspond to smooth and rough walls, respectively (Hui et al., 1984). The first term of Eq. 14
 221 represents the stress in the granular flow approaching the boundary, the second term is the rate of
 222 tangential momentum transferred to the wall by particles collisions and the third term represents
 223 the frictional stress due to the sliding particles, which is calculated by applying Coulomb friction law
 224 to the particles that slide at the boundary (Li and Benyahia, 2012).

225 The specularity coefficient ϕ can be also explained as the fraction of the collision that transfer
 226 significant amount of average tangential momentum to the wall (Hui et al., 1984):

227

$$228 \quad \overline{M_{t,w}} = \phi \rho_s \pi d^3 U_{sl} / 6 \quad 15$$

229

230 Li and Benyahia (Li and Benyahia, 2012) proposed a predictive expression for ϕ , which was obtained
 231 from numerical integration data based on the rigid-body theory:

232

$$233 \quad \phi = \begin{cases} -7\sqrt{6\pi}(\phi_0)^2 r + \phi_0 & r \leq \frac{4k}{7\sqrt{6\pi}\phi_0} \\ \frac{2}{7} \frac{k}{r\sqrt{6\pi}} & r > \frac{4k}{7\sqrt{6\pi}\phi_0} \end{cases} \quad 16$$

234

235 where r is equal to $U_{sl}/\sqrt{3\theta}$ (the normalized slip velocity at the wall characterizing the mean impact
 236 angle of particles), k is equal to $\frac{7}{2} \tan \delta_w (1 + e_w)$ and ϕ_0 states for ϕ value when r goes to zero:

237

$$\begin{aligned} 238 \quad \phi_0 = & -0.0012596 + 0.1064551k - 0.04281476k^2 + 0.0097594k^3 - 0.0012508258k^4 + \\ 239 \quad & 0.0000836983k^5 - 0.00000226955k^6 \end{aligned} \quad 17$$

240

241 The Johnson and Jackson boundary condition with Li and Benyahia modification for the calculation
242 of ϕ is referred to in this paper as “revisited Johnson and Jackson BC”.

243 The boundary condition for the granular energy is obtained from the balance of granular energy
244 over a control volume (Johnson and Jackson, 1987):

245

$$246 \quad -\mathbf{n}_1 \cdot \mathbf{q} = D + \mathbf{U}_{sl} \cdot \mathbf{S}_c^b \quad 18$$

247

248 where \mathbf{S}_c^b corresponds to the second term of Eq. 14 and D is the rate of dissipation of granular
249 energy due to inelastic particles-wall collisions, which is given by:

250

$$251 \quad D = \frac{1}{4} \pi \rho_s \theta (1 - e_w^2) \frac{\sqrt{3\theta}}{\left[\left(\frac{\varepsilon_s^*}{\varepsilon_s} \right)^{\frac{1}{3}} - 1 \right]} \frac{1}{\left(\frac{\varepsilon_s^*}{\varepsilon_s} \right)^{\frac{2}{3}}} \quad 19$$

252

253 The model proposed by Jenkins (1992) consists of relationships for the shear stress and granular
254 energy flux at the wall in two limiting case: small-friction/all-sliding limit and the large-friction/no-
255 sliding limit. The only limit case currently implemented in MFIx is the small-friction/all-sliding limit,

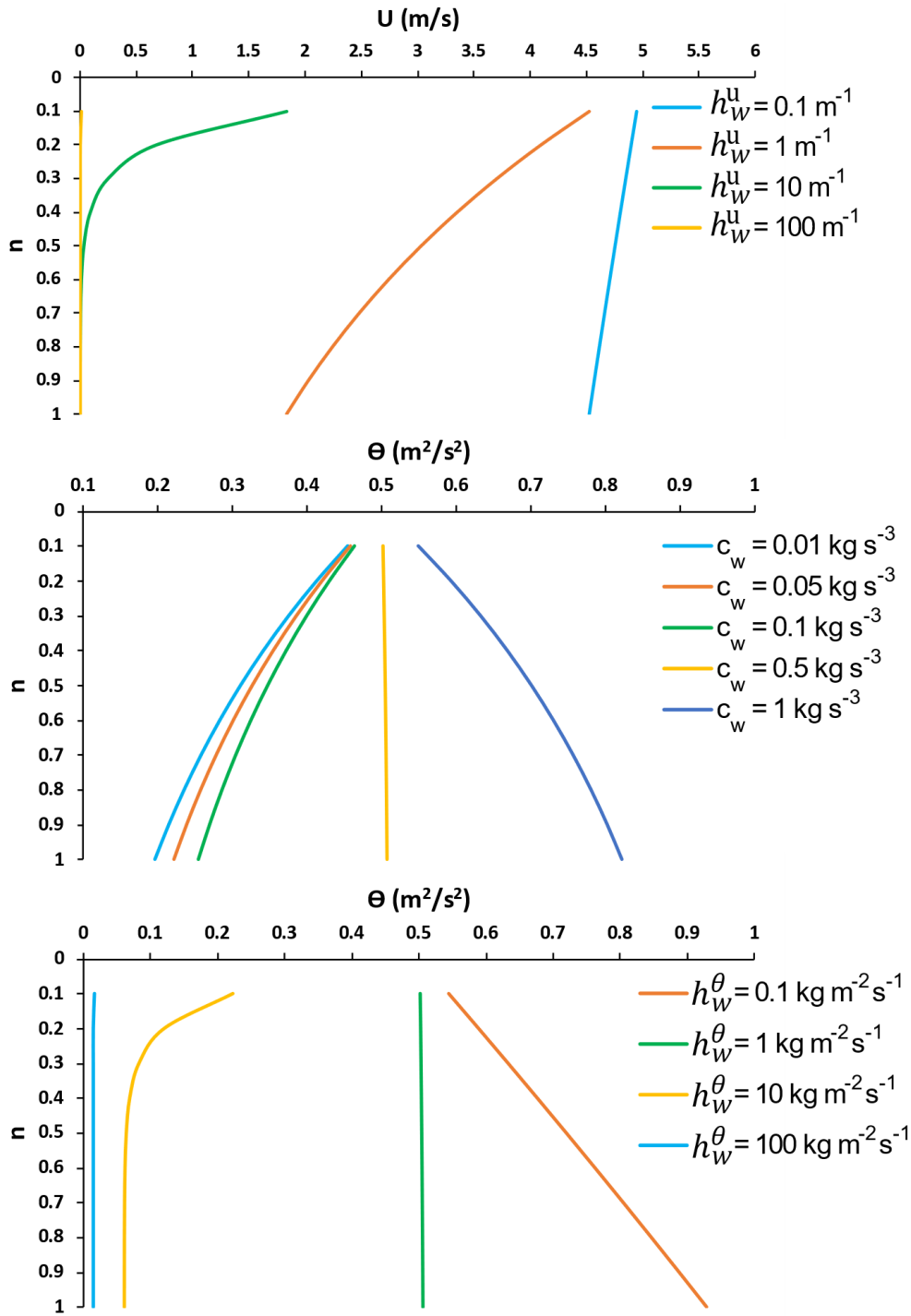
256 for which all collisions involve sliding and the ratio of shear to normal stress, is equal to the wall
257 friction coefficient:

258

$$259 \quad \frac{q}{P_s^k \sqrt{3\theta}} = \tan^2 \delta_w (1 + e_w) \frac{21}{16} - \frac{3}{8} (1 - e_w) \quad 20$$

260

261 To better understand the effect of h_w^u , h_w^θ and c_w on the solid-wall interactions in the simulations,
262 we analytically solved Eqs. 12 and 13 and plotted the U and θ vs. n (Fig. 1), setting for the velocity
263 profile equation (Eq. 12) $U = 5.0 \text{ m s}^{-1}$ and $U_w = 0.0 \text{ m s}^{-1}$ and for granular temperature profiles
264 equation (Eq. 13) $\theta = 0.5 \text{ m}^2 \text{ s}^{-2}$ and $\theta_w = 0.01 \text{ m}^2 \text{ s}^{-2}$.



265 Figure 1. Flow velocities (U) and granular temperatures (θ) plotted against the normal fluid-to-wall (n).

266

267 Figure 1 shows that the higher h_w^u , the sharper the velocity gradients. Indeed, $h_w^u = 0.1 \text{ m}^{-1}$ yields a
 268 velocity gradient with constant angular coefficient resulting in high velocities (close to $U = 5 \text{ m s}^{-1}$),
 269 whereas $h_w^u = 100 \text{ m}^{-1}$ results in velocities equal to U_w (0.0 m s^{-1}), freezing the particle at the wall.
 270 Therefore, in the limit of h_w^u approaching 0 the partial-slip boundary condition reduces to a free-slip

271 condition for the solid phase; on the other hand, large values of h_w^u leads to a no-slip condition.
 272 Furthermore, h_w^u ranging between $1 - 10 \text{ m}^{-1}$ produces concave velocity profiles facing to the right.
 273 h_w^θ and c_w show two different trends at changing θ . For $h_w^\theta > 1 \text{ kg m}^{-2}\text{s}^{-1}$ and $c_w < 0.5 \text{ kg s}^{-3}$ the
 274 granular temperatures decrease more or less quickly in the direction towards the wall, whereas for
 275 $h_w^\theta < 1 \text{ kg m}^{-2}\text{s}^{-1}$ and $c_w > 0.5 \text{ kg s}^{-3}$ an opposite trend is observed and the granular temperature
 276 increases at the wall. The inverse trend is physically unrealistic when compared to granular flows
 277 where the basal part is dominated by enduring contacts between particles (Sulpizio et al., 2016).
 278 Indeed, $h_w^\theta = 10 \text{ kg m}^{-2}\text{s}^{-1}$ and $c_w \leq 0.1 \text{ kg s}^{-3}$ result in profiles closer to the experimentally measured
 279 ones (Sarno et al., 2018b).

280

Partial-slip wall condition	Johnson and Jackson (1987)	Jenkins (1992)
$\frac{dU}{dn} + h_w^u(U - U_w) = 0$ <p style="text-align: center;"><i>where</i></p> $h_w^u = \frac{COL}{\mu_s^k} \quad \varepsilon_s \leq \varepsilon_s^{min}$ $h_w^u = \frac{COL+FRI}{\mu_s^k + \mu_s^f} \quad \varepsilon_s > \varepsilon_s^{min}$	$COL = \frac{\phi\sqrt{3}\theta\pi\rho_s\varepsilon_s g_0}{6(1 - \varepsilon_s^*)}$	$COL = \frac{\tan \delta_w P_s^k}{U_{sl}}$
$\frac{d\theta}{dn} + h_w^\theta(\theta - \theta_w) = c_w$	$h_w^\theta = \frac{1}{4}\pi\rho_s(1 - e_w^2)\frac{\sqrt{3}\theta}{(1 - \varepsilon_s^*)}$ $c_w = U_{sl} \cdot S_c^b$	$h_w^\theta = \frac{3}{8}(1 - e_w)P_s^k\sqrt{3}\theta\frac{1}{\theta}$ $c_w = \tan^2 \delta_w(1 + e_w)\frac{21}{16}P_s^k\sqrt{3}\theta$

281 Table 2. Summary of the partial-slip wall conditions as implemented in MFIX. *COL* and *FRI* represent collisional and
 282 frictional contribute to the wall, respectively. *FRI* is equal for the Johnson and Jackson and Jenkins boundary conditions,
 283 i.e. equals to the Coulomb law.

284

285 **2.2.1 Sensitivity analysis of the boundary conditions for the solid phase**

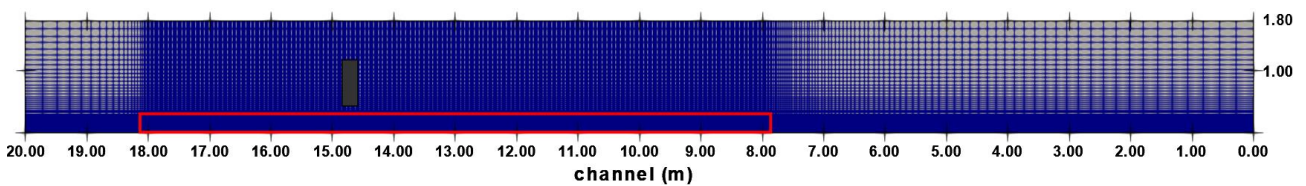
286 In sections 2.2.2, 2.2.3 and 2.2.4, we present results of the sensitivity analysis of the wall boundary
287 conditions for the solid phase. We first focus on the effect of varying the specularity coefficient
288 when using the Johnson and Jackson BC (Johnson and Jackson, 1987). We then analyse the influence
289 of particle size on the simulated flows using Jenkins (Jenkins, 1992). We also show the effect of
290 manually changing the parameters of the partial-slip boundary condition h_w^θ , h_w^u and c_w (Eqs. 12
291 and 13). Finally, we compare results obtained by the different configurations of the partial-slip wall
292 condition in MFIX (manual, Johnson and Jackson, Jenkins). In all the simulations discussed in Section
293 2.2.2, 2.2.3 and 2.2.4, the computational domain consists of a rectangle of 20.0 m length x 1.8 m
294 height discretized with a finer grid with rectangular cells of 0.02 m x 0.005 m in the focus area and
295 by a coarser one close to the walls (Fig. 2).

296

297

298

299



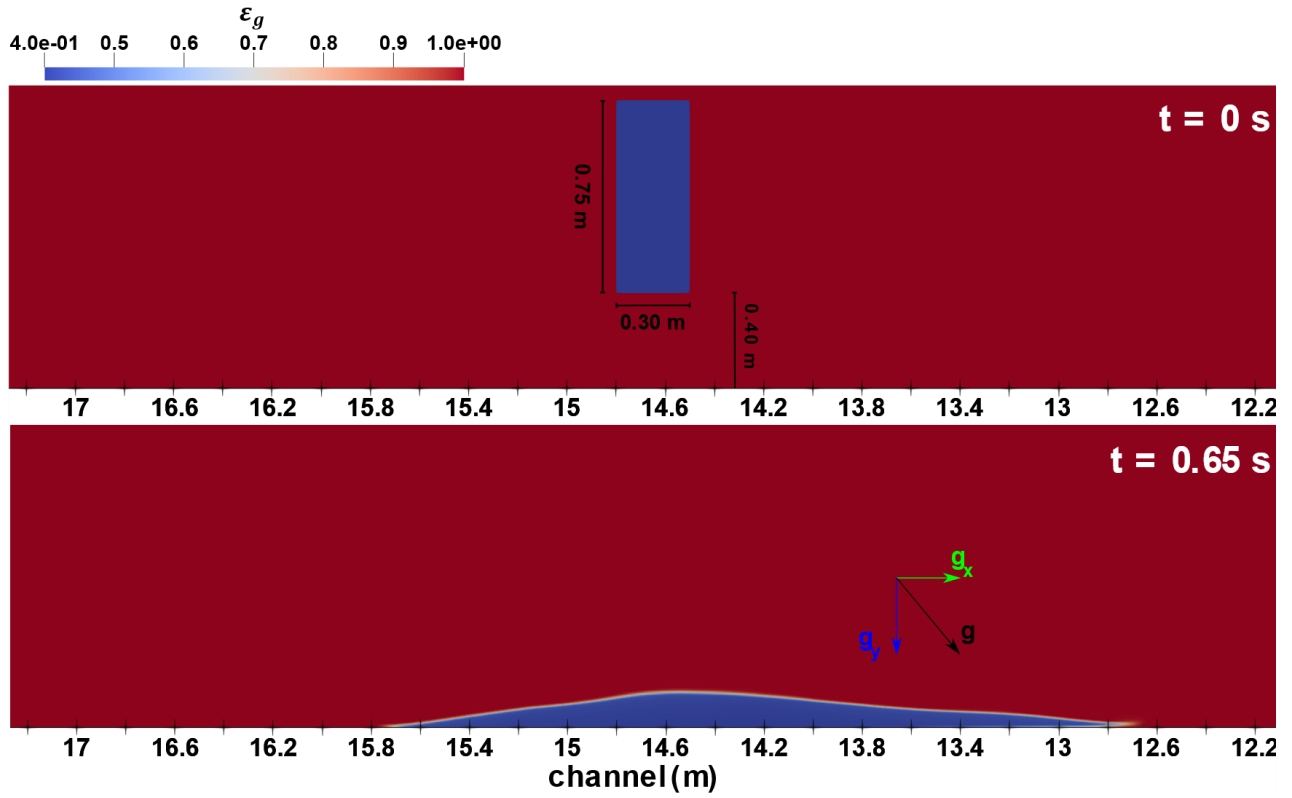
300 Figure 2. Grid layout for the computational domain. The granular material is shaded grey and the focus area is outlined
301 by the solid red line.

302

303 The simulations were carried out by dropping granular material from a height of 0.40 m on a 40°
304 sloped channel. This was reproduced through tilting the components of gravity acceleration at the

305 instant of granular material impacting on the channel surface (Fig. 3). The physical parameters for
 306 the solid and fluid phases are reported in Table 3.

307



308 Figure 3. Gas volume concentration (ϵ_g) at $t=0$ s and $t=0.65$ s. The green and blue arrows denote the gravitational
 309 accelerations in the x and y direction, while the black arrow indicates the resulting gravitational acceleration.

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Parameters (unit)	Sensitivity analysis	Experimental granular flow simulations
-------------------	----------------------	---

Solid density (kg/m ³)	2000	2300
Particles diameter (m)	0.1-0.5-1 x 10 ⁻³	1 x 10 ⁻³
Particle-particle restitution coefficient	0.9	0.9
Particle-wall restitution coefficient	0.7	0.7
Internal friction angle (°)	35°	33°
Basal friction angle (°)	11°	11°
Max packing fraction	0.65	0.65
Fluid density (kg/m ³)	1.2	1.2
Fluid dynamic viscosity (Pa s)	1.8 x 10 ⁻⁵	1.8 x 10 ⁻⁵

316 Table 3. Solid and fluid phase parameters used in the simulations.

317

318 **2.2.2 Sensitivity analysis of Johnson and Jackson boundary condition to specularity** 319 **coefficient and particles diameter**

320 Simulations of a mono-disperse granular flow sliding on a 40° sloped channel were carried out
321 varying the value of the specularity coefficient ϕ and the particle diameter d . For the simulations at
322 varying ϕ the solid phase size was set to 0.5 mm, while for the simulations at changing d the
323 specularity coefficient was set to 0.1. Profiles of solid volume concentration, solid velocity in x -
324 direction (u_s) and granular temperature at a simulation time (t) of 1.25 s are reported in Figure 4.

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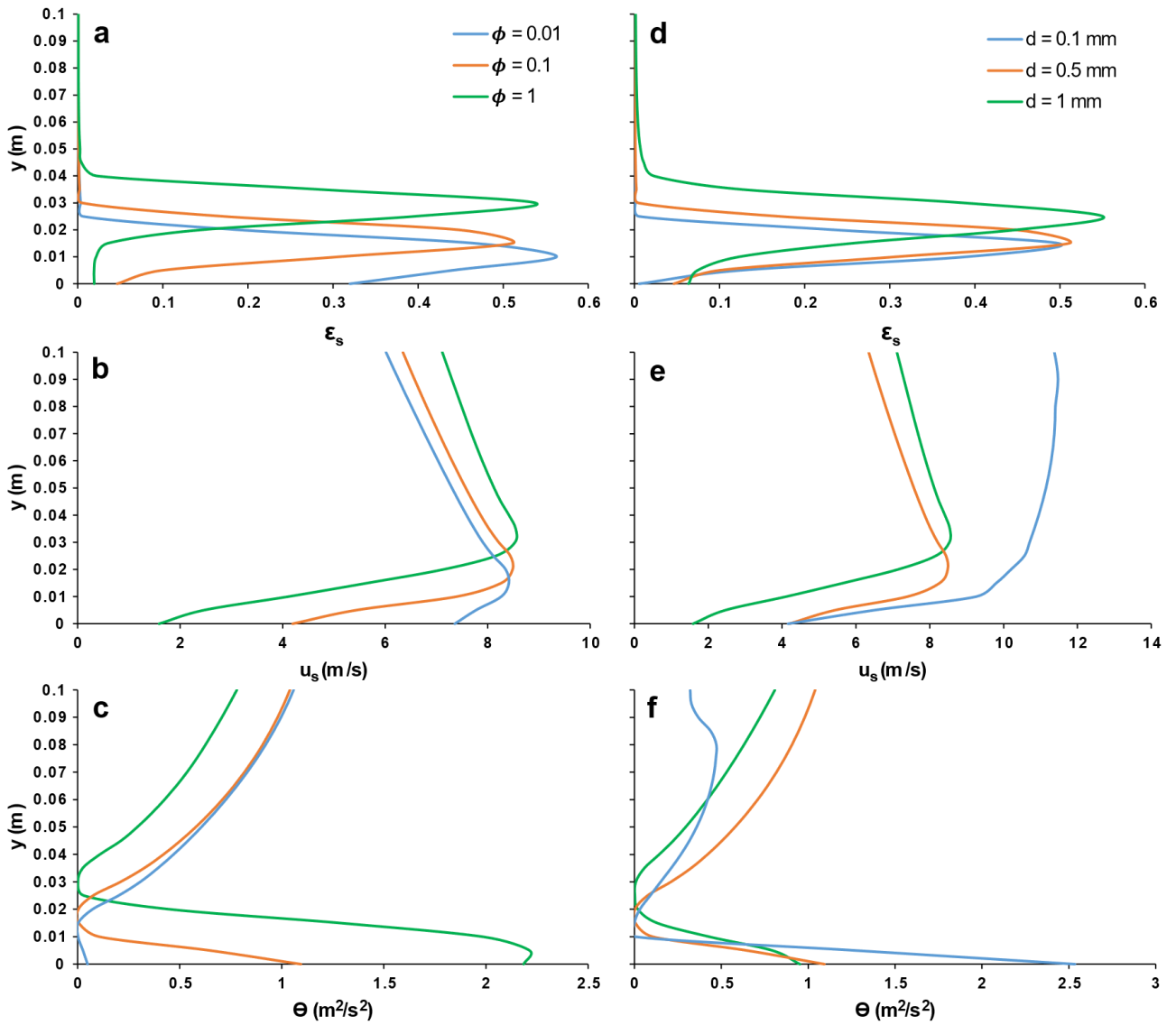
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341 Figure 4. Profiles of solid volume concentration (a, d), solid velocity in x -direction (b, e) and granular temperature (c, f)
 342 at 9 m from the right side of the domain (or 5.5 m downstream the initial position of the granular material) against the
 343 distance from the wall at changing ϕ and d .

344

345 The vertical profiles of ϵ_s (Figs. 4a and 4d) show the formation of a flow basal layer at the wall where
 346 particle concentration is less than the peak concentration in the flow. Hereafter we refer to this
 347 feature as “air-cushion”. We observed that the air-cushion is sensitive to the particles diameters
 348 and to the specularity coefficient. In fact, the greater ϕ and d , the thicker the air-cushion at the flow
 349 base. In particular, ϕ has a greater impact on the air-cushion, with values of ϵ_s at the wall that range
 350 from 0.03 ($\phi = 1$) to 0.32 ($\phi = 0.01$) and thickness ranging between 0.01 m – 0.03 m (Fig. 4a).

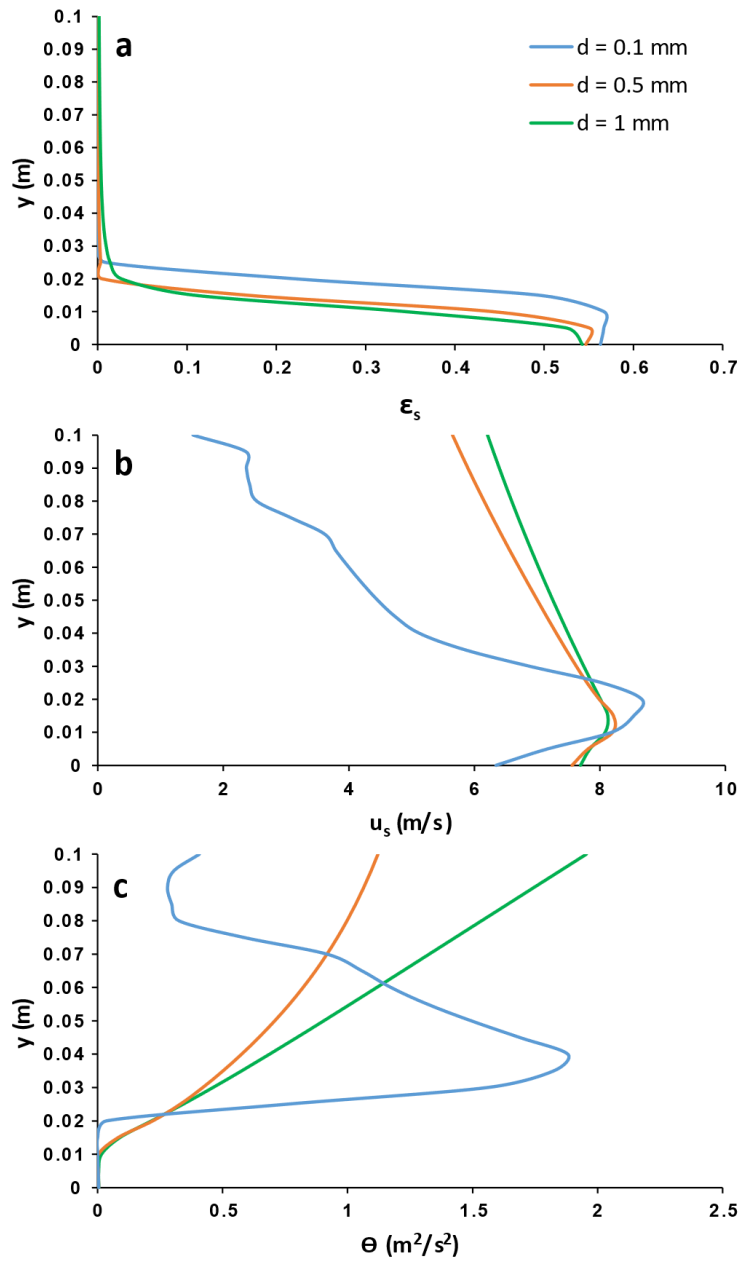
351 Velocity profiles of the solid phase in the x -direction (u_s) exhibit maximum velocities that range from
352 8.4 m s^{-1} to 8.5 m s^{-1} (Figs. 4b and 4e), with the exception of the maximum velocity of 11.45 m s^{-1}
353 recorded by the granular flow with particles diameter of 0.1 mm (Fig. 4e). For all the simulations, u_s
354 linearly decreases from the maximum to the top of the flow (Fig. 4b). The air-cushion affects u_s at
355 the wall increasing its gradient.

356 θ is significantly influenced by changing ϕ and d , with the highest values of $2.2 \text{ m}^2 \text{ s}^{-2}$ and $2.5 \text{ m}^2 \text{ s}^{-2}$
357 at the wall obtained for $\phi = 1$ and $d = 1 \text{ mm}$, respectively (Figs. 4c and 4f). All profiles show a
358 minimum of the granular temperature in the region where ε_s and u_s are at their peak (Figs. 4b and
359 4e), while θ increases towards the top of the flow where ε_s decreases. This can be attributed to the
360 particle fluctuations being inhibited or almost suppressed in the most concentrated regions of the
361 flow where ε_s is maximum, and enhanced in the top and basal part of the flow that is more diluted.

362

363 **2.2.3 Particle diameter sensitivity analysis of Jenkins boundary condition**

364 The specular coefficient is not used in the Jenkins boundary condition (see Table 2 and Eq. 20)
365 and, hence, we focused on the effects of varying the solid particles mean size. Profiles of gas and
366 solid volume concentration, solid velocity in the x -direction and granular temperature at t of 1.25 s
367 are reported in Figures 5.



368 Figure 5. Profiles of solid volume concentration (a), solid velocity in x -direction (b) and granular temperature (c) at 9 m
 369 from the right side of the domain (or 5.5 m downstream the initial position of the granular material) against the distance
 370 from the wall at changing d .

371

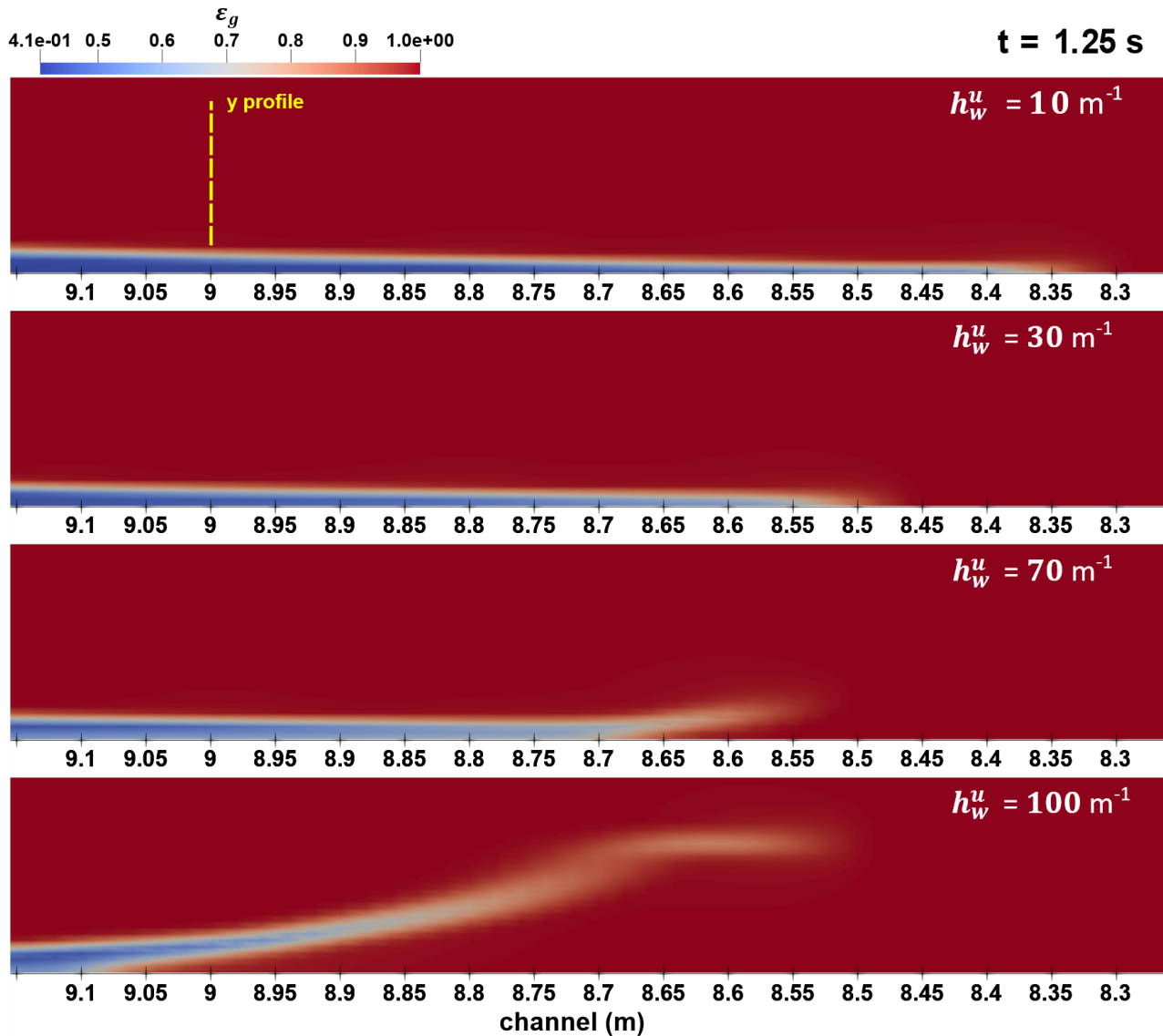
372 ϵ_s profiles and plots show flow thickness ranging between 0.020 m – 0.026 m with the thickest
 373 simulated flow obtained with the smallest particles ($d = 0.1$ mm) (Figs. 5a). In particular, the profiles
 374 do not exhibit the air-cushion at the flow base, which can then be attributed to the Johnson and
 375 Jackson boundary condition. The vertical u_s profiles exhibit maximum velocities ranging between

376 $8.18 \text{ m s}^{-1} - 8.67 \text{ m s}^{-1}$, with the highest velocity for $d = 0.1 \text{ mm}$ (Fig. 5b). All θ profiles are
377 characterised by a basal region with $\theta = 0 \text{ m}^2 \text{ s}^{-2}$, which coincides with the concentrated part of the
378 simulated flow (Fig. 5c). θ profile for $d = 0.1 \text{ mm}$ exhibits the most relevant variations with regards
379 to profiles for $d = 0.5 \text{ mm} - 1 \text{ mm}$, recording a peak at around 40% of the flow thickness in proximity
380 of the diluted part of the flow, which enhances the particle fluctuations.

381

382 **2.2.4 Sensitivity analysis to user-defined h_w^θ , h_w^u , c_w**

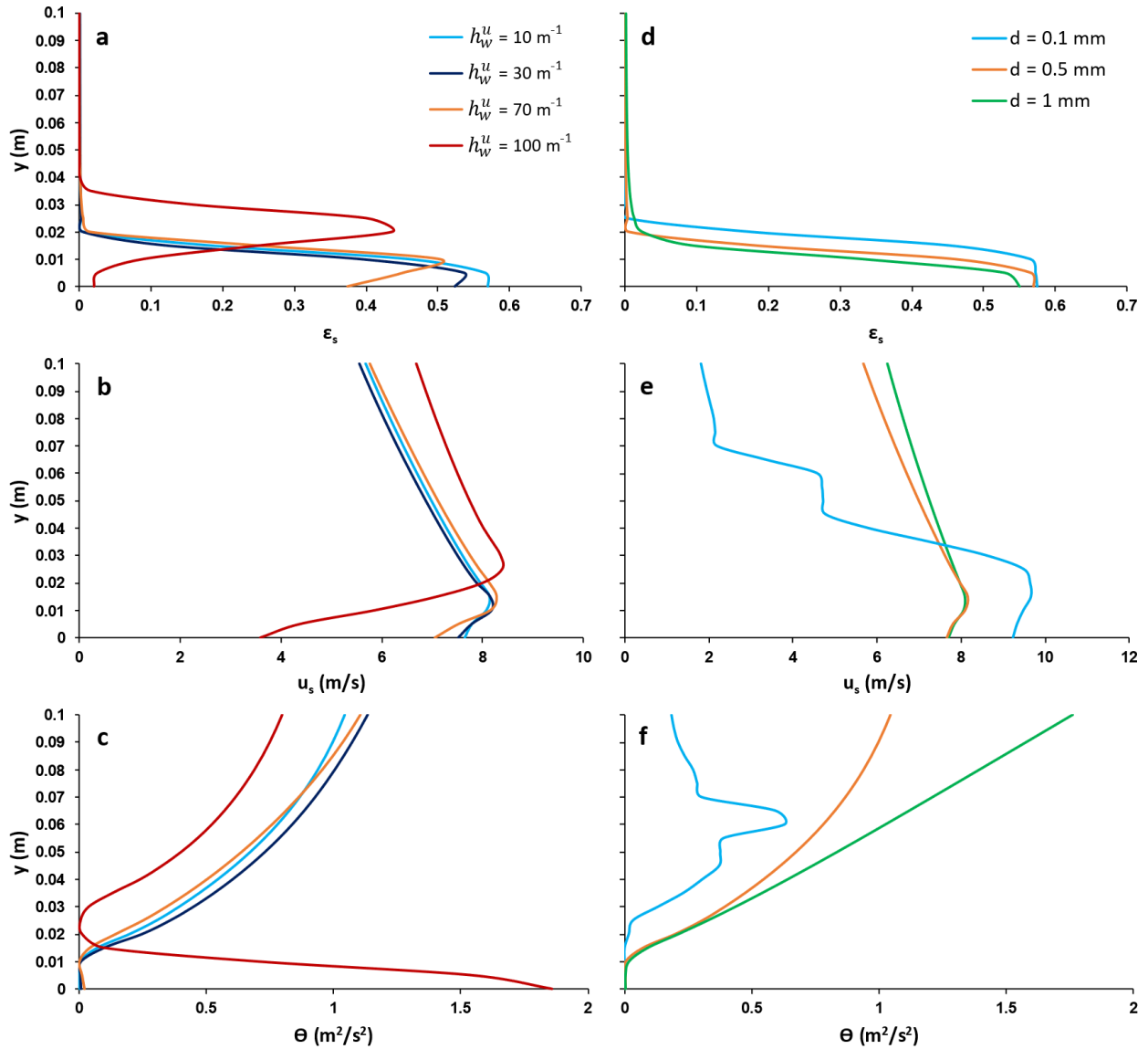
383 The Johnson and Jackson (1987) and Jenkins (1992) boundary conditions for solid phase (Table 2)
384 are used in MFIX to calculate the local flow-dependent values of h_w^θ , h_w^u and c_w coefficients, which
385 are required by the partial-slip wall condition equations (Eqs. 12 and 13). To better understand the
386 role played by these coefficients in controlling the simulated granular flows and the solid phase-wall
387 dynamics, we carried out simulations of mono-disperse granular flows with particle size of 0.5 mm
388 by manually setting h_w^θ , h_w^u and c_w to all the wall in the whole computational domain and for the
389 entire duration of the simulation. Plots of gas volume concentration and vertical profiles of solid
390 volume concentration, solid velocity in the x -direction and granular temperature at t of 1.25 s are
391 reported in Figures 6 and 7.



392 Figure 6. Plots of gas volume concentration (ϵ_g) at changing h_w^u . The yellow dotted line marks the profiles position
 393 shown below. t = simulation time.

394

395



396 Figure 7. Profiles of solid volume concentration (a, d), solid velocity in x -direction (b, e) and granular temperature (c, f)
 397 at 9 m from the right side of the domain (or 5.5 m downstream the initial position of the granular material) against the
 398 distance from the wall at changing h_w^u and d . On the basis of the analytical profiles of θ and U (Section 2.3), c_w and h_w^θ
 399 were set to 0.1 kg s^{-3} and $10 \text{ kg m}^{-2}\text{s}^{-1}$, respectively.

400

401 The vertical profiles of ϵ_s , u_s and θ at increasing h_w^u show the air-cushion is generated for $h_w^u \geq 70$
 402 m^{-1} , which leads to a flow thickness increase from 0.015 m to 0.030 m (Figs. 6 and 7a); the basal
 403 layer affected by the air-cushion results in lower u_s , which decreases from 7.65 m s^{-1} ($h_w^u = 10 \text{ m}^{-1}$)
 404 to 3.59 m s^{-1} ($h_w^u = 100 \text{ m}^{-1}$) (Fig. 7b); θ values are significantly influenced by varying h_w^u , with the
 405 highest value of $1.86 \text{ m}^2 \text{ s}^{-2}$ recorded at the boundary for the granular flow that generates the

406 thickest air-cushion ($h_w^u = 100 \text{ m}^{-1}$) (Fig. 7c). Instead, the simulations at increasing show flow
407 thicknesses that decrease from 0.15 m to 0.05 m (Fig 7d) and maximum values decreasing from 9.65
408 m s^{-1} to 8.15 m s^{-1} (Fig. 7e). Furthermore, the vertical velocity profile for $d = 0.1 \text{ mm}$ is affected by a
409 staircase-like trend with reducing values to the channel surface (Fig. 7e). Profiles for $d = 0.5, 1 \text{ mm}$
410 show a gradual decrease to the base of the flow with values close to $0 \text{ m}^2 \text{ s}^{-2}$, while profile for $d =$
411 0.1 mm is more complex and exhibits almost neutral values near the channel surface that gradually
412 increase in the flow centre reaching a granular temperatures peak at around 65 % of the flow height
413 and then decrease to the flow top (Fig. 7f). The velocity staircase-like profile and the granular
414 temperature peak are probably associated to the vortex activity, which interacts with the velocity
415 of the finest solid phase ($d = 0.1 \text{ mm}$).

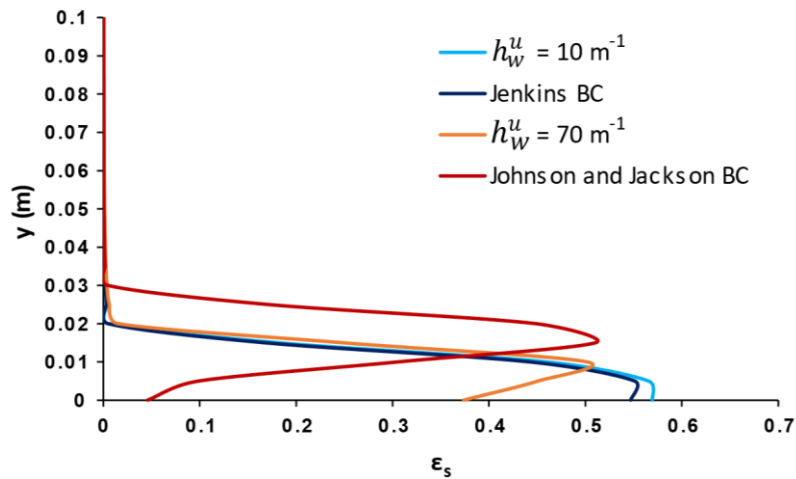
416 These simulations were repeated by changing h_w^θ and c_w and by dropping the mono-disperse
417 granular material both on the sloped (40°) and horizontal channel. Results can be found in the
418 Supplementary Material (Appendix).

419

420 **3. Comparison between the different boundary conditions**

421 The results of ε_s for the different boundary conditions (Section 2.2.2, 2.2.3 and 2.2.4) showed the
422 generation of an air-cushion layer at the base of the simulated granular flows either using the
423 Johnson and Jackson boundary condition with $\phi \geq 0.1$ (Fig. 4) or manually setting h_w^u to values
424 higher than 70 m^{-1} (Fig. 8). ε_s profiles recorded by granular flows with $d = 0.5 \text{ mm}$ for the different
425 boundary conditions are compared in the Figure 8.

426



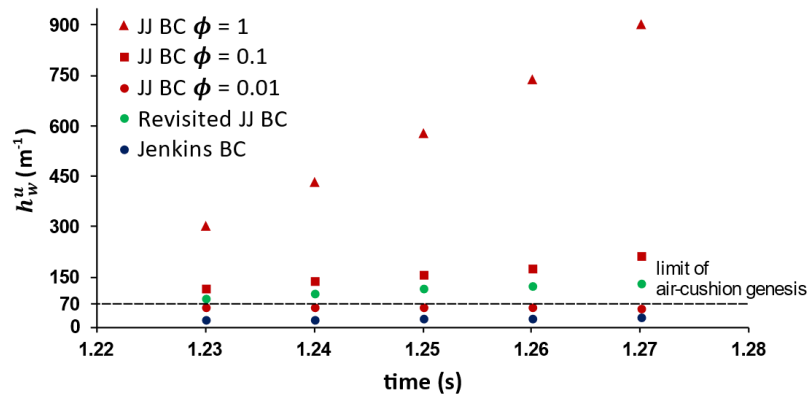
427 Figure 8. Profile of solid volume concentration for different boundary conditions at 9 m from the right side of the domain
428 (or 5.5 m downstream the initial position of the granular material) against the distance from the wall. BC = boundary
429 condition.

430

431 The comparison suggests the air-cushion dependence on high values of h_w^u . In order to verify this
432 observation, in the simulations with mono-disperse granular material ($d = 0.5$ mm) we tracked the
433 value of h_w^u at a fixed location (the boundary cell at 9 m of the sloped channel) over the duration at
434 changing boundary conditions (Fig. 9). In addition to Johnson and Jackson and Jenkins boundary
435 conditions, the Johnson and Jackson BC revisited by Li and Benyahia (2012) was also tested, which
436 allows a predictive local calculation of ϕ (Eq. 16). The effects of the predictive ϕ on h_w^u calculation
437 and consequently, on the air-cushion propagation at the flow base are well captured by the
438 comparing plots of the gas volume concentration between the different boundary conditions (Fig.
439 10).

440

441



442 Figure 9. h_w^u iteratively calculated as a function of time. The plotted values refer to a position of 9 m of the sloped
 443 channel. The dotted line indicates the limit of air-cushion formation located to $h_w^u = 70 \text{ m}^{-1}$. BC = boundary condition. JJ
 444 = Johnson and Jackson.

445

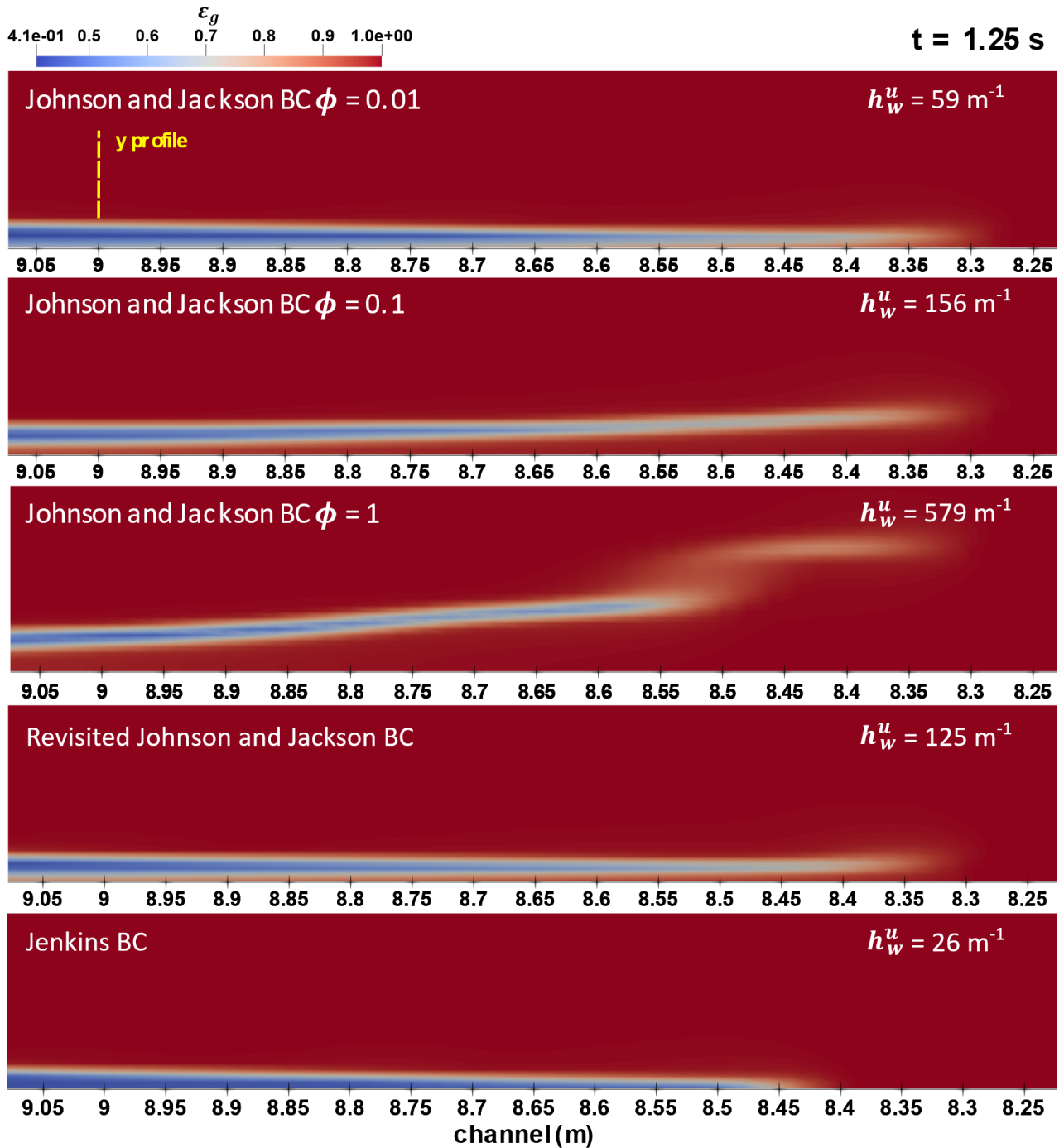
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451 Figure 10. Plot of gas volume concentration (ε_g) of revisited and standard (by varying ϕ) Johnson and Jackson and
 452 Jenkins boundary conditions (BC). The yellow dotted line marks the profiles position shown in Figure 5, 7, 8 and 9. $t =$
 453 simulation time.

454

455 The Johnson and Jackson BC with $\phi \geq 0.1$ and the revisited Johnson and Jackson BC computed
 456 values of h_w^u that increase over time during the granular flow front passage from the control
 457 position. The values of h_w^u are significantly higher than the previously identified limit of the air-

458 cushion formation at $h_w^u = 70 \text{ m}^{-1}$ (Fig. 9). On the other hand, the Johnsons and Jackson BC with $\phi =$
459 0.01 and the Jenkins BC generate values of h_w^u lower than 70 m^{-1} , which resulted in simulated mono-
460 disperse granular flows without the air-cushion at the flow base (Fig. 10). This proves the positive
461 correlation between the air-cushion and the wall velocity transfer coefficient h_w^u . Furthermore, the
462 iteratively calculated ϕ by Li and Benyahia equation (Eq. 16) slightly affect the simulations, resulting
463 in lower h_w^u and in a less developed air-cushion (Fig. 10).

464

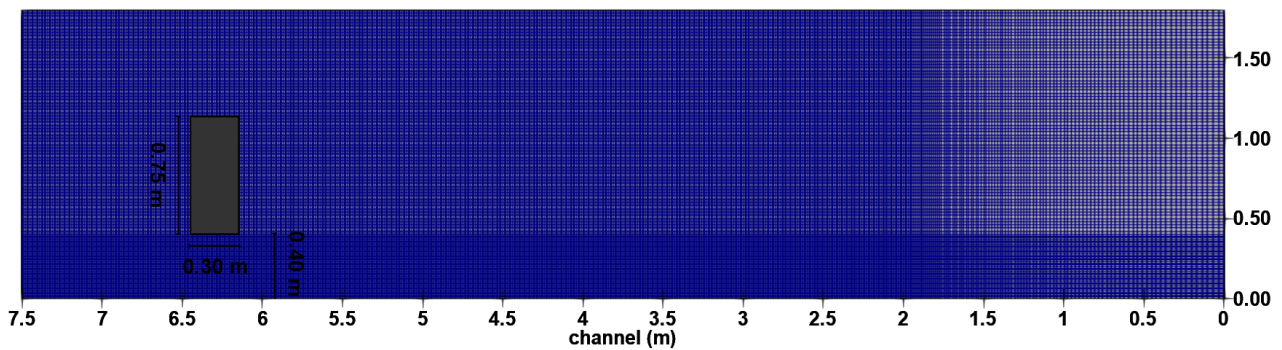
465 **4. Comparing MFIX simulations with one large-scale experiment**

466 The Johnson and Jackson (1987) and the Jenkins (1992) boundary conditions for the solid phase
467 were used to model one of the granular flows produced at the large-scale flume facility at the
468 University of San Luis Potosì (UASLP, Mexico) (Sulpizio et al., 2016). This represents a preliminary
469 test of the ability of a specific boundary condition to quantify the velocities of the granular flow at
470 the wall.

471 The instrumental apparatus used for the large-scale experiment comprises a hopper with a remotely
472 controlled gate located 0.40 m above the hopper inlet of a 5-m long and 0.30-m wide flume with a
473 40° slope. More details on the apparatus and granular flows experiments are available in the works
474 of Rodriguez-Sedano et al. (2016) and of Sulpizio et al. (2016). In the analysed experiment, 41.4 kg
475 of solid particles of volcanic origin with a density $\rho_s \cong 2300 \text{ kg/m}^3$ sieved within the diameter
476 interval of 1 mm - 2 mm were used. Internal friction angle of the solid mixture (δ_{int}) was
477 experimentally measured to be 33° . Granular flow front velocities were detected by seven laser
478 barriers deployed along the whole channel flume length starting from 1.65 m downstream and
479 evenly spaced of 0.45 m.

480 The numerical simulations were conducted by reproducing the particle release from the hopper via
481 the collapse of a volume composed of mono-disperse mixture with $d = 1$ mm from a height of 0.40
482 m on a 40° inclined channel, which in turn was reproduced by tilting the acceleration components
483 as seen in Section 2.2.1 (Fig. 3). The lower limit of the experimental diameter interval was selected
484 to obtain the finest grid (0.01 m x 0.01 m) maintaining the TFM assumption on the size of the control
485 volume that has to be at least ten times greater to the particles one. The rectangular computational
486 domain of 7.5 m x 1.8 m was discretised via variable-sized rectangular cells with decreasing size
487 down to square cells of 0.01 m side in the compacting and sliding zone (Fig. 11).

488

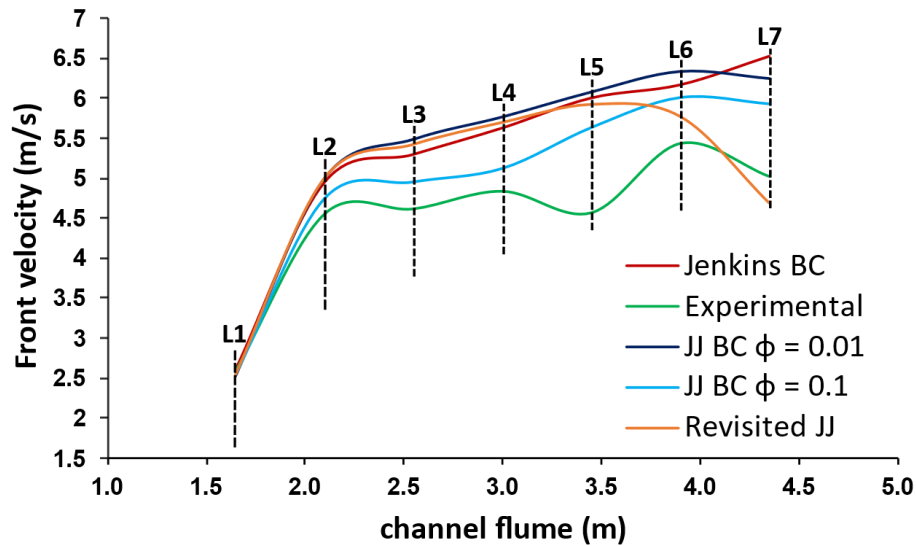


489 Figure 11. Grid layout for the computational domain. The granular material is shaded grey.

490

491 We performed the simulations by setting the partial-slip wall boundary condition for the solid phase
492 and varying the partial-slip wall boundary conditions (Jenkins (1992) and Johnson and Jackson
493 (1987)) and, when using the Johnsons and Jackson BC, by varying ϕ .

494 We compared experimental and simulated granular flow front velocities and those are reported in
495 Fig. 12.



496 Figure 12. Simulated and experimental granular flow front velocities plotted along the channel flume. The black dotted
 497 lines indicate the laser detectors (L) position along the channel. JJ = Johnson and Jackson. BC = boundary condition.

498

499 In the experiment, the kinetic energy of the granular material released from the hopper is redirected
 500 along the channel flume upon impact on the channel, resulting in flow elongation and fast velocity
 501 increase in the first two meters of runout. The rapid velocity increase is followed by an oscillatory
 502 trend of front propagation velocities around ca. 4.0 m s^{-1} with a final larger velocity peak of 5.4 m s^{-1} .
 503 The simulated profiles show different behaviours upon changing the boundary conditions (Fig.
 504 12). Jenkins BC and Johnson and Jackson BC with $\phi = 0.1$ (air-cushion-forming), well mimic the
 505 experimental oscillatory trend from L2 to L4, with a better match for Johnson and Jackson BC, which
 506 develops a mean square error of $0.36 \text{ m}^2 \text{ s}^{-2}$ against an error of $0.88 \text{ m}^2 \text{ s}^{-2}$ obtained for Jenkins BC.
 507 Further downstream, the simulated velocities obtained with Jenkins BC and Johnson and Jackson
 508 BC increase reaching maximum values of 6.5 m s^{-1} and 6.0 m s^{-1} , respectively (Fig. 12). On the other
 509 hand, the Johnson and Jackson BC with $\phi = 0.01$ (not air-cushion-forming) does not capture the
 510 experimental velocity oscillations showing a linear velocity increase, with a maximum velocity of
 511 6.25 m s^{-1} reached at L6 (Fig. 12) and with a mean square error of $0.93 \text{ m}^2 \text{ s}^{-2}$. Finally, the revisited
 512 Johnson and Jackson BC follows the trend of the previous one up to L5 and then decreases

513 approaching a velocity of 4.7 m s^{-1} (Fig. 12), resulting in a mean square error of $0.53 \text{ m}^2 \text{ s}^{-2}$. Therefore,
514 the boundary conditions air-cushion-forming seem to provide better results than BC not air-cushion
515 forming nonetheless this phenomenon was not detected in the experimental granular flow.

516

517 **5. Discussion and conclusions**

518 Sensitivity analysis of the model to the different partial-slip boundary conditions for the solid phase
519 available in the current version of MFIX were performed. The analysis showed that an air-cushion,
520 at the contact between the solid phase and the wall, is generated when using the Johnson and
521 Jackson (1987) boundary condition, while it never occurs when using Jenkins BC. The size (thickness)
522 of the air-cushion was found to depend on the solid phase size and on to the specular coefficient,
523 a fact that is associated to the increase of the tangential momentum transferred to the wall by the
524 solid phase collision as these parameters increase (second term of Eq. 14 and Eq. 15), which
525 minimises the amount of slip at the wall, promoting diffuse collisions (greater ϕ) and eventually
526 solid phase overpassing to the top flow. This in turn causes a decrease of the solid volume
527 concentration, allowing the air-cushion formation and its maintenance during the flow slip. The flow
528 sensitivity on the chosen value of ϕ was also demonstrated by other authors (Benyahia et al., 2005;
529 Li et al., 2010b, 2010a). Additional simulations, with user-defined values of wall velocity transfer
530 coefficient h_w^u for the solid phase, showed that this parameter plays a crucial role in the generation
531 of the air-cushion, which occurs when $h_w^u > 70 \text{ m}^{-1}$ are used; the thickness of the air-cushion
532 increases at increasing h_w^u . We further verified this by tracking h_w^u calculated by MFIX at specific
533 location and time when using Johnson and Jackson and Jenkins boundary conditions and by
534 comparing these values with the limit of the air-cushion formation ($h_w^u = 70 \text{ m}^{-1}$; Fig. 9). In fact,
535 simulations with Johnson and Jackson BC for ϕ of 1, 0.1 and 0.01 resulted in h_w^u of 579 m^{-1} , 156 m^{-1}
536 and 59 m^{-1} , respectively, while simulations with Jenkins BC developed h_w^u of 26 m^{-1} (Fig. 10), hence

537 confirming that the air-cushion is not formed or is roughly generated for boundary conditions
538 predicting low values of h_w^u . The significantly different behaviour of these two boundary conditions
539 is hence attributed to h_w^u calculation, which in the Johnson and Jackson BC strongly depends on the
540 specular coefficient ϕ (Table 2), which in turn represents an input data affected by great
541 uncertainties since it is difficult to measure or estimate and usually is specified adjusting this
542 parameter to fit some experimental data. The Johnson and Jackson boundary condition revisited by
543 Li and Benyahia (2012), which calculates local values of the specular coefficient (Eq. 16), was also
544 tested resulting in h_w^u lower than those ones obtained by the standard Johnson and Jackson BC, but
545 still greater than h_w^u of 70 m^{-1} (Figs. 9 and 10). Therefore, the revisited Johnson and Jackson BC does
546 not avoid the air-cushion generation, but nonetheless reduce it controlling h_w^u calculation by means
547 of a modelled ϕ . This again confirms the correlation between the air-cushion formation and the wall
548 velocity transfer coefficient h_w^u . The possibility to manually set h_w^u , h_w^θ and c_w proved to be a
549 powerful instrument to better understand the implication of h_w^u calculation on the air-cushion
550 formation. However, the use of constant coefficients limits the model predictivity, considering that
551 the manually set h_w^u , h_w^θ and c_w are time-independent and applied to all the partial-slip wall
552 boundary conditions of the whole computational domain.

553 All granular flows reproduced by Sulpizio et al. (2016) and by Rodriguez-Sedano et al. (2016),
554 including the here presented one, did not detect the air-cushion phenomenon, showing instead a
555 basal layer that slip in frictional contact with the basal surface. However, it should be noted that the
556 air-cushion could be difficult to experimentally capture, because the laboratory instruments (e.g.
557 laser detectors, high-speed cameras, load cells etc.) are not adequate or not able to detect a
558 phenomenon acting in a very limited basal region. Recently, Lube et al. (2019) showed by coupling
559 large-scale experiments on dilute pyroclastic density currents and numerical multiphase modelling
560 (MFIx-DEM) the generation of air lubrication at the base of the flow. Despite the dilute pyroclastic

561 density currents and granular flows being very different, the work by Lube and co-workers lead to
562 think to the air-cushion as a real phenomenon not detected during the granular flows experiments
563 of Sulpizio et al. (2016) and of Rodriguez-Sedano et al. (2016). Many experiments on granular flows
564 with different granulometries are still required to better evaluate the nature and the magnitude of
565 the air-cushion phenomenon.

566 We finally carried out a benchmark of the boundary conditions implemented in MFIX against the
567 experimental ones observed in a large-scale flume (Rodriguez-Sedano et al., 2016; Sulpizio et al.,
568 2016). It should be noted that this benchmark study represents a preliminary analysis, since several
569 experiments should be considered for a full investigation. The experimental flow front velocities
570 exhibited a flow acceleration in the first two metres of the sloped channel followed by an oscillatory
571 trend (Fig. 12). The initial flow acceleration is given by the redirection of the falling material kinetic
572 energy along the channel flume, causing the flow elongation. The latter increases the frictional
573 forces at the base promoting the overpassing of the coarser particles with great inertia into the
574 upper layer and into the granular flow front. The high inertia held by the coarser particles and their
575 upward and forward movement result in thicker and faster granular flow, which in turn promotes
576 the flow elongation and the frictional forces at the flow base. Thinning and thickening alternance
577 given by frictional and inertial forces competition explains the oscillatory velocity trend of the
578 experimental granular flow front (Fig. 12). This velocity fluctuation was detected by MFIX
579 simulations when using the Jenkins and the Johnson and Jackson models. In particular, simulations
580 with Johnson and Jackson setting $\phi = 0.1$ (air-cushion forming) resulted in the best match with the
581 experimental data (Fig. 12) (mean square error of $0.36 \text{ m}^2 \text{ s}^{-2}$), unlike the simulation with $\phi = 0.01$
582 (not air-cushion-forming), which resulted in the worst match (Fig. 12) (mean square error of 0.93 m^2
583 s^{-2}). The revisited Johnson and Jackson BC (mean square error of $0.93 \text{ m}^2 \text{ s}^{-2}$) developed a velocity
584 decrease in proximity of the last two laser detectors, which is likely due to the fact that this boundary

585 condition includes an expression for the specularity coefficient, which therefore responds to local
586 changes of the flow parameters, influencing the simulated flow velocity. Generally, all the
587 simulations resulted in velocities greater than observed ones. It should be note that: 1) since we are
588 running a 2D simulation of a 3D phenomenon, we are neglecting the friction effects due to the
589 sidewalls and adjacent particles; 2) the wall friction angle of 11° is probably not realistic for the case
590 under analysis that is characterized by a channel roughness. In conclusion, the boundary conditions
591 forming the air-cushion developed the best results nonetheless this phenomenon was not detected
592 in the real granular flow. This outcome is probably due to a more realistic transfer of tangential
593 momentum to the wall ruled by the specularity coefficient, which promotes the air-cushion
594 formation and strongly influences the flow velocity. This preliminary analysis would seem to suggest
595 the use of the Johnson and Jackson BC to replicate dense granular flows, even though additional
596 comparisons between simulated and experimental data are required to exhaustively define which
597 of the studied boundary conditions is the more appropriate to study this type of flows.

598

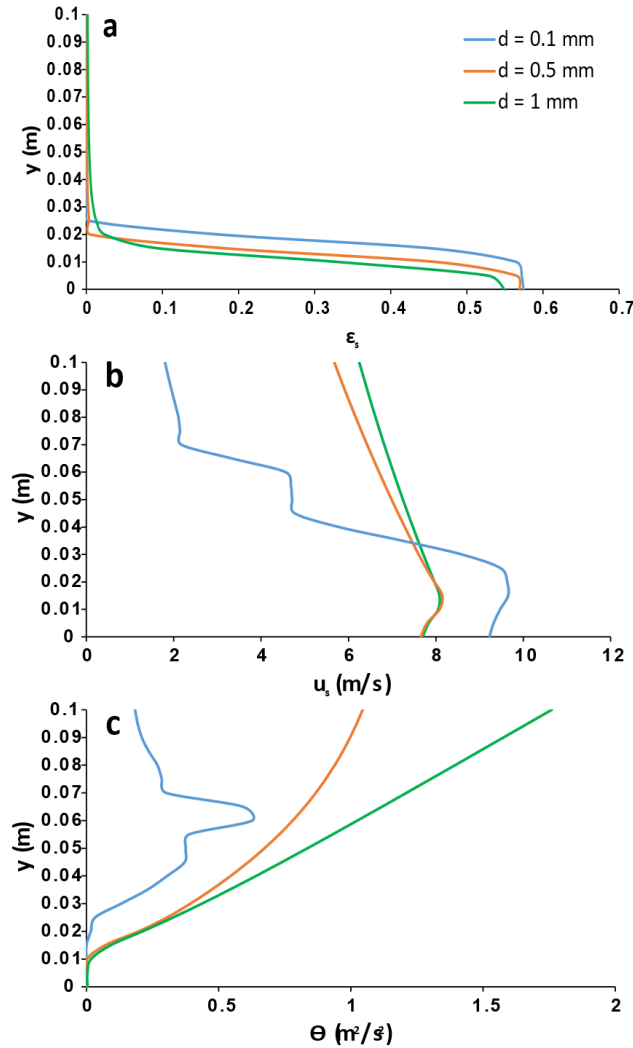
599 **Acknowledgment**

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601 was in part funded by the British Geological Survey University Funding Initiative (BUFI) PhD
602 studentship (S385). This work is published with permission of the Executive Director of British
603 Geological Survey (UKRI).

604

605 **Appendix**

606 In addition to the analysis of the influence of h_w^u , simulations with different d were conducted
 607 setting h_w^u to 10 m^{-1} and simulating the fall of a mono-disperse granular material of 0.5 mm on a 40°
 608 sloped channel. Results are reported in Figure 13.



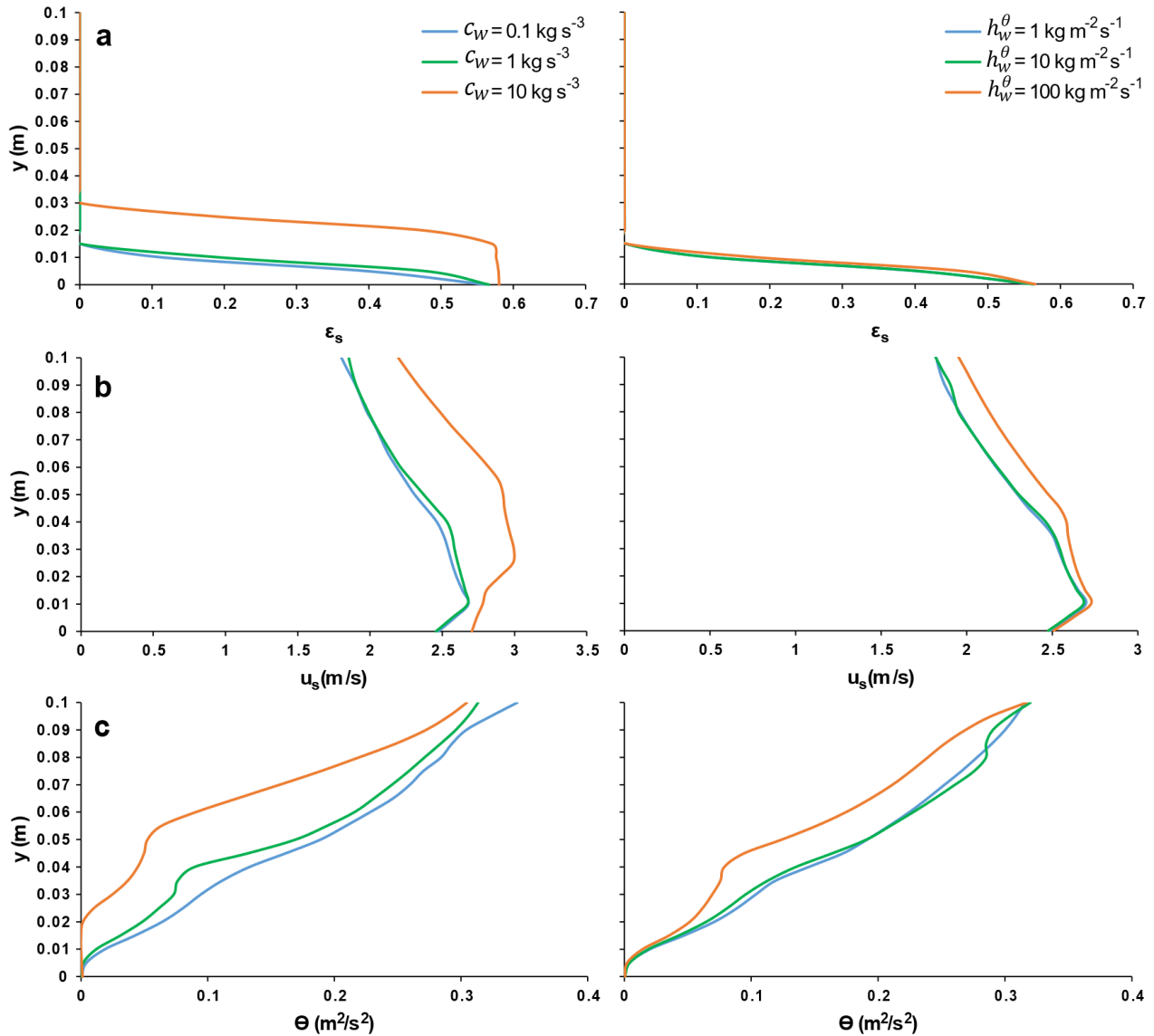
609 Figure 13. Profiles of solid volume concentration (a), solid velocity in x -direction (b) and granular temperature (c) at 9
 610 m from the right side of the domain (or 5.5 m downstream the initial position of the granular material) against the
 611 distance from the wall at changing d . On the basis of the analytical profiles of θ and v (Section 2.3), c_w was set to 0.1 kg
 612 s^{-3} and h_w^θ was set to $10 \text{ kg m}^{-2}\text{s}^{-1}$. $t = 1.25 \text{ s}$.

613

614 ϵ_s profiles for the different solid phase sizes have very similar shapes with thicker flows for the
 615 smaller particles (Fig. 13a). u_s profiles exhibit greater velocities for particles diameter of 0.1 mm,

616 which is affected by a staircase-like trend with decreasing values to the channel surface (Fig. 13b).
617 θ profiles for d equals to 0.5 mm and 1 mm show a gradual decrease to the basal layer with values
618 close to 0, while the granular flow with $d = 0.1$ mm records a granular temperatures peak (Fig. 13c).
619 The velocity staircase-like profile and the granular temperatures peak are probably associated to
620 the vortex activity, which negatively interacts with the solid phase velocity.

621 Numerical simulations at changing h_w^θ and c_w were run simulating mono-disperse granular material
622 of 0.5 mm falling both on sloped (40°) and horizontal channel. Profiles obtained for the sloped
623 channel at changing coefficients were almost identical between them and very similar to the
624 horizontal ones. For this reason, we only reported the simulations results for the horizontal channel
625 for h_w^θ equal to 1 kg m⁻²s⁻¹, 10 kg m⁻²s⁻¹, 100 kg m⁻²s⁻¹ and c_w equal to 0.1 kg s⁻³, 1 kg s⁻³ and 10 kg s⁻³
626 (Fig. 14).



627 Figure 14. Profiles of solid volume concentration (a), solid velocity in x -direction (b) and granular temperature (c) at 9
 628 m from the right side of the domain (or 5.5 m downstream the initial position of the granular material) against the
 629 distance from the wall at changing h_w^θ and c_w . On the basis of the analytical profiles of θ and v (Section 2.3), c_w was set
 630 to 0.1 kg s^{-3} for simulations changing h_w^θ , and h_w^θ was set to $10 \text{ kg m}^{-2}\text{s}^{-1}$ for simulations changing c_w . h_w^u was set to 10
 631 m^{-1} for the same reason. $t = 1.25 \text{ s}$.

632

633 The solid volume concentration profiles show almost imperceptible variations for simulations with
 634 different h_w^θ and slight difference for simulations changing c_w . In particular, $c_w = 10 \text{ kg s}^{-3}$ results in
 635 a simulated flow 0.014 m thicker than simulations with lower c_w (Fig. 14a). u_s profiles for all values
 636 of h_w^θ and c_w exhibit very similar trends, with the profile for $c_w = 0.1 \text{ kg s}^{-3}$ and $h_w^\theta = 100 \text{ kg m}^{-2}\text{s}^{-1}$

637 that show the greatest velocities (Fig. 14b). Finally, θ shows trends that linearly decrease to the
638 basal part until values close to $0 \text{ m}^2 \text{ s}^{-2}$ (Fig. 14c).

639

640 **References**

641 Anderson, T.B., Jackson, R., 1967. Fluid Mechanical Description of Fluidized Beds. *Ind. Eng.*
642 *Chem. Fundam.* 6, 527–539. <https://doi.org/10.1021/i160024a007>

643 Benyahia, S., Syamlal, M., O'Brien, T.J., 2005. Evaluation of boundary conditions used to
644 model dilute, turbulent gas/solids flows in a pipe. *Powder Technol.* 156, 62–72.
645 <https://doi.org/10.1016/j.powtec.2005.04.002>

646 Boyle, E.J., Massoudi, M., 1989. A kinetic theory derivation of the stress tensor for granular
647 material that includes normal stress effects, *Tech. Rep. DOE/METC-89/4088, DE89 00,977, 66*
648 *pp.*, U.S. Dep. of Energy, Washington, D. C.

649 Branney, J.M., Kokelaar, P., 2002. Pyroclastic density currents and the sedimentation of
650 ignimbrites, *Geological Society Memoir No. 27*. <https://doi.org/10.1086/427850>

651 Breard, E.C.P., Dufek, J., Roche, O., 2019. Continuum Modeling of Pressure-Balanced and
652 Fluidized Granular Flows in 2-D: Comparison With Glass Bead Experiments and Implications
653 for Concentrated Pyroclastic Density Currents. *J. Geophys. Res. Solid Earth* 1–27.
654 <https://doi.org/10.1029/2018JB016874>

655 Campbell, C.S., 1990. Rapid Granular Flows. *Annu. Rev. Fluid Mech.* 22, 57–90.
656 <https://doi.org/10.1146/annurev.fl.22.010190.000421>

657 Cundall, P.A., Strack, O.D.L., 1979. A discrete numerical model for granular assemblies.
658 *Geotechnique* 29, 47–65. <https://doi.org/10.1680/geot.1979.29.1.47>

659 Dartevelle, S., 2004. Numerical modeling of geophysical granular flows: 1. A comprehensive
660 approach to granular rheologies and geophysical multiphase flows. *Geochemistry, Geophys.*
661 *Geosystems* 5. <https://doi.org/10.1029/2003GC000636>

662 Garg, R., Galvin, J., Li, T., Pannala, S., 2012. Open-source MFIx-DEM software for gas-solids
663 flows: Part I-Verification studies. *Powder Technol.* 220, 122–137.
664 <https://doi.org/10.1016/j.powtec.2011.09.019>

665 Ge, W., Lu, L., Liu, S., Xu, J., Chen, F., Li, J., 2015. Multiscale Discrete Supercomputing – A
666 Game Changer for Process Simulation? *Chem. Eng. Technol.* 38, 575–584.

667 Gera, D., Syamlal, M., O’Brien, T.J., 2004. Hydrodynamics of particle segregation in fluidized
668 beds. *Int. J. Multiph. Flow* 30, 419–428.
669 <https://doi.org/10.1016/j.ijmultiphaseflow.2004.01.003>

670 Hanes, D.M., Inman, D.L., 1985. Observations of rapidly flowing granular-fluid materials. *J.*
671 *Fluid Mech.* 150, 357–380.

672 Harnett, C.E., Thomas, M.E., Purvance, M.D., Neuberg, J., 2018. Using a discrete element
673 approach to model lava dome emplacement and collapse. *J. Volcanol. Geotherm. Res.* 359,
674 68–77.

675 Hui, K., Haff, P.K., Ungar, J.E., Jackson, R., 1984. Boundary conditions for high-shear grain
676 flows. *J. Fluid Mech.* 145, 223–233. <https://doi.org/10.1017/S0022112084002883>

677 Iverson, R.M., 1997. The Physics of Debris Flows. *Rev. Geophys.* 35, 245–296.
678 <https://doi.org/10.1029/97RG00426>;

679 Iverson, R.M., Vallance, J.W., 2001. New views of granular mass flows. *Geology* 29, 115–118.
680 [https://doi.org/10.1130/0091-7613\(2001\)029<0115:NVOGMF>2.0.CO;2](https://doi.org/10.1130/0091-7613(2001)029<0115:NVOGMF>2.0.CO;2)

681 Jaeger, H.M., Nagel, S.R., Behringer, R.P., 1996. The physics of granular materials. *Phys. Today*
682 49, 32–38. <https://doi.org/10.1063/1.881494>

683 Jenike, A.W., 1987. A theory of flow of particulate solids in converging and diverging channels
684 based on a conical yield function. *Powder Technol.* 50, 229–236.
685 [https://doi.org/10.1016/0032-5910\(87\)80068-2](https://doi.org/10.1016/0032-5910(87)80068-2)

686 Jenkins, J.T., 1992. Boundary conditions for rapid granular flow: Flat, frictional walls. *J. Appl.*
687 *Mech. Trans. ASME.* <https://doi.org/10.1115/1.2899416>

688 Johnson, P.C., Jackson, R., 1987. Frictional-collisional constitutive relations for granular
689 materials, with application to plane shearing. *J. Fluid Mech.* 176, 67–93.
690 <https://doi.org/10.1017/S0022112087000570>

691 Jop, P., Forterre, Y., Pouliquen, O., 2005. Crucial role of sidewalls in granular surface flows:
692 Consequences for the rheology. *J. Fluid Mech.* 541, 167–192.
693 <https://doi.org/10.1017/S0022112005005987>

694 Li, T., Benyahia, S., 2012. Revisiting Johnson and Jackson boundary conditions for granular
695 flows. *AIChE J.* 58, 2058–2068. <https://doi.org/10.1002/aic.12728>

696 Li, T., Garg, R., Galvin, J., Pannala, S., 2012. Open-source MFIx-DEM software for gas-solids
697 flows: Part II - Validation studies. *Powder Technol.* 220, 138–150.
698 <https://doi.org/10.1016/j.powtec.2011.09.020>

699 Li, T., Grace, J., Bi, X., 2010a. Study of wall boundary condition in numerical simulations of
700 bubbling fluidized beds. *Powder Technol.* 203, 447–457.

701 Li, T., Zhang, Y., Grace, J.R., Bi, X., 2010b. Numerical investigation of gas mixing in gas-solid
702 fluidized beds. *AIChE J.* 56, 2280–2296.

703 Louge, M.Y., Turnbull, B., Carroll, C., 2012. Volume growth of a powder snow avalanche. *Ann.*
704 *Glaciol.* 53, 57–60. <https://doi.org/10.3189/2012AoG61A030>

705 Lube, G., Breard, E.C., Jones, J., Fullard, L., Dufek, J., Cronin, S.J., Wang, T., 2019. Generation
706 of air lubrication within pyroclastic density currents. *Nat. Geosci.* 12, 381–386.

707 Lun, C.K.K., Savage, S.B., Jeffrey, D.J., Chepuruiy, N., 1984. Kinetic theories for granular flow:
708 Inelastic particles in Couette flow and slightly inelastic particles in a general flowfield. *J. Fluid*
709 *Mech.* 140, 223–256. <https://doi.org/10.1017/S0022112084000586>

710 Neglia, F., Sulpizio, R., Dioguardi, F., Capra, L., Sarocchi, D., 2020. Shallow-water models for
711 volcanic granular flows: A review of strengths and weaknesses of TITAN2D and FLO2D
712 numerical codes. *J. Volcanol. Geotherm. Res.* 107146.

713 Pritchett, J.W., Blake, T.R., Garg, S.K., 1978. Numerical model of gas fluidized beds, in: *AIChE*
714 *Symp Ser.*

715 Rodriguez-Sedano, L.A., Sarocchi, D., Sulpizio, R., Borselli, L., Campos, G., Moreno Chavez, G.,
716 2016. Influence of particle density on flow behavior and deposit architecture of concentrated
717 pyroclastic density currents over a break in slope: Insights from laboratory experiments. *J.*
718 *Volcanol. Geotherm. Res.* <https://doi.org/10.1016/j.jvolgeores.2016.10.017>

719 Sarno, L., Carleo, L., Papa, M.N., Villani, P., 2018a. Experimental Investigation on the Effects of
720 the Fixed Boundaries in Channelized Dry Granular Flows. *Rock Mech. Rock Eng.* 51, 203–225.
721 <https://doi.org/10.1007/s00603-017-1311-2>

722 Sarno, L., Carravetta, A., Tai, Y.C., Martino, R., Papa, M.N., Kuo, C.Y., 2018b. Measuring the
723 velocity fields of granular flows – Employment of a multi-pass two-dimensional particle image
724 velocimetry (2D-PIV) approach. *Adv. Powder Technol.* 29, 3107–3123.

725 <https://doi.org/10.1016/j.apr.2018.08.014>

726 Savage, S.B., 1998. Analyses of slow high-concentration flows of granular materials. *J. Fluid*
727 *Mech.* 377, 1–26. <https://doi.org/10.1017/S0022112098002936>

728 Savage, S.B., Sayed, M., 1984. Stresses developed by dry cohesionless granular materials
729 sheared in an annular shear cell. *J. Fluid Mech.* 142, 391–430.

730 Schaeffer, D.G., 1987. Instability in the evolution equations describing incompressible
731 granular flow. *J. Differ. Equ.* [https://doi.org/10.1016/0022-0396\(87\)90038-6](https://doi.org/10.1016/0022-0396(87)90038-6)

732 Srivastava, A., Sundaresan, S., 2003. Analysis of a frictional-kinetic model for gas-particle flow.
733 *Powder Technol.* 129, 72–85. [https://doi.org/10.1016/S0032-5910\(02\)00132-8](https://doi.org/10.1016/S0032-5910(02)00132-8)

734 Sulpizio, R., Capra, L., Sarocchi, D., Saucedo, R., Gavilanes-Ruiz, J.C., Varley, N.R., 2010.
735 Predicting the block-and-ash flow inundation areas at Volcán de Colima (Colima, Mexico)
736 based on the present day (February 2010) status. *J. Volcanol. Geotherm. Res.* 193, 49–66.
737 <https://doi.org/10.1016/j.jvolgeores.2010.03.007>

738 Sulpizio, R., Castioni, D., Rodriguez-Sedano, L.A., Sarocchi, D., Lucchi, F., 2016. The influence
739 of slope-angle ratio on the dynamics of granular flows: insights from laboratory experiments.
740 *Bull. Volcanol.* 78, 77. <https://doi.org/10.1007/s00445-016-1069-5>

741 Syamlal, M., Rogers, W., O'Brien, T.J., 1993. MFIx documentation theory guide. DOE/METC-
742 94/1004, DE9400,097. USDOE Morgant. Energy Technol. Center, WV.
743 <https://doi.org/10.2172/10145548>

744 Valentine, G.A., 2020. Initiation of dilute and concentrated pyroclastic currents from
745 collapsing mixtures and origin of their proximal deposits. *Bull. Volcanol.* 82.
746 <https://doi.org/10.1007/s00445-020-1366-x>

747 Valentine, G.A., Sweeney, M.R., 2018. Compressible Flow Phenomena at Inception of Lateral
748 Density Currents Fed by Collapsing Gas-Particle Mixtures. *J. Geophys. Res. Solid Earth* 123,
749 1286–1302. <https://doi.org/10.1002/2017JB015129>

750 Zanchetta, G., Sulpizio, R., Pareschi, M.T., Leoni, F.M., Santacroce, R., 2004. Characteristics of
751 May 5-6, 1998 volcanoclastic debris flows in the Sarno area (Campania, southern Italy):
752 Relationships to structural damage and hazard zonation. *J. Volcanol. Geotherm. Res.* 133,
753 377–393. [https://doi.org/10.1016/S0377-0273\(03\)00409-8](https://doi.org/10.1016/S0377-0273(03)00409-8)

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