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1 Conditions for segregation of a crystal-rich layer within  
2 a convective magma ocean

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9 **Abstract**

10 The vigor of the thermal convection in a terrestrial magma ocean tends to  
11 prevent the sedimentation of the solid grains. Understanding of the overall dy-  
12 namical behavior of this solid phase segregation is required to anticipate the  
13 solidification mechanisms in the early Earth mantle. We develop numerical  
14 models using COMSOL Multiphysics to monitor the crystal fraction evolution  
15 of a convecting magmatic reservoir. Our models show that the ability of the  
16 crystal fraction to disperse within the domain strongly depends on the crystal  
17 size, the density difference and the magma viscosity. Two regimes can be identi-  
18 fied: sedimentation or suspension regime. We show that the critical value of the  
19 convection/buoyancy stress ratio separating these two regimes is smaller than  
20 proposed by *Solomatov et al.* (1993). Hence, during the early crystallization of  
21 a magma ocean, suspension should be the dominant process.

22

23 We then investigate the implications of our models on the mechanism of  
24 magma ocean solidification after a major melting event on an Earth-like planet.  
25 We define the relevant set of parameters; including the P-V-T equations of  
26 state of coexisting melt and bridgmanite in the mushy MO. We observe that  
27 bridgmanite grains are unlikely to segregate in a mantle of pyrolite composition.

28 However, bridgmanite segregation is more likely to occur at the bottom of a  
29 MO enriched in SiO<sub>2</sub>, compared to pyrolite. When a solidifying layer contains  
30 60% of bridgmanite and 40% of melt, we observe a significant SiO<sub>2</sub> enrichment  
31 with increasing mantle depth in a primitive mantle compatible with seismic and  
32 geochemical observations.

33 *Keywords:* Early Earth, thermal evolution, magma ocean, numerical  
34 modeling, two-phase flow, convection

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## 35 1. Introduction

36 During its early history, the Earth has experienced several episodes where  
37 a significant volume fraction of its mantle was molten. These melting events  
38 were enhanced by radiogenic heating (*Yoshino et al.*, 2003), viscous dissipation  
39 during core formation (*Monteux et al.*, 2009; *Samuel et al.*, 2010) and kinetic  
40 energy converted into heat during large impacts (*Tonks and Melosh*, 1993). The  
41 giant impact leading to the Earth/Moon system could even be responsible for  
42 the complete melting of the Earth mantle (*Nakajima and Stevenson*, 2015) and  
43 the subsequent formation of a nearly 3000 km thick magma ocean.

44  
45 Extremely vigorous convection is likely to occur within such a molten reser-  
46 voir (*Solomatov*, 2015; *Monteux et al.*, 2016). The variations in temperature  
47 are strong enough to generate a significant natural convection flow. Moreover  
48 the potentially large thickness of a molten-silicate reservoir coupled with low  
49 viscosity material (*Karki and Stixrude*, 2010; *Xie et al.*, 2021) leads to Rayleigh  
50 numbers (comparing advective and diffusive timescales) ranging between 10<sup>20</sup>  
51 to 10<sup>30</sup> (*Patočka et al.*, 2020) while the current Rayleigh number of the Earth  
52 mantle is ranging between 10<sup>6</sup> and 10<sup>8</sup> (*Ricard*, 2007). The cooling and solidifi-  
53 cation dynamics are difficult to monitor within such an environment. However,  
54 recent numerical models agree on the characteristic cooling timescales that is

55 constrained to several thousands of years (*Lebrun et al.*, 2013; *Monteux et al.*,  
56 2016).

57

58 The study of particle sedimentation in vigorously convecting fluids and, by  
59 extension, the study of crystal behaviour in convecting magmas is a debated  
60 subject in fluid dynamics (*Lavorel and Le Bars*, 2009) and in Earth Sciences  
61 (*Jaupart and Tait*, 1995). A large number of study has been dedicated to the  
62 crystal settling in magma chambers using laboratory experiments (*Martin and*  
63 *Nokes*, 1988; *Sturtz et al.*, 2021), numerical modelling (*Höink et al.*, 2005; *Ver-*  
64 *hoeven and Schmalzl*, 2009) or both (*Weinstein et al.*, 1988). All these studies  
65 point out the importance of particle deposition and the subsequent differenti-  
66 ation mechanisms that may occur within large plutonic reservoirs. In magma  
67 oceans, the physical context is quite different with potentially more vigorous  
68 convection related to much thicker reservoirs. Recent numerical models from  
69 *Patočka et al.* (2020) constrained the settling of inertial particles in turbulent  
70 Rayleigh-Bénard convection without considering the re-entrainment process.  
71 In particular, *Patočka et al.* (2020) identified different settling regimes and de-  
72 rived characteristic residence timescales. For their range of particule sizes and  
73 densities, their results show that the settling should be rapid, much shorter  
74 than the typical time scales for the solidification of a whole-mantle terrestrial  
75 magma ocean supporting the idea of a fully fractional crystallisation. However,  
76 using analog models, *Solomatov et al.* (1993) introduced the conditions for par-  
77 ticle re-entrainment after sedimentation at the bottom of a convecting reservoir.  
78 For sufficiently high Rayleigh numbers, their models illustrate that the parti-  
79 cles might be re-entrained by the viscous stress produced by thermal plumes  
80 emphasising that entrainment of crystals cumulated within dunes was likely at  
81 the bottom magma oceans. Such a re-entrainment process could hence favour

82 equilibrium crystallisation. More recent laboratory experiments from (*Lavorel*  
83 *and Le Bars*, 2009) confirmed the founding from *Solomatov et al.* (1993) and  
84 characterized the influence of the density ratio between fluid and crystals and  
85 the temperature difference driving thermal convection.

86

87 Several parameters likely influence the settling dynamics: (1) the density  
88 difference between the settling crystal and the surrounding convecting magma  
89 ocean, (2) the crystal size that is a strong function of the magma ocean cooling  
90 rate and (3) the viscosity of the magma ocean which value may cover several  
91 orders of magnitude depending on the pressure/temperature conditions within  
92 the early magma ocean. Recently, *Caracas et al.* (2019) proposed that the ac-  
93 cumulation of crystals might occur near the depth of neutral buoyancy between  
94 crystals and the coexisting melt. They localised this neutral buoyancy depth for  
95 different partition coefficients iron partitioning and solid fractions. They show  
96 that the crystals may cumulate and form a mushy layer inside the magma ocean  
97 separating a shallow MO and a basal MO. Here, we monitor the stability of a  
98 thin mushy layer cumulated within a magma ocean. We consider grain sizes,  
99 the density differences between the crystals and the surrounding magma ocean  
100 and viscosities of the magma ocean derived from petrological experiments. In  
101 particular, we aim at determining if the crystal layer will be sedimented at the  
102 bottom of the reservoir or will be efficiently mixed in the convective reservoir.

103

104 The hypothesis of a fully molten mantle is difficult to reconcile with geochem-  
105 ical data and the need for hidden reservoirs (*Boyet and Carlson*, 2005). However,  
106 the cooling and solidification processes occurring within large partially molten  
107 silicate reservoirs may lead to important chemical differentiation events and to  
108 chemical segregation. The depth at which solidification initiates is governed

109 by the crossing between the early geotherm and the melting curves. Crystal  
110 settling could then occur towards neutral buoyancy depths where crystals are  
111 paradoxically more easily entrained by the flow (*Caracas et al.*, 2019). Both  
112 chemical composition and temperature contribute to the buoyancy of a crystal  
113 layer within a convecting reservoir. The chemical differentiation occurring after  
114 a large melting event is strongly related to the ability of the crystal fraction to  
115 sink or float within the convective reservoir. This ability is itself governed by  
116 the propension of the crystallised minerals to integrate in their structure heavy  
117 elements such as Fe (*Nomura et al.*, 2011; *Andrault et al.*, 2012). Depending  
118 on the crystal buoyancy relative to the molten magma, different scenarios may  
119 emerge with a bottom/up solidification (*Monteux et al.*, 2016) or a mid-mantle  
120 solidification making a basal magma ocean possible (*Labrosse et al.*, 2007). In  
121 our study, we will discuss the implications of our model on the mechanism of  
122 magma ocean solidification after a major Moon forming impact on an Earth-like  
123 planet.

124

125 In the following study, we have developed a numerical model to monitor  
126 the cooling, segregation and chemical evolution of the early Earth mantle. Our  
127 study is organised as follows. In section 2, we present our physical and numerical  
128 models. In section 3, we present the main numerical results from our systematic  
129 parametric study emphasising the influence of the melt viscosity, the crystal size  
130 and the density difference between crystals and melt. Section 4 details a criterion  
131 for the stability of a crystallising layer. Finally section 5 describes the evolution  
132 of mushy material in the context of a progressive magma ocean crystallisation.  
133 We discuss our results and conclude in section 6.

## 134 **2. Physical and numerical models**

### 135 *2.1. Governing equations*

136 We monitor the stability of a horizontal mushy layer composed of solid crys-  
137 tals within an initially convecting fully molten magma reservoir. For this pur-  
138 pose, we consider the Euler-Euler model which is an accurate dispersed mul-  
139 tiphase flow model describing both the crystal and the liquid phases. We dis-  
140 tinguish two non-miscible phases in our models: the continuous phase (with  
141  $c$  subscript) that represents the liquid magma ocean and the dispersed phase  
142 (with  $d$  subscript) that represents the crystal phase. Both phases behave as  
143 Newtonian and incompressible fluids. The local volume fraction of the fluid  
144 continuous phase  $\phi_c$  and the dispersed solid phase  $\phi_d$  are the local average vol-  
145 ume of melt and crystals respectively ( $\phi_c = 1 - \phi_d$ ).

146

147 The dynamical and thermal evolution of the mushy layer and ambient liquid  
148 are governed by the Navier-Stokes and heat transfer equations. We initially  
149 solve the equations for the continuous phase heat in 2D rectangular geometry  
150 using the Rayleigh-Bénard system. Once it reaches a steady state, we then solve  
151 the dynamical evolution of the mushy layer within the convective reservoir. The  
152 Euler-Euler flow model defines one set of Navier-Stokes equations for each phase:

- 153 • The mass conservation:

$$\nabla \cdot (\phi_c \mathbf{u}_c + \phi_d \mathbf{u}_d) = 0, \quad (1)$$

154

$$\nabla \cdot (\phi_d \mathbf{u}_d) = 0 \quad (2)$$

155 with  $\mathbf{u}_d$  and  $\mathbf{u}_c$  represent of the dispersed phase and the continuous phases  
156 fluid velocity vector respectively ( $\text{m}\cdot\text{s}^{-1}$ ).

157

- The momentum conservation:

$$\rho_c \left( \frac{\partial \mathbf{u}_c}{\partial t} + \mathbf{u}_c \cdot \nabla \mathbf{u}_c \right) = \nabla \cdot [-P \mathbf{I} + \eta_c (\nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T)] + \rho_c \mathbf{g} + \frac{\mathbf{F}_{m,c}}{\phi_c} \quad (3)$$

$$\rho_d \left( \frac{\partial \mathbf{u}_d}{\partial t} + \mathbf{u}_d \cdot \nabla \mathbf{u}_d \right) = \nabla \cdot [-P \mathbf{I} + \eta_d (\nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T)] + \rho_d \mathbf{g} + \frac{\mathbf{F}_{m,d}}{\phi_d} \quad (4)$$

158

with  $\rho_c$  the melt density ( $\text{kg.m}^{-3}$ ),  $\rho_d$  the solid phase density,  $\eta_c$  the melt

159

viscosity (Pa.s),  $\eta_d$  the solid phase viscosity (Pa.s),  $t$  the time (s),  $P$  the

160

fluid pressure (Pa),  $\mathbf{g}$  the gravitational acceleration ( $\text{m.s}^{-2}$ ) and  $\mathbf{I}$  the

161

identity matrix.  $F_{m,c}$  and  $F_{m,d}$  are the drag forces ( $N/m^3$ )

162

163

- The heat conservation:

$$\rho_c C_p \left[ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right] + \nabla \cdot [-k \nabla T] = 0 \quad (5)$$

164

with  $C_p$  the heat capacity at constant pressure ( $\text{J.kg}^{-1}.\text{K}^{-1}$ ),  $T$  the fluid

165

temperature (K),  $\mathbf{u}$  the fluid velocity vector ( $\text{m.s}^{-1}$ ),  $k$  the thermal con-

166

ductivity ( $\text{W.m}^{-1}.\text{K}^{-1}$ ). No heat source is considered in our models (e.g.

167

radiogenic, tidal or latent heat). For simplicity, we consider that both

168

the continuous and dispersed phases have the same heat capacities and

169

thermal conductivities.

170

For each fluid parcel, the viscosity ranges between the viscosity of the fully

171

molten phase  $\eta_c$  that is imposed for each simulation (see Tab. 1 for values) and

172

the viscosity of the solid dispersed phase. In between the mixture viscosity  $\eta$



173 depends on the dispersed solid phase volume fraction  $\phi_d$ . For the mixture, we  
 174 consider a Krieger-type dynamic viscosity:

$$\eta = \eta_c \left(1 - \text{MIN}\left(\frac{\phi_d}{\phi_{d,max}}, 0.999\right)\right)^{-2.5\phi_{d,max}} \quad (6)$$

175 where  $\phi_{d,max}$  is the maximum packing concentration.  $\phi_{d,max}$  depends on the  
 176 geometry of the crystals within the system and on the shear rate. For mono-  
 177 dispersed systems with spheres and low shear rates,  $\phi_{d,max}$  ranges between 0.5  
 178 and 0.7 (*Dörr et al.*, 2013). We consider in our models that  $\phi_{d,max}$  is fixed to  
 179 0.6 meaning that  $\phi_c$  can locally range between 40 and 100% while  $\phi_d$  can locally  
 180 range between 0 and 60%.

181

182 To compute the drag force  $\mathbf{F}_m$ , we consider the Schiller-Naumann drag model  
 183 (*Schiller and Naumann*, 1935; *Ibrahim and Meguid*, 2020) that is relevant for  
 184 dispersed rigid spheres and for the range of Reynolds number (comparing inertial  
 185 and viscous forces) values in our study (lower than  $10^4$ ).  $\mathbf{F}_m$  is defined as:

$$\mathbf{F}_{m,c} = -\mathbf{F}_{m,d} = \beta(\mathbf{u}_d - \mathbf{u}_c) \quad (7)$$

186 with  $\beta$  the momentum transfer coefficient (in  $\text{kg m}^{-3} \text{s}^{-1}$ ) between fluid and  
 187 solid particles (*Ibrahim and Meguid*, 2020)

$$\beta = \frac{3}{4} \frac{\rho_c \phi_d C_D (\mathbf{u}_d - \mathbf{u}_c)}{D_d} \quad (8)$$

188  $D_d$  is the particle diameter (m) and  $C_D$  is the drag coefficient for a single  
 189 particle. For  $Re < 1000$ :

$$C_D = \frac{24(1 + 0.15Re^{0.687})}{Re} \quad (9)$$

190 For  $Re > 1000$ ,  $C_D = 0.44$  (*Wen and Yu, 1966*).

191 The density of the magma ocean is supposed to vary linearly with tempera-  
192 ture in the buoyancy term of the momentum equation following the Boussinesq  
193 approximation. The density calculation accounts for the contrast related to the  
194 thermal effects and the phase influence. It is calculated as:

$$\rho_c = \rho_{c,0}(1 - \alpha(T - T_0)) \quad (10)$$

195 where  $T_0$  is the reference temperature (in K) and  $\alpha$  is the thermal expansion  
196 coefficient ( $K^{-1}$ ). The initial reference temperature of the reservoir is highly  
197 influenced by the full thermal history of the early earth as well as its depth  
198 within the Earth mantle. Here we fix  $T_0 = 4000$  K. The particle density is  
199 calculated as:

$$\rho_d = \rho_c + \Delta\rho \quad (11)$$

200 with  $\Delta\rho$  the intrinsic density difference between the molten silicates and the  
201 solid crystals.

## 202 *2.2. Non dimensional parameters*

203 Before considering the stability of a crystal layer within the molten reser-  
204 voir, we first solve only the equations relative to thermal convection within the  
205 reservoir. In our geophysical investigation, the main parameter is the magma  
206 ocean viscosity which ranges widely in value. Here we use viscosities for the  
207 continuous phase ( $\eta_{c,0}$ ) ranging between 0.1 and 10 Pa.s (*Karki and Stixrude,*  
208 *2010; Xie et al., 2021*). The convection flow induced within the magma ocean  
209 is characterised by the thermal Rayleigh number ( $Ra$ ) describing the vigor of  
210 convection as a consequence of basal heating:

$$Ra = \frac{\alpha \rho_c g \Delta T H^3}{\eta_c \kappa} \quad (12)$$

211 with  $\kappa$  the heat diffusivity of the convective fluid (see Tab. 1 for value).  
 212 This leads to  $Ra$  values ranging between  $1.8 \times 10^6$  and  $1.8 \times 10^8$ . From our  
 213 purely thermally convective models, we monitor the surface heat flux  $F$  which  
 214 is proportional to the average value of the temperature gradient at the surface  
 215 of the reservoir. We obtain  $F$  as a function of time for the range of  $Ra$  values  
 216 considered in our study. We stop our thermally convective simulations once  
 217 the surface heat flux has converged to a constant value and use this value to  
 218 calculate the corresponding Nusselt number  $Nu$ :

$$Nu = \frac{HF}{k\Delta T} \quad (13)$$

219 Fig. 1 shows the  $Nu$ - $Ra$  relation obtained from our models and compares our  
 220 numerical results with the scalings obtained from *Turcotte and Schubert* (1982)  
 221 and *Wolstencroft et al.* (2009). Our results show an agreement with these 2  
 222 scalings and we obtain  $Nu = 0.14Ra^{0.34}$ . For each  $Ra$  value used in our models  
 223 we obtain a temperature field that will be used as the initial temperature field  
 224 for the Euler-Euler model in order to study the stability of a thin mushy layer  
 225 with different characteristics ( $D_d$  and  $\Delta\rho$ ).

### 226 2.3. Numerical model

227 We used the commercial software COMSOL Multiphysics (version 5.4) pre-  
 228 viously validated for two phase flow applications (*Qaddah et al.* (2019, 2020)).  
 229 We consider a 2D domain with a thickness  $H$  and a width of  $4H$  (See Fig. 2). As  
 230 a first attempt to characterise the stability of a thin newly formed mushy layer  
 231 within a convective magma ocean, we arbitrarily consider that the thickness of  
 232 this mushy layer is  $h = H/10$ . The mush thickness is set constant in all our

233 models. Within the mushy layer, the crystals are considered as spheres with a  
 234 fixed diameter  $D_d$ . In our models, this diameter ranges between  $10^{-4}$  and  $10^{-2}$   
 235 m. The initial volume fraction of crystal  $\phi_{d,0}$  is also set to a constant value  
 236 ( $\phi_{d,0} = 0.1$ ). For the dynamics, we use free-slip conditions at all the system  
 237 boundaries for both the dispersed and continuous phases. For the temperature,  
 238 we consider no flux conditions at lateral boundaries. We fix the temperature  
 239 to 4100 K at the bottom boundary and to 4000 K at the top boundary (i.e.  
 240  $\Delta T = 100K$ ).

241

242 The COMSOL Multiphysics software employs the finite-element method on  
 243 a grid mesh to solve the set of equations (Eqs. 1 to 5). In order to study  
 244 the sensitivity analysis of mesh size on the main results of this paper, we run  
 245 several models varying the size of the mesh (between 1.6 mm and 50 mm). In  
 246 these resolution tests we consider the overturn of a mushy layer with  $h = H/10$ ,  
 247  $\phi_{d,0} = 0.5$ ,  $\eta_c = 10$  ( $Ra = 1.8 \times 10^6$ ) and  $\Delta\rho = 30 \text{ kg.m}^{-3}$ . Fig. 3 shows  
 248 the average value  $\phi_{d,average}$  along a horizontal profile located at the bottom of  
 249 the reservoir at  $t = 600\text{s}$  when the mushy layer is fully sedimented.  $\phi_{d,average}$   
 250 increases when decreasing the mesh size from 0.05 m to 0.01m. Then, below a  
 251 mesh size value of 0.01 m,  $\phi_{d,average}$  converges to a constant value of 0.45. In  
 252 order to save computational time, we consider a mesh size of 0.08 which leads to  
 253 an error of 7.7% relative to the converged value obtained for the smallest mesh  
 254 size. In addition, we decrease the size of the mesh by a factor 2 in the lowermost  
 255 part of the reservoir where crystal-rich patches are likely to settle or within the  
 256 whole reservoir for the most vigorously convective contexts. Therefore, the  
 257 calculation domain is composed of 100 000 to 180 000 cells. We list the details  
 258 of our models in Tab. 2. Each run presented in this study represents (for the  
 259 Euler-Euler flow model only) 12 to 72 hours computation time on a bi-processor,

260 8-cores, 3.2-GHz workstation.

#### 261 2.4. Reference case

262 In this subsection, we detail the case corresponding to simulation no. 47 in  
263 Tab. 2. For this reference case, we consider the case with  $Ra = 4.4 \times 10^6$  (cor-  
264 responding to  $\eta_c = 4$  Pa.s),  $\Delta\rho = 50 \text{ kg.m}^{-3}$  ( $\Delta\rho/\rho_{c,0} = 1.7\%$ ) and  $D_d = 10^{-3}$   
265 m. Fig. 4 illustrates the thermal and dynamical time evolutions of the convec-  
266 tive magma ocean and the mushy crystal layer. Because of negative buoyancy,  
267 the crystal layer rapidly sinks. Fig. 4 shows that an overturn rapidly occurs  
268 concentrating the crystals in the lower part of the reservoir during the first hun-  
269 dreds of seconds after the layer formation. The crystal fraction is first diluted  
270 in the lower reservoir then starts to organise in patches where the concentration  
271 is much higher than the initial concentration. This early stage limits the heat  
272 transfer from the bottom surface to the reservoir leading to a transient cooling  
273 of the magma.

274

275 To monitor the evolution of the average concentration  $C$  (particles/m<sup>3</sup>) in  
276 crystals in the upper mid reservoir for the reference case, we define:

$$e = \frac{\int_{H/2}^H \int_0^{4H} C dx dz}{\int_0^H \int_0^{4H} C dx dz} \quad (14)$$

277 *Höink et al.* (2005) refers to this parameter as the relative entrainment. Fig. 5  
278 illustrates the time evolution of  $e$  for our reference case and shows that during  
279 2000 s, the upper reservoir is depleted in crystals. After nearly 10 000 s, large  
280 hot plumes formed at the bottom of the reservoir (see Fig. 4) transport the  
281 crystals back in the upper reservoir. Hence the concentration in crystals in the  
282 upper reservoir increases. This second phases leads to an efficient mixing in the  
283 whole reservoir and the crystal concentration gets back and slightly oscillates

284 around its initial value. Fig. 5 shows that the initial concentration in the upper  
285 reservoir is slightly larger than its theoretical value of 0.01. This is due to  
286 the mesh properties that encompasses a larger volume of crystals leading to an  
287 initial value of  $e = 0.0105$ .

### 288 **3. Parametric study**

289 In the following section, we monitor the influence of the density difference  
290 between the crystals and the magma, the crystal size, and the magma viscosity  
291 on the settling dynamics within a convecting magma ocean.

#### 292 *3.1. Influence of the density difference $\Delta\rho$*

293 During the solidification of the magma ocean, the density of the crystal phase  
294 potentially increases (or decreases) relative to the molten phase depending on  
295 its ability to integrate dense chemical elements in its structure. Within the fully  
296 molten mantle, the first crystal to form is a crystal of bridgmanite. This first  
297 crystal is Fe-poor, and becomes chemically neutrally buoyant close to the core  
298 mantle boundary (*Caracas et al.*, 2019). Then, the relative Fe content increases  
299 in the melt potentially leading to the formation of a basal magma ocean overlaid  
300 by a thick layer of bridgmanite. The front of neutral buoyancy moves towards  
301 the shallow mantle as the solidification proceeds (*Solomatov*, 2000; *Boukaré*  
302 *et al.*, 2015; *Caracas et al.*, 2019). This scenario potentially leads to a fractional  
303 crystallisation of the early mantle (*Patočka et al.*, 2020). However, when ac-  
304 counting for re-entrainment enhanced by vigorous convection, crystal dispersion  
305 might be an efficient process that should favor batch (or equilibrium) crystalli-  
306 sation of the early mantle (*Solomatov et al.*, 1993). The melt-crystal density  
307 crossover in both these scenarios is discussed by *Caracas et al.* (2019). Here, we  
308 monitor the influence of the chemical density difference on the settling dynamics  
309 considering relatively small chemical density differences ( $10 - 100 \text{ kg.m}^{-3}$ ) which

310 is relevant in the early stages of mantle solidification. The chemical density dif-  
311 ference is fixed in each simulation and is superimposed to the thermal density  
312 difference which can evolve during the cooling. We note here that in our models,  
313 the density difference related to temperature differences ( $\alpha\rho\Delta T = 3 \text{ kg.m}^{-3}$ ) is  
314 smaller than the density difference between the magma and the crystals.

315

316 In Fig. 6, we considered the reference case illustrated in Fig. 4 in which  
317 we increased the density difference from  $\Delta\rho = 50 \text{ kg.m}^{-3}$  to  $\Delta\rho = 100 \text{ kg.m}^{-3}$ .  
318 As already illustrated in Fig. 4, Fig. 6 shows that because of negative buoy-  
319 ancy, the crystal layer rapidly sinks. After a rapid settling at the bottom of the  
320 reservoir, particles entrainment occurs from the dunes (10 000 s after the initi-  
321 ation of the settling). However, because of a larger density difference between  
322 the dispersed phase and the continuous phase, efficient mixing is prevented.  
323 Particle entrainment nearly vanishes and the layer is fully sedimented at the  
324 bottom of the reservoir (28 000 s after the initiation of the settling). Again,  
325 the sedimented layer acts as an insulating layer by limiting the heat transfer  
326 from the bottom of the reservoir. As a consequence, the mean temperature is  
327 significantly lower due to bottom insulation when full sedimentation is achieved.

328

329 Fig. 5 compares the time evolution of the concentration of particles in the  
330 upper part of the reservoir for the two density differences illustrated in Fig. 4 and  
331 6. During all the simulation, the concentration for the case with  $\Delta\rho = 50 \text{ kg.m}^{-3}$   
332 remains larger than the concentration for the case with  $\Delta\rho = 100 \text{ kg.m}^{-3}$ . This  
333 feature is in agreement with *Lavorel and Le Bars (2009)* who monitored the  
334 relative number of particles in suspension as a function of the fluid/particle  
335 density difference during the first 1000 s after being uniformly distributed within  
336 the reservoir. Fig. 5 also shows that increasing the density difference decreases

337 both the minimum value of the particle concentration in the upper reservoir and  
 338 the time at which this minimum is reached. This feature is in agreement with  
 339 the theoretical overturn timescale derived for a viscous layer of thickness  $\delta$  from  
 340 *Hess and Parmentier (1995)* and modified to account for the thermal buoyancy  
 341 contribution:

$$t_{\text{overturn}} = \frac{4\pi^2\eta_{\text{lay},0}}{(\phi_{d,0}\Delta\rho - \alpha\rho_{\text{lay},0}\Delta T)g\delta} \quad (15)$$

342 where  $\eta_{\text{lay},0}$  is the initial viscosity of the crystal rich layer (see Eq.6) and  
 343  $\rho_{\text{lay},0}$  is the initial density of the crystal rich layer ( $= \phi_{d,0}\rho_d + (1 - \phi_{d,0})\rho_c$ ).  
 344 The overturn timescales decreases with increasing density differences as shown  
 345 in Fig. 5.

### 346 3.2. Influence of the crystal size

347 Upon solidifying, crystals form following the nucleation and growth mecha-  
 348 nisms (*Solomatov, 2015*). The crystal size reached at equilibrium depends on  
 349 the nature of the mineral and on the cooling rate within the convecting reservoir.  
 350 The grain size may range between  $10^{-4}\text{m}$  and  $10^{-2}\text{m}$  in typical magma ocean  
 351 conditions (*Solomatov, 2015*). Here, we monitor the influence of the crystal size  
 352 in our models. To that aim, we compare the reference case (with  $D_d = 10^{-3}\text{m}$ )  
 353 to cases with crystals larger ( $D_d = 10^{-2}\text{m}$ ) and smaller ( $D_d = 10^{-4}\text{m}$ ). Fig. 7  
 354 shows the time evolution of the crystal fraction in the upper part of the reservoir  
 355 for the three particle diameters  $D_d$  considered. Fig. 7 illustrates that, even for  
 356 the wide range of crystal sizes considered (2 orders of magnitude), the overturn  
 357 timescale is poorly sensitive to the particle diameter  $D_d$  (factor 3 in difference).  
 358 This result is in agreement in agreement with Eq. 15.

359

360 However, Fig. 7 shows that the final behaviour of the reservoir in terms  
 361 of sedimentation/suspension is dependent on the crystal size. Indeed, for the



362 parameters chosen for the reference case ( $\eta_c = 4$  Pa.s and  $\Delta\rho = 50$  kg.m<sup>-3</sup>), Fig.  
363 7 shows that when the particle size is equal to  $10^{-2}$  m, the suspension regime is  
364 not reached after the overturn. For smaller particle diameters ( $D_d = 10^{-4}$  and  
365  $D_d = 10^{-3}$ ), the overturn process is rapidly followed by a suspension regime  
366 where the particles are efficiently mixed within the convecting reservoir.

### 367 3.3. Influence of the viscosity

368 The viscosity of the molten phase ( $\eta_c$ ) is a key parameter governing the cool-  
369 ing dynamics of the magma ocean and in particular the solidification timescales  
370 (Monteux *et al.*, 2016). According to Karki and Stixrude (2010),  $\eta_c$  for liquid  
371 anhydrous MgSiO<sub>3</sub> may decrease down to 0.048 Pa.s at mid-mantle conditions  
372 ( $P = 70$  GPa and  $T = 4000$  K along the magma ocean isentrope). For molten  
373 peridotite, Xie *et al.* (2021) obtained a viscosity ranging between 0.017 and  
374 0.038 Pa.s. To maintain a laminar flow, (i.e. with low Reynolds number), we  
375 consider  $0.1 \leq \eta_c \leq 10$  Pa.s.

376

377 Fig. 8 shows that the continuous phase viscosity governs the ability of the  
378 solid phase to mix or sediment at the bottom of the reservoir. The interesting  
379 feature arises from the non linearity of the process. Indeed Fig. 8 shows that for  
380 the lowest viscosity, the crystal layer rapidly mix with the convecting reservoir.  
381 Then for  $0.4 \leq \eta_c \leq 1$ , the rapid overturn process is not followed by a mixing  
382 process and the final concentration within the upper part of the reservoir does  
383 not reach the typical value synonymous of efficient mixing. Finally, for  $\eta_c > 1$   
384 Pa.s, the overturn process is followed by a vigorous mixing process similarly to  
385 the case with  $\eta_c = 0.1$  Pa.s.

386

387 Fig. 8 shows that the molten phase viscosity also governs the early overturn  
388 timescale (i.e. the time needed for the particle concentration in the upper part

389 of the reservoir to reach the minimal value). This overturn time increases from  
390 nearly 40s (for  $\eta_c = 0.1$  Pa.s) up to 2000s (for  $\eta_c = 10$  Pa.s). We represent  
391 these overturn timescales in Fig. 9 and compare them with the scaling law from  
392 Eq. 15. Fig. 9 shows that the overturn timescales from our models is 5 to  
393 40 times larger than the overturn timescale from Eq. 15. We attribute this  
394 discrepancy to two points: (1) Eq. 15 is related to an overturn timescale while  
395 Fig. 9 represents the time from which the concentration in the upper part of  
396 the reservoir re-increases after the overturn which is closer to a re-entrainment  
397 timescale and (2) the mixing dynamics tends to dilute the concentration in  
398 particles within the overturning layer during its sinking. Initially the particle  
399 concentration in the layer is  $\phi_{d,0}$ . As illustrated in Figs. 4 and 6 (second  
400 line), the vigorous convection redistribute the particles within the reservoir even  
401 during the early overturn. As a consequence the density of the mushy layer  
402 relative to the ambient fluid decreases from its initial value. The mushy layer  
403 settles with a timescale that is larger than if the layer could maintain its initial  
404 structure.

#### 405 **4. A criterion for the stability of a crystallising layer**

406 We have illustrated the separated influence of the density difference between  
407 crystals and melt, grain size and melt viscosity on the behaviour of a crystallising  
408 layer within a magma ocean. We now aim at anticipating the ability of the flow  
409 generated from the convection within magma ocean to initiate the motion and  
410 suspension of sedimented crystals and to lead to efficient mixing within the  
411 magma ocean. We introduce the Shields number  $Sh$  that is the ratio between  
412 the tangential stress from convective flow over the buoyancy stress relative to  
413 density difference between the crystals and the melt (*Solomatov et al., 1993*):

$$Sh = \left( \frac{\eta_c \alpha g F}{C_p} \right)^{1/2} \frac{1}{\Delta \rho g D_d} \quad (16)$$

414 Large  $Sh$  values favor a suspension regime while small  $Sh$  values favor a  
 415 sedimentation regime. The two regimes are separated by a critical Shields num-  
 416 ber value  $Sh_c$ . From their analog experiments, *Solomatov et al.* (1993) have  
 417 estimated a critical value  $Sh_c = 0.1 - 0.2$ . We have run a total of 76 numer-  
 418 ical models (with values listed in Tab. 2) considering different sets of  $D_d$ ,  $\Delta\rho$   
 419 and  $\eta_c$  with value ranges in Tab. 1. Each model corresponds to a  $Sh$  value  
 420 calculated considering the combination of Eq. 12, Eq. 13 and the expression  
 421  $Nu = 0.14Ra^{0.34}$  obtained from Fig. 1 to compute the heat flow  $F$  (See Tab. 2  
 422 for values). Monitoring the concentration of grains in the upper reservoir ( $e(t)$ )  
 423 in each models enables to decipher if the models end up in the suspension or  
 424 sedimentation regime.

425

426 In Fig. 10, we illustrate the  $Sh$  values as a function of the molten phase  
 427 viscosity  $\eta_c$ . A case where the grain concentration in the upper part of the  
 428 reservoir ( $e$ ) never reaches back its initial value is considered in the sedimen-  
 429 tation regime. Oppositely, a case where the grain concentration in the upper  
 430 part of the reservoir gets back to its initial value is considered in the suspen-  
 431 sion regime. As shown in Fig. 8, some cases may end up in an intermediate  
 432 regime where the final concentration is  $0.005 < e < 0.01$ . We consider that these  
 433 intermediate cases fall out in the sedimentation regime. Sedimentation and sus-  
 434 pension regimes are separated by the critical Shields number value ( $Sh_c$ ).

435

436 According to Fig. 10, the  $Sh_c$  value is a non-linear function of the continuous  
 437 molten phase viscosity. For  $\eta_c > 1$ ,  $Sh_c$  seems to be constant and independent  
 438 of the  $\eta_c$  value. However, when  $\eta_c < 1$ , the  $Sh_c$  value decreases with decreasing

439 values of the viscosity following  $Sh_c = 0.1\eta_c^{0.45}$ . As a consequence  $Sh_c$  is not  
 440 influenced by the increase of Rayleigh number up to  $Ra = 1.8 \times 10^7$ . For  $Ra$   
 441 values larger than  $1.8 \times 10^7$  the increase of the kinetic energy induced by the  
 442 vigorous convection in the system results in a decrease of  $Sh_c$  following:

$$Sh_c = 184.Ra^{-0.45} \quad (17)$$

443 The non-linear dependence of  $Sh_c$  on the viscosity explains why the crystal  
 444 settling behaviour may vary back and forth between sedimentation and suspen-  
 445 sion regimes when the viscosity increases. Indeed Fig. 10 shows with the red  
 446 dotted line the path followed for the models detailed in Fig. 8. Moreover, Fig.  
 447 10 shows that  $Sh_c$  is smaller than the range of values proposed by *Solomatov*  
 448 *et al.* (1993) (0.1 – 0.2). This feature is particularly visible for the lowest range  
 449 of viscosities used in our models. For a magma ocean viscosity value of 0.1 Pa.s,  
 450 the  $Sh_c$  value may decrease down to 0.04 which means that the crystal settling  
 451 is difficult to envision in such a convecting environment especially regarding the  
 452 typical viscosity values for a magma ocean (*Karki and Stixrude, 2010; Xie et al.,*  
 453 *2021*). Decreasing the viscosity down to the lowest values proposed by *Xie et al.*  
 454 (2021) may enhance this feature.

## 455 **5. Fate of mushy material in the context of a progressive magma** 456 **ocean crystallisation**

### 457 *5.1. Parameters controlling the solidification of a magma ocean on a Earth-like* 458 *planet*

459 We now investigate the implication of our model on the mechanism of magma  
 460 ocean (MO) solidification on Earth. More precisely, we investigate the possi-  
 461 bility of Bridgmanite (Bg) segregation depending on its buoyancy (positive or  
 462 negative). To that aim, we compare the density difference between the MO

463 and the solid crystal  $\Delta\rho_{MO}$  calculated for different compositions and the crit-  
 464 ical density contrast  $\Delta\rho_{crit}$  above which crystal segregation is likely to occur.  
 465  $\Delta\rho_{crit}$  is derived from Eq. 16 by calculating:

$$\Delta\rho_{crit} = \left( \frac{\eta_c \alpha g F}{C_p} \right)^{1/2} \frac{1}{Sh_c g D_d} \quad (18)$$

466 and considering  $Sh_c = 0.1$  which is a conservative value regarding a magma  
 467 ocean viscosity of 0.1 Pa.s or less (*Xie et al.*, 2021). At a given depth ( $z$ ), a  
 468  $\Delta\rho_{MO}$  larger than the critical value  $\Delta\rho_{crit}$  would yield an efficient Bg sedimen-  
 469 tation to the bottom of the MO. By extension, we also consider that Bg would ef-  
 470 ficiently segregate into a solid layer above a basal magma ocean if  $\Delta\rho_{MO}/\Delta\rho_{crit}$   
 471 is smaller than  $-1$ . Calculating  $\Delta\rho_{MO}$  requires a number of assumptions:

- 472 1. We use pyrolite as a model of reference for the mantle composition. Py-  
 473 rolite is obtained by adding some crust component to the present-day  
 474 depleted (peridotitic) upper mantle (*Ringwood*, 1975). To implement flex-  
 475 ibility on the possible mantle compositions, we add or subtract a compo-  
 476 nent of bridgmanite (Bg) to pyrolite; it yields less or more mafic mantle  
 477 material, respectively. Later, we will argue that the composition of the  
 478 primitive upper mantle (PUM) should be close to pyrolite, as this is widely  
 479 accepted.
- 480 2. The composition of the bulk silicate Earth (BSE) is still not well estab-  
 481 lished, because a number of deep mantle reservoirs could have a com-  
 482 position different than pyrolite: The large low seismic velocity provinces  
 483 (LLSVP) seem to present a different mineralogy (e.g. *Vilella et al.* (2021)),  
 484 the deep lower mantle could be more bridgmanitic than pyrolite (*Mu-  
 485 rakami et al.*, 2012) and there could be relics above the core-mantle bound-  
 486 ary (CMB) of a basal magma ocean (*Labrosse et al.*, 2007) or of early  
 487 mantle overturns (e.g. *Boukaré et al.* (2015)). In our models, we give a

488 large freedom of size of the possible Bg-rich or mafic reservoirs that could  
489 have segregated in the deep mantle during the MO solidification. The  
490 flexibility of BSE composition is achieved by adding or subtracting up to  
491 40% of Bg to the pyrolite mantle reference. This is a much broader range  
492 of chemical variation than the uncertainty remaining today on the major  
493 elements concentration in BSE.

494 3. The Bg composition is calculated by equilibrating it with the melt in  
495 the mushy MO, using partitioning coefficients  $K(Al)^{Bg/Melt} = 0.5$  and  
496  $K(Fe)^{Bg/Melt} = 0.1$  or  $0.25$ . The value of  $K(Al)^{Bg/Melt}$  does not impact  
497 our calculations significantly.  $K(Fe)^{Bg/Melt}$  remains controversial as it is  
498 reported between  $\sim 0.07$  to  $\sim 0.5$  (*Andrault et al., 2012; Nomura et al.,*  
499 *2011*). The former value could be underestimated as it was measured in a  
500 sample presenting extreme chemical segregation in a temperature gradient,  
501 which artificially promotes the Fe-depletion of Bg at the highest temper-  
502 ature. In the latter study, the experimental conditions corresponded to  
503 solidus-like temperatures, at which Fe is more compatible in Bg. Relevant  
504 temperatures for MO solidification evolve from liquidus-like to intermedi-  
505 ate between liquidus and solidus. Therefore, we perform our calculations  
506 for  $K(Fe)^{Bg/Melt}$  values of 0.1 or 0.25.

507 4. As a reference model for the mushy MO, we use Bg grain diameter ( $D_{Bg}$ )  
508 of 0.1 to 10 mm, viscosity ( $\eta$ ) of 0.1 Pa.s (*Xie et al., 2020*), intrinsic  
509 conductivity ( $k$ ) of 5 W/m/K (*Hofmeister, 1999*) and heat capacity ( $Cp$ )  
510 of 1800 J/Kg/K (*Asimow, 2018*). We consider that the melt has the same  
511 composition at all depths because of efficient mixing in the turbulent MO.

512 5. We consider that the term  $\Delta T$  used in  $F$  calculation from Eq. 18 is the  
513 temperature difference between the Earth's surface and the bottom of the  
514 MO, after correcting for the adiabatic increase of temperature with mantle  
515 depth. We first fix the surface temperature ( $T_{surf}$ ) to 500 K (*Lebrun et al.,*

516 2013; *Monteux et al.*, 2020), however, we will investigate later  $T_{surf}$  of 1000  
 517 and 1500 K. We consider that the bottom of the MO ( $z_{MO}$ ) is the depth  
 518 where the mantle solidification is achieved for a mixture of 60% of Bg and  
 519 40% of melt. During the mantle solidification,  $z_{MO}$  evolves from the CMB  
 520 depth towards the surface. We assume that the temperature at a depth  
 521  $z_{MO}$  follows the solidus temperature profile of pyrolite ( $T_{sol}(z_{MO})$ ) (*Pierru*  
 522 *et al.*, *subm.*). We note that using the solidus profile yields a conservative  
 523  $\Delta T$ , compared to the true temperature that should be between solidus  
 524 and liquidus. Then, we calculate  $\Delta T(z_{MO})$  of a MO extending from a  
 525 depth  $z_{MO}$  to the Earth surface using the following equation:

$$\Delta T(z_{MO}) = T_{sol}(z_{MO}) - T_{surf} - \Delta T_{ad}(z_{MO}) \quad (19)$$

526 where  $\Delta T_{ad}(z_{MO})$  is the temperature difference between  $T_{sol}(z_{MO})$  and  
 527 the corresponding potential surface temperature extrapolated from  $T_{sol}(z_{MO})$   
 528 to the surface along the MO adiabatic temperature profile. The adiabatic  
 529 gradient in the MO is calculated using the equations of state available for  
 530 different silicate melt compositions (*Asimow*, 2018).  $\Delta T(z_{MO})$  is found  
 531 to range between  $\sim 1300$  K and  $\sim 2000$  K for MO extending from 660 km  
 532 (24 GPa) to 2800 km (135 GPa), respectively (see Fig. 11).

533 6. We calculate the density of Bg ( $\rho_{Bg}$ ) along the mantle solidus, using the  
 534 equations of state (EoS) of  $\text{MgSiO}_3$ ,  $\text{FeSiO}_3$  and  $\text{Al}_2\text{O}_3$  end-members  
 535 (*Matas et al.*, 2007). The decomposition in end-members assumes Bg  
 536 of  $(\text{Mg}_{1-x-y}\text{Fe}_x\text{Al}_y)(\text{Si}_{1-y}\text{Al}_y)\text{O}_3$  stoichiometry with a dominant fraction  
 537 of  $\text{Fe}^{2+}$  over  $\text{Fe}^{3+}$  at lower mantle conditions, in agreement with pre-  
 538 vious works (e.g. *Andrault et al.* (2018)). This assumption has little  
 539 impact on the Bg density; the dominating parameter is the global Fe con-  
 540 tent in Bg, itself controlled by  $K(\text{Fe})^{Bg/Melt}$  (discussed above). At the

541 same P-T conditions, we calculate the MO density ( $\rho_{Melt}$ ) and thermal  
 542 expansion ( $\alpha_{Melt}$ ) using the EoS of the end-member molten  $MgSiO_3$  en-  
 543 statite,  $Mg_2SiO_4$  forsterite,  $Fe_2SiO_4$  fayalite,  $CaMgSi_2O_6$  diopside, and  
 544  $CaAl_2Si_2O_8$  anorthite (Asimow, 2018). These calculations yield the Bg-  
 545 to-melt density contrast ( $\Delta\rho_{MO} = \rho_{Bg} - \rho_{Melt}$ , Fig. 12) along the mantle  
 546 solidus:  $\Delta\rho$  decreases with increasing pressure whatever is the composi-  
 547 tion of the mushy mantle, because the melt is more compressible than  
 548 Bg.

549 7. We do not attempt to model the latest stages of MO crystallization, when  
 550 the bottom of the MO is shallower 660 km depth, because the phase  
 551 relations rely on the melting diagrams at upper mantle P-T conditions.

## 552 5.2. Conditions for segregation of Bg in the mushy magma ocean

### 553 5.2.1. Effect of melt composition

554 We now calculate the ratio of density differences  $\chi_\rho = \Delta\rho_{MO}/\Delta\rho_{crit}$  at all  
 555 lower mantle depths using the parameters defined above. First, we fix the grain  
 556 size of Bg to 1 mm,  $K(Fe)^{Bg/Melt}$  to 0.1 or 0.25, and vary the MO composition  
 557 from pyrolite -40% of Bg to pyrolite +40% of Bg (i.e. 70% of pyrolite and 30%  
 558 of Bg).  $\chi_\rho$  is found to be positive or negative (Fig. 13), depending on the solid-  
 559 melt density difference (Fig. 12). A  $\Delta\rho_{MO}$  value larger than  $\Delta\rho_{crit}$  (i.e.  $\chi_\rho > 1$ )  
 560 indicates an efficient Bg segregation to the bottom of the MO. Our calculations  
 561 show that Bg segregation happens in shallow MOs for all chemical compositions  
 562 investigated. For pyrolite, this is in agreement with a previous work dedicated  
 563 to the determination of the MO viscosity (Xie et al., 2020). The higher is the Bg  
 564 content in the MO, the earlier (the deeper) Bg segregation occurs during the MO  
 565 solidification; this is because  $\Delta\rho_{MO}$  is larger when the bulk Fe-content is lower.  
 566 As expected, lower  $K(Fe)^{Bg/Melt}$  favors a denser melt, and thus lower  $\Delta\rho_{MO}$ .  
 567 Still, our calculations show a moderate impact on the results of  $K(Fe)^{Bg/Melt}$



568 variations from 0.1 to 0.25. Finally, efficient Bg segregation could occur above  
569 a dense MO for a MO composition highly depleted in Bg; this is suggested by  
570  $\chi_\rho < -1$  for pyrolite -40%Bg at pressures larger than  $\sim 120$  GPa, for a Bg grain  
571 size of 1 mm (Fig. 13).

### 572 5.2.2. Effect of grain size

573 We now investigate the role of the Bg grain size, for five different mantle  
574 compositions (Fig. 14). We first focus on a melt of pyrolite composition.  $\chi_\rho$   
575 is found positive at most of the mantle depths, because  $\Delta\rho_{MO}$  is also positive  
576 (Fig. 12), except in the lowermost mantle for  $K(Fe)^{Bg/Melt} = 0.1$ . Still,  $\chi_\rho$   
577 can only be larger than 1 for  $D_{Bg}$  larger than 0.5 mm; Bg-grains of e.g. 2 mm  
578 segregate when pressure (depth) is larger than 70 GPa (1650 km). Grain size  
579 in a crystallizing MO remains a complicated issue (Solomatov, 2015): (i) as  
580 long as the MO is fully liquid close to the planetary surface, grains are often  
581 remolten within the large scale convection movements and, therefore, grain size  
582 is controlled by nucleation processes; (ii) When the crystallization zone reaches  
583 the surface, it enables some grains to grow indefinitely. According to the shape  
584 of mantle solidus and liquidus, this change of mechanism could happen when  
585 the bottom of the MO reaches a depth of 1000 km ( 40 GPa) (see Xie *et al.*  
586 (2020)). In this article, we aim at modelling the chemical segregation in the  
587 first stages of the MO solidification, when grain size is controlled by nucleation  
588 processes.  $D_{Bg}$  in these conditions depends largely on the cooling rate of the  
589 MO, with estimated values of 0.1 to 1 mm (Solomatov, 2015). For 1 mm grain  
590 size,  $\chi_\rho$  is larger than unity at pressures (depths) larger than 45GPa (1100  
591 km) (Fig. 13). As a result, it appears unlikely that Bg grains could segregate  
592 in a crystallizing MO of pyrolite composition for a depth larger than  $\sim 1100$  km.

593

594 A BSE composition enriched in Bg yields a lighter melt on the first stages

595 of the MO solidification, and thus a larger  $\Delta\rho_{MO}$ . It makes it easier the segregation  
596 of Bg at the bottom of the mushy MO. For a melt composition enriched  
597 with 20% or 40% of Bg, Bg grains of 1 mm could efficiently segregate at pressures  
598 (depths) of 55 GPa (1350 km) or 65 GPa (1550 km), respectively (Fig.  
599 14 a and b). From a geochemical point of view, an early segregation of Bg  
600 to the CMB requires a BSE composition enriched in Bg if the late shallow MO  
601 should be of pyrolite composition; we will discuss this matter later in the article.

602

603 Alternatively, a BSE composition depleted in Bg yields a denser melt in the  
604 mushy MO, as discussed in several works (*Boukaré et al., 2015; Ballmer et al.,*  
605 *2017a; Caracas et al., 2019*). Our calculations of  $\chi_\rho$  for melt compositions of  
606 pyrolite -20% and -40% of Bg show that Bg is indeed less dense than the melts in  
607 a large fraction of the lower mantle (Fig. 12). Bg remains always denser at low  
608 pressures, due to its very high bulk modulus. For Bg grain size of 1 mm, values  
609 of  $\chi_\rho$  are found lower than -1 at pressures (depths) larger than 120 GPa (2600  
610 km) for a melt composition of pyrolite -40% of Bg (Fig. 14 e). The pressure  
611 (depth) at which Bg could segregate upwards decreases with increasing the Bg  
612 grain size. From a geochemical point of view, an early segregation close to the  
613 CMB of a Bg-depleted melt requires a BSE composition depleted in Bg, if the  
614 shallow MO were to be pyrolitic.

### 615 5.2.3. Effect of temperature

616 Another important parameter in  $\Delta\rho_{crit}$  is  $\Delta T$  (Eq. 19), which is intrinsically  
617 related to the rate of MO cooling. During the mushy stage of a MO solidifica-  
618 tion, the surface temperature is  $\approx 500$  K, which yields to final MO solidification  
619 in 100-200 thousands years after the Moon forming impact (*Lebrun et al., 2013;*  
620 *Monteux et al., 2020*). Presence of a blanketing atmosphere atop the MO would  
621 induce a larger surface temperature and a lower rate of cooling (*Sleep et al.,*

2014; *Salvador et al.*, 2017). We note that the formation of a blanketing atmo-  
sphere is unlikely to affect the first stages of the MO solidification for different  
reasons: (i) H<sub>2</sub>O (a most efficient blanketing compound) is efficiently vaporized  
to the atmosphere only after a high level of MO solidification (*Elkins-Tanton*,  
2008; *Salvador et al.*, 2017). (ii) a surface temperature larger than 1500K yields  
an atmosphere dominated by rock-vapor, which is inefficient to stop the surface  
cooling by thermal radiation (*Sleep et al.*, 2014). For these reasons, we also per-  
form calculations of  $\Delta\rho_{MO}$  for surface temperatures of 500K, 1000K and 1500  
K (Fig. 15).

631

Calculations show that larger surface temperatures yield more extreme posi-  
tive and negative values of  $\chi_\rho$  and therefore easier Bg segregation. This is be-  
cause larger  $T_{surf}$  corresponds to smaller temperature difference  $\Delta T$  (Eq. 19)  
and thus a less turbulent MO. Still, the impact remains modest; for a pyrolite  
mantle, variation of  $T_{surf}$  from 500 to 1500 K yields Bg segregation at pressures  
(depths) lower than 45 GPa (1100 km) and 67 GPa (1600 km), respectively.

### 5.3. Possible scenarios of MO solidification

#### 5.3.1. Conditions for Bg segregation at the bottom of the MO

Geochemical scenarios of the Earth’s formation involve building blocks of  
chondritic composition. Uncertainties remain about the composition of the  
primitive ”chondritic-type” mantle after the core-mantle segregation. Still, it  
is very likely that it would be enriched in SiO<sub>2</sub>, compared to pyrolite (*Allègre*  
*et al.*, 1995; *Javoy*, 1995; *McDonough and Sun*, 1995). Such enrichment raised  
long-term discussions about how much the core could contain some Si and how  
much the deep mantle could be enriched in SiO<sub>2</sub>, compared to the present day  
upper mantle. A high MgSiO<sub>3</sub>/MgO ratio in the lower mantle is compatible  
with results from inversions of seismic profiles based on elastic parameters of

649 minerals (*Samuel et al.*, 2005; *Matas et al.*, 2007; *Murakami et al.*, 2012).

650

651 Our model shows that increasing the Bg content in BSE favors the segregation  
652 of Bg in a deep MO (Fig. 14 a and b). Bg grains of 1mm diameter  
653 segregate efficiently (i.e.  $\chi_\rho > 1$ ) at pressures (depths) lower than 45GPa (1100  
654 km), 55 GPa (1350 km) and 65 GPa (1550 km) for pyrolite, pyrolite with ad-  
655 dition of +20%Bg and +40%Bg, respectively. Still, Bg grains would segregate  
656 at the early stages of the solidification if the grain size would be 5 mm or more.  
657 Such big grains are not expected in a very thick MO (*Solomatov*, 2015). Bg  
658 segregation becomes possible when the MO is shallower and the greater the  
659 Bg enrichment, the earlier (the deeper) the Bg-segregation. For a grain size of  
660 1mm, a Bg layer could form at MO depths of 1100 to 1550 km, depending on  
661 the BSE composition. Such thin MO could also favor grain growth, because  
662 the MO is partially crystallized up to the Earth's surface (*Solomatov*, 2015; *Xie*  
663 *et al.*, 2020). Such Bg-layer could yield silica-enriched domains (*Ballmer et al.*,  
664 2017b). Unfortunately, our models are not adapted to address the thickness of  
665 layer, because of too many adjustable parameters. Segregation of some Bg in  
666 the lower mantle would drive the MO toward a pyrolite mantle, for a BSE is  
667 enriched in Bg. Decreasing the Bg-content makes the segregation of Bg grains  
668 less efficient (Fig. 13).

### 669 5.3.2. Solidification of a pyrolite-type bulk silicate Earth

670 A pyrolite-like BSE would solidify with no Bg segregation from the melt, as  
671 long as the Bg grain size always remains lower than 0.5 mm (Fig. 14 c). Bg  
672 segregation could still happen in the uppermost lower mantle if the Bg grain  
673 size gets larger. We note, however, that the grain growth of olivine and other  
674 minerals of the upper mantle may have a moderate impact on the grain size of  
675 Bg in the lower mantle. Modelling the mechanism of MO solidification in the

676 upper mantle is beyond the scope of this article.

677

678 Interestingly, absence of Bg segregation does not imply a chemically homo-  
679 geneous mantle once it is entirely solidified. The origin of this effect is that the  
680 solidified mantle contains  $\sim 60\%$  of Bg and  $\sim 40\%$  of melt, while the overlying  
681 mushy MO contains a different fraction of the two phases. Here we assume  
682 the rate of mushy-mantle compaction (with extraction of the melt) significantly  
683 slower than the rate of MO solidification, following a previous work (*Soloma-*  
684 *tov, 2015*). To model the chemical stratification resulting from homogeneous  
685 solidification, we proceed as follows: (i) we choose a BSE composition close to  
686 pyrolite. Still, we keep its Bg content adjustable, to enable a final shallow MO  
687 (thickness of  $\sim 660$  km) composition as close as possible from pyrolite. (ii) At  
688 each time step of the progressive MO solidification, we estimate the fraction of  
689 Bg grains in the MO above the bottom of the MO ( $\phi_{MO}$ ) based on our previ-  
690 ous model of progressive MO solidification (Fig. 3 of *Monteux et al. (2016)*).  
691 (iii) We calculate the composition of the coexisting melt and Bg grains, fixing  
692  $K(Fe)^{Bg/Melt} = 0.25$ . Anyway, the value of  $K(Fe)^{Bg/Melt}$  has no significant  
693 impact on this calculation. (iv) Starting from the CMB, we cool the mantle and  
694 calculate the composition of a mixture of 60% of Bg grains and 40% of melt  
695 which solidifies at the bottom of the MO. The chemical content of this bottom  
696 layer is then subtracted to the composition of the overlying mushy MO, before  
697 a next step of the solidification is performed within a thinner MO.

698

699 This calculation shows significant changes of the  $\text{SiO}_2$ , FeO and CaO con-  
700 tents with depth in the solidified mantle (Fig. 16). They occur due to Bg pre-  
701 senting higher  $\text{SiO}_2$  and lower FeO and CaO contents, compared to the melt.  
702 The shallow MO presents a chemical composition close to pyrolite, when the

703 BSE composition is adjusted to 80% of pyrolite and 20% of Bg. The SiO<sub>2</sub> con-  
704 tent in the deep mantle is found to decrease from ~46 to 39%, which translate  
705 into a decrease from ~90 to 70% of the Bg-content, with decreasing depth from  
706 2900 to 660 km, respectively. The Fe-content also increases with decreasing  
707 depth, because of its incompatible character; this effect is found even larger  
708 when using  $K(Fe)^{Bg/Melt} = 0.1$ , instead of  $K(Fe)^{Bg/Melt} = 0.25$ . Still, the  
709 overlying mushy MO does not become denser than the solidified layers, because  
710 Bg is denser than the melt at all mantle depth for Bg-enriched BSE composition  
711 (Fig. 12).

712

713 Such a chemical layering would only survive as such in a mantle that would  
714 be stagnant after its solidification. Instead, one could expect important ver-  
715 tical mixing in mushy mantle presenting a relatively low viscosity and with a  
716 major heat flux from the core to the surface (*Monteux et al., 2016*). Another  
717 effect that can moderate the chemical stratification is a simultaneous mantle  
718 solidification in a large range of mantle depths. Upon cooling, the tempera-  
719 ture profile becomes almost parallel to the solidus (*Miller et al., 1991; Stixrude*  
720 *et al., 2009; Monteux et al., 2016*), which could yield to a bulk solidification.  
721 Still, these effects may not suppress entirely the chemical gradients, in partic-  
722 ular between a shallow MO and the lower mantle. The progressive enrichment  
723 of Bg with mantle depth is in good agreement with the mineralogical models  
724 (*Samuel et al., 2005; Matas et al., 2007; Murakami et al., 2012*), as well as with  
725 the difference between shallow the mantle composition today (pyrolite) and a  
726 "chondritic-type" BSE (see above).

727

728 We note that the scenario of Bg-segregation in the lowermost mantle does  
729 not help explaining the LLSVPs atop the CMB. Several origins were proposed

730 for the LLSVP, in particular some primitive mantle that did not melted upon  
731 the Moon forming impact. Primitive mantle compositions imply a relatively low  
732 proportion of ferropericlase, which is compatible with the comparison between  
733 the LLSVP seismic signature and the elastic parameters of the minerals (*Vilella*  
734 *et al.*, 2021). Still, LLSVPs represent a quite small fraction of the mantle vol-  
735 ume, typically 1.5 to 2.5 % (*Burke et al.*, 2008). Therefore, our models would  
736 not be much different if some primitive mantle would have survived to melting  
737 at the Moon Forming impact.

### 738 5.3.3. Conditions for the formation of a primary basal magma ocean

739 The segregation of large Bg grains to the bottom of a pyrolite mantle would  
740 yield a mafic Fe-enriched overlying MO. Following this scenario, it has been pro-  
741 posed that the melt could become denser than the underlying mantle and induce  
742 early mantle overturns (*Boukaré et al.*, 2015; *Ballmer et al.*, 2017a; *Caracas*  
743 *et al.*, 2019). Such a reversal could result in a secondary MO with a composi-  
744 tion typical of a shallow MO. Our results do not strongly support this scenario,  
745 because the lower the Bg-content in the mushy MO, the less efficient the Bg  
746 segregation (Fig. 14). Therefore, bulk solidification should rapidly be favored,  
747 after some Bg-segregation may have occurred in a thick MO. Mantle overturns  
748 may still occur due to the crystallization processes in the upper mantle; this  
749 should be investigated in further works based on analyses of the melting dia-  
750 grams in the upper mantle.

751

752 Formation of a basal MO during the solidification process (i.e. a primary  
753 basal-MO) would require the efficient segregation of Bg in an overlying solid  
754 layer (*Labrosse et al.*, 2007). This conditions translates into  $\chi_\rho < -1$  in our  
755 model. Such condition is reached for mafic BSE composition, which present a  
756 lower Bg content, compared to pyrolite (Fig. 14 c and d). Still, our calculations

757 show that Bg segregation upwards is only expected (i) in the lowermost part of  
758 a MO (ii) for a BSE composition depleted of more than -20% of Bg, compared  
759 to pyrolite and (iii) for Bg grain size larger than 0.5 mm. We note that low  
760  $K(Fe)^{Bg/Melt}$  value at these conditions help making the melt denser than Bg  
761 (Fig. 13, *Nomura et al.* (2011)). For a MO composed of pyrolite -40%Bg, Bg  
762 grains of 1 mm diameter would aggregate efficiently to a Bg-rich layer that  
763 would be located pressure (depth) of 120 GPa (2600 km). For a MO composed  
764 of pyrolite -20%Bg, only Bg grains of 5 mm diameter could segregate efficiently  
765 upwards. The simultaneous formation of a basal MO and a solid layer of Bg may  
766 maintain mafic the composition of the overlying MO. No further Bg segregation  
767 should be expected above  $\sim 2500$  km (i.e. 100-110 GPa) in a mafic MO, for  
768 a reasonable Bg grain size. In case the MO would be further depleted in Bg  
769 due to the mechanism of "at equilibrium fractionation" described above (Fig.  
770 16), it would make it even more mafic. At this point, it is difficult to imagine  
771 which geological process could lead to the disappearance of such a major volume  
772 of early mafic MO. The path to pyrolite-type upper mantle seems difficult to  
773 achieve. It makes the formation of a primary basal MO simultaneous to MO  
774 solidification relatively unlikely.

## 775 6. Conclusion

776 The solidification within a deep convecting magma ocean (MO) is a key pro-  
777 cess that significantly shaped the Earth's interior (*Ballmer et al.*, 2017a) and  
778 likely the early mantle evolution for several planetary contexts : Mars (*Elkins-*  
779 *Tanton et al.*, 2005), Mercury (*Mouser et al.*, 2021) or the Moon (*Elkins-Tanton*  
780 *et al.*, 2011; *Dygert et al.*, 2017). This process is responsible for the separation  
781 between compatible elements that prefer the solid phase (e.g., Mg, Si) and in-  
782 compatible elements which prefer the liquid phase (e.g., Al, Na, Fe). The solidi-



783 fication depth is governed by the geotherm and the melting curves. With density  
784 profiles of the melt and bridgmanite crystals crossing in the lower mantle, crys-  
785 tal settling could then occur towards neutral buoyancy depths where crystals  
786 are paradoxically more easily entrained by the flow. Both chemical composition  
787 and temperature contribute to the buoyancy of a crystal layer within a convect-  
788 ing reservoir. Hence different scenarios may emerge: Bottom/up solidification  
789 or mid-mantle solidification making a basal magma ocean possible.

790

791 In our study we have shown that the ability of the crystal fraction to sed-  
792 iment or to disperse within the domain is the result of a combination of the  
793 influence of the crystal size, the density difference between the crystals and the  
794 magma and the magma viscosity. We have shown that this ability is a func-  
795 tion of the ratio of the convection over the buoyancy stress (expressed as the  
796  $Sh$  dimensionless number). From a relevant range of parameters we observe  
797 that the critical  $Sh_c$  separating suspension and sedimentation regimes exhibits  
798 values lower than proposed by *Solomatov et al.* (1993). As a consequence, our  
799 results strengthen the idea that suspension mechanism should be the dominant  
800 process during the magma ocean solidification compared to sedimentation and,  
801 as a consequence, equilibrium crystallisation should be favoured compared to  
802 fractional crystallisation.

803

804 In our models, we consider a particule size range ( $10^{-4} - 10^{-2}$  m) and a den-  
805 sity difference range between the magma and the particles ( $10 - 100 \text{ kg.m}^{-3}$ ),  
806 which are probably closer to the relevant MO conditions (see e.g.  $\Delta\rho = -200$  to  
807  $200 \text{ kg/m}^3$  in Fig. 12) than the range of parameters proposed by *Patočka et al.*  
808 (2020) ( $0.5 \times 10^{-3} - 10^{-2}$  m and  $10 - 3000 \text{ kg.m}^{-3}$ ). Moreover, their models  
809 neglect the re-entrainment process by eliminating the particles that reach the

810 bottom of the reservoir. Hence, it is not surprising that their models favour a  
811 rapid crystal settling and a fractional crystallisation. *Patočka et al. (2020)*  
812 identified three settling regimes: "stone-like", bi-linear and "dust-like" regimes  
813 depending on the ratio between the crystal terminal velocity and the average  
814 vertical velocity of the flow. It appears that the models we run mostly fall out  
815 in the "dust-like regime" where the terminal velocity of a particle is smaller  
816 than the average velocity within the convective reservoir. In the "dust-like"  
817 regime the particles from the models developed by *Patočka et al. (2020)* appear  
818 uniformly distributed in the reservoir in agreement with our models.

819

820 We have also considered in our models different end-members for the chem-  
821 ical composition of the early mantle adding or subtracting up to 40% of Bg to a  
822 pyrolite mantle reference. Exploring the early mantle composition within such  
823 a range leads to a wide range of density difference between the molten and the  
824 solid phases. Hence the chemical composition also influences the ability of the  
825 crystals to cumulate at the bottom or in the middle of the magma ocean. Our  
826 models emphasize that (1) Bg grains are unlikely to segregate in a mantle of  
827 pyrolite composition, except in a shallow MO when the grain size may increase  
828 to 1 mm and more, (2) Bg grains are likely to segregate at the bottom of a MO  
829 enriched in SiO<sub>2</sub>, compared to pyrolite and (3) the formation of a basal MO  
830 simultaneous to mantle solidification could be possible for mafic BSE composi-  
831 tions (difficult to reconcile with the Earth's geochemical models). We also note  
832 that a homogeneous bottom-up solidification of the MO is expected to produce  
833 a significant SiO<sub>2</sub> enrichment with increasing mantle depth in a primitive man-  
834 tle (compatible with seismic observations) and a higher SiO<sub>2</sub> content in BSE  
835 compared to pyrolite (compatible with Earth's geochemical models).

836

837 This study is a supplementary step toward a more realistic approach that  
838 should account for several other major processes. In our models we have not  
839 consider the time evolution of the crystal size, of the crystal fraction and of the  
840 density of the crystals during their growth. If crystal settling is likely to occur  
841 close to mechanical boundaries (CMB or solidified wall) where the velocity is  
842 lower than in the middle of the magma ocean ( within "calm" conditions ), future  
843 models should explore parameters compatible with the center of the magma  
844 ocean (i.e. larger Rayleigh numbers). This would imply much higher Reynolds  
845 number and would require to consider the inertial forces and the turbulence  
846 equations in our model. The likeliness of a thick magma ocean and the presence  
847 of a large Moon much closer to the Earth than today should also lead us to  
848 consider te influence of the Coriolis forces (*Solomatov, 2000*).

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854 XXX.

#### 855 **Data availability**

856 The data that support the findings of this study were obtained using the com-  
857 mercial software COMSOL Multiphysics (version 5.4). COMSOL Multiphysics  
858 is a simulation platform that provides fully coupled multiphysics and single-  
859 physics modeling capabilities. COMSOL Multiphysics (version 5.4) has been  
860 previously validated for two phase flow applications (*Qaddah et al. (2019, 2020)*).  
861 To compute our simulations we used the Heat Transfer ([https://www.comsol.com/heat-  
862 transfer-module](https://www.comsol.com/heat-transfer-module)) and Computational Flow Dynamics ([https://www.comsol.com/cfd-  
863 module](https://www.comsol.com/cfd-module)) modules in addition to the main Multiphysics platform ([34](https://www.comsol.com/comsol-</a></p></div><div data-bbox=)

864 multiphysics). All the parameters used in our simulation are listed and described  
865 in the manuscript. The open source software used for data visualisation was  
866 Xmgrace (<https://plasma-gate.weizmann.ac.il/Grace/>). Data obtained can be  
867 downloaded on the following link: <https://drive.uca.fr/d/2f9684aae96c4947b3cf/>

### 868 **Code availability**

869 The software used for this study is the commercial software COMSOL Multi-  
870 physics (version 5.4) previously validated for two phase flow applications (*Qad-*  
871 *dah et al.* (2019, 2020)). A trial version of COMSOL Multiphysics may be  
872 requested (see <https://www.comsol.com>).

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Figure 1: Nusselt number as a function of the Rayleigh number during the phase the first phases where only the thermal convection is considered (no settling of particles). Results from our models are represented with black circles. For comparison, we plot the scaling laws proposed by *Wolstencroft et al. (2009)* and *Turcotte and Schubert (1982)* with blue and green dashed lines respectively. The red dashed line represents the result from a power-law fitting of our numerical results. Corresponding scaling laws are detailed in the legend of the figure.

Figure 2: Schematic representation of the computational domain of our study. Blue material represents the continuous phase (molten silicates) and green material represent the initially mixed continuous and dispersed phases. A close-up view is illustrated in the right panel.

Figure 3: Dispersed fraction averaged along an horizontal profile at the bottom of the computational domain as a function of the mesh size. In these models,  $h = H/10$ ,  $\phi_{d,0} = 0.5$ ,  $\eta_c = 10$  Pa.s and  $\Delta\rho = 30$  kg.m<sup>-3</sup>. The red dashed line represents the asymptotic value at which  $\phi_{d,average}$  is converging for high-resolutions (i.e. small mesh size) models.

Figure 4: Time evolution (from top to bottom) of the dispersed volume concentration (left) and the temperature (right) for the reference case (with  $Ra = 4.4 \times 10^6$  (corresponding to  $\eta_c = 4$  Pa.s),  $\Delta\rho = 50$  kg.m<sup>-3</sup> and  $D_d = 10^{-3}$ m).

Figure 5: Time evolution of the particles concentration in the upper part of the reservoir with  $Ra = 4.4 \times 10^6$  (corresponding to  $\eta_c = 4$  Pa.s) and  $D_d = 10^{-3}$ m. The red line illustrates the case where  $\Delta\rho = 50$  kg.m<sup>-3</sup> and the green line the case where  $\Delta\rho = 100$  kg.m<sup>-3</sup>. Vertical dashed lines illustrate the time when the minimum value of  $e$  is obtained, which is referred in the text as the overturn time.

Figure 6: Time evolution (from top to bottom) of the dispersed volume concentration (left) and the temperature (right) for the case with  $Ra = 4.4 \times 10^6$  (corresponding to  $\eta_c = 4$  Pa.s),  $\Delta\rho = 100$  kg.m<sup>-3</sup> and  $D_d = 10^{-3}$ m.

Figure 7: Time evolution of the particles concentration in the upper part of the reservoir with  $Ra = 4.4 \times 10^6$  (corresponding to  $\eta_c = 4$  Pa.s) and  $\Delta\rho = 50$  kg.m<sup>-3</sup>. The red line illustrates the case with  $D_d = 10^{-3}$ m, the green line the case with  $D_d = 10^{-4}$ m and the blue line the case with  $D_d = 10^{-2}$ m. Vertical dashed lines illustrate the time when the minimum value of  $e$  is obtained, which is referred in the text as the overturn time.

Figure 8: Time evolution of the particles concentration in the upper part of the reservoir with  $\Delta\rho = 50 \text{ kg.m}^{-3}$  and  $D_d = 10^{-3}\text{m}$ . The different color lines illustrate with cases with different viscosities of the continuous phase ranging from 0.1 to 10 Pa.s. Vertical dashed lines illustrate the time when the minimum value of  $e$  is obtained, which is referred in the text as the overturn time. The corresponding values of the overturn times are plotted in Fig. 9. We note we have tested the case with  $\eta_c = 0.1$  Pa.s with two different meshes (a 6 and 8 mm mesh) and the difference between the two curves is not significative.

Figure 9: Overturn timescale as a function of the molten phase viscosity. Black symbols illustrate the results from our numerical models. The dashes lines show the overturn timescale obtained from Eq. 15 (with 1 to 100  $t_{\text{overturn}}$ ). We note we have tested the case with  $\eta_c = 0.4$  Pa.s with two different meshes (a 4 and 8 mm mesh) and the difference between the two timescales is not significative.

Figure 10: Shields number value ( $Sh$ ) as a function of the molten continuous phase viscosity ( $\eta_c$ ) (or  $Ra$  for the top x-axis). Square symbols correspond to the models run in this study (see Tab. 2 for values). Empty black symbols represent cases where the suspension regime is reached. Filled green symbols represent cases where the sedimentation regime is reached. The two regimes are separated by dashed lines (green for  $\eta_c \leq 1$ , blue for  $\eta_c \geq 1$ ) illustrating the critical Shields number ( $Sh_c$ ). Red symbols and dotted lines illustrate the values for the cases represented in Fig. 5, Fig. 7 and Fig. 8 respectively. We calculate the  $Sh$  values considering the combination of Eq. 12, Eq. 13 and the expression  $Nu = 0.14Ra^{0.34}$  obtained from Fig. 1 to compute the heat flow  $F$  within Eq. 16.

Figure 11: Temperature profiles corresponding to (grey thick line) the solidus of the pyrolite mantle (*Pierru et al.*, subm.) and (colored lines) adiabatic gradients of MO for potential surface temperature from 1800 to 2500 K.

Figure 12: Solid-melt density difference ( $\Delta\rho_{MO} = \rho_{Bg} - \rho_{melt}$ ) calculated using the P-V-T equation of state of Bg (*Matas et al.*, 2007) and MO (*Asimow*, 2018), after decomposition in end-members. Calculations are performed for several MO compositions by adding or subtracting a fraction of Bg to a pyrolite-based mantle reference, and for Fe partition coefficient between Bg and MO ( $K(Fe)^{Bg/Melt}$ ) of 0.1 or 0.25. Positive value indicates lighter melt.

Figure 13: Density contrast ratio  $\Delta\rho_{MO}/\Delta\rho_{crit}$  in the MO. Values larger than 1, or smaller than -1, indicate efficient Bg segregation below, or above, a mushy MO, respectively.

Figure 14: Density contrast ratio  $\Delta\rho_{MO}/\Delta\rho_{crit}$  in the MO calculated as a function of the Bg grain size, from 0.1 to 5 mm, for 5 different melt compositions, from pyrolite -40%Bg to pyrolite +40%Bg. Values larger than 1 or lower than -1 indicate efficient Bg segregation below, or above, the mushy MO, respectively.  $\chi_\rho = 0$  is found for  $\Delta\rho_{MO} = 0$  (Fig. 12). It indicates infinite value of  $Sh$  and perfect crystal suspension (Fig. 10). Continuous and dashed lines indicate  $K(Fe)^{Bg/Melt}$  of 0.1 or 0.25, respectively.

Figure 15: Density contrast ratio  $\Delta\rho_{MO}/\Delta\rho_{crit}$  calculated for various surface temperatures (Eq. 19). Thick, intermediate and thin lines correspond to 500, 1000 and 1500 K, respectively. The calculations are also performed for various mantle compositions and  $K(Fe)^{Bg/Melt}$  values.

Figure 16: Chemical profiles obtained in the case of no Bg segregation from the melt. The chemical gradient comes from the solidification of  $\sim 60\%$  of Bg and  $40\%$  of the melt at the bottom of the MO. These profiles assume no mantle mixing once the mantle layers are eventually solidified. "BSE" and "s-MO" are bulk silicate Earth and a shallow MO extending up to 660 km depth, respectively. Here, the BSE composition is adjusted to 80% pyrolite and 20% of Bg.

Table 1: Symbol definitions and values of the physical parameters used in this study.

	Symbol	Value or range
Magma ocean density	$\rho_{c,0}$	3000 kg/m <sup>3</sup>
Crystals density	$\rho_d$	$\rho_{c,0} + \Delta\rho$
Density difference	$\Delta\rho = \rho_d - \rho_c$	5-100 kg/m <sup>3</sup>
Magma ocean viscosity	$\eta_c$	0.1- 10 Pa.s
Crystal diameter	$D_d$	$10^{-4}$ - $10^{-2}$ m
Heat capacity	$C_p$	1000 J.kg <sup>-1</sup> .K <sup>-1</sup>
Thermal conductivity	$k$	5 W.m <sup>-1</sup> .K <sup>-1</sup>
Thermal diffusivity	$\kappa = k/(\rho_{c,0}C_p)$	$1.7 \times 10^{-6}$ m <sup>2</sup> .s <sup>-1</sup>
Thermal expansion coefficient	$\alpha$	$10^{-5}$ K <sup>-1</sup>
Reference temperature	$T_0$	4000 K
Temperature difference	$\Delta T$	100 K

Table 2: Parameters for all performed simulations used in this study. We calculate the  $Sh$  value from Eq. 16 considering the combination of Eq. 12, Eq. 13 and the expression  $Nu = 0.14Ra^{0.34}$  obtained from Fig. 1 to compute the heat flow  $F$ .

	$\eta_c(Pa.s)$	$Ra$	$D_d$ (m)	$\Delta\rho$ (kg/m <sup>3</sup> )	$Sh$
#1	0.1	$1.8 \times 10^8$	$10^{-4}$	5	4.16
#2	0.1	$1.8 \times 10^8$	$10^{-4}$	10	2.08
#3	0.1	$1.8 \times 10^8$	$10^{-4}$	20	1.04
#4	0.1	$1.8 \times 10^8$	$10^{-4}$	30	0.69
#5	0.1	$1.8 \times 10^8$	$10^{-4}$	40	0.52
#6	0.1	$1.8 \times 10^8$	$10^{-4}$	50	0.42
#7	0.1	$1.8 \times 10^8$	$10^{-3}$	5	0.41
#8	0.1	$1.8 \times 10^8$	$10^{-3}$	10	0.2
#9	0.1	$1.8 \times 10^8$	$10^{-3}$	20	0.1
#10	0.1	$1.8 \times 10^8$	$10^{-3}$	30	0.07
#11	0.1	$1.8 \times 10^8$	$10^{-3}$	40	0.052
#12	0.1	$1.8 \times 10^8$	$10^{-3}$	50	0.042
#13	0.1	$1.8 \times 10^8$	$10^{-3}$	80	0.026
#14	0.1	$1.8 \times 10^8$	$10^{-3}$	100	0.02
#15	0.1	$1.8 \times 10^8$	$10^{-2}$	5	0.041
#16	0.1	$1.8 \times 10^8$	$10^{-2}$	10	0.02
#17	0.1	$1.8 \times 10^8$	$10^{-2}$	20	0.01
#18	0.1	$1.8 \times 10^8$	$10^{-2}$	30	0.007
#19	0.2	$9. \times 10^7$	$10^{-3}$	50	0.052
#20	0.2	$9. \times 10^7$	$10^{-3}$	60	0.044
#21	0.4	$4.4 \times 10^7$	$10^{-3}$	5	0.65
#22	0.4	$4.4 \times 10^7$	$10^{-3}$	10	0.33
#23	0.4	$4.4 \times 10^7$	$10^{-3}$	20	0.16
#24	0.4	$4.4 \times 10^7$	$10^{-3}$	30	0.11
#25	0.4	$4.4 \times 10^7$	$10^{-3}$	40	0.082
#26	0.4	$4.4 \times 10^7$	$10^{-3}$	50	0.065
#27	0.7	$3. \times 10^7$	$10^{-3}$	40	0.1
#28	0.7	$3. \times 10^7$	$10^{-3}$	50	0.081
#29	1.	$1.8 \times 10^7$	$10^{-4}$	5	8.9
#30	1.	$1.8 \times 10^7$	$10^{-4}$	10	4.45
#31	1.	$1.8 \times 10^7$	$10^{-4}$	20	2.22
#32	1.	$1.8 \times 10^7$	$10^{-4}$	30	1.48
#33	1.	$1.8 \times 10^7$	$10^{-4}$	40	1.1
#34	1.	$1.8 \times 10^7$	$10^{-4}$	50	0.089
#35	1.	$1.8 \times 10^7$	$10^{-3}$	10	0.44
#36	1.	$1.8 \times 10^7$	$10^{-3}$	20	0.22
#37	1.	$1.8 \times 10^7$	$10^{-3}$	30	0.148



Table 2: Part 2

	$\eta_c(Pa.s)$	$Ra$	$D_d$ (m)	$\Delta\rho$ (kg/m <sup>3</sup> )	$Sh$
#38	1.	$1.8 \times 10^7$	$10^{-3}$	35	0.127
#39	1.	$1.8 \times 10^7$	$10^{-3}$	40	0.111
#40	1.	$1.8 \times 10^7$	$10^{-3}$	50	0.09
#41	1.	$1.8 \times 10^7$	$10^{-3}$	100	0.044
#42	1.	$1.8 \times 10^7$	$10^{-2}$	5	0.089
#43	1.	$1.8 \times 10^7$	$10^{-2}$	10	0.044
#44	1.	$1.8 \times 10^7$	$10^{-2}$	20	0.022
#45	1.	$1.8 \times 10^7$	$10^{-2}$	30	0.015
#46	4.	$4.4 \times 10^6$	$10^{-4}$	50	1.4
#47	4.	$4.4 \times 10^6$	$10^{-3}$	50	0.14
#48	4.	$4.4 \times 10^6$	$10^{-3}$	70	0.1
#49	4.	$4.4 \times 10^6$	$10^{-3}$	80	0.0875
#50	4.	$4.4 \times 10^6$	$10^{-3}$	100	0.07
#51	4.	$4.4 \times 10^6$	$10^{-2}$	50	0.014
#52	10	$1.8 \times 10^6$	$10^{-4}$	5	19
#53	10	$1.8 \times 10^6$	$10^{-4}$	10	9.51
#54	10	$1.8 \times 10^6$	$10^{-4}$	20	4.76
#55	10	$1.8 \times 10^6$	$10^{-4}$	30	3.17
#56	10	$1.8 \times 10^6$	$10^{-4}$	40	2.37
#57	10	$1.8 \times 10^6$	$10^{-4}$	50	1.9
#58	10	$1.8 \times 10^6$	$10^{-4}$	100	0.95
#59	10	$1.8 \times 10^6$	$10^{-3}$	5	1.9
#60	10	$1.8 \times 10^6$	$10^{-3}$	10	0.95
#61	10	$1.8 \times 10^6$	$10^{-3}$	20	0.47
#62	10	$1.8 \times 10^6$	$10^{-3}$	30	0.31
#63	10	$1.8 \times 10^6$	$10^{-3}$	40	0.24
#64	10	$1.8 \times 10^6$	$10^{-3}$	50	0.19
#65	10	$1.8 \times 10^6$	$10^{-3}$	100	0.095
#66	10	$1.8 \times 10^6$	$10^{-2}$	5	0.19
#67	10	$1.8 \times 10^6$	$10^{-2}$	10	0.095
#68	10	$1.8 \times 10^6$	$10^{-2}$	15	0.063
#69	10	$1.8 \times 10^6$	$10^{-2}$	20	0.047
#70	10	$1.8 \times 10^6$	$10^{-2}$	30	0.032
#71	10	$1.8 \times 10^6$	$10^{-2}$	50	0.019
#72	10	$1.8 \times 10^6$	$10^{-2}$	100	0.0095

Figure 1.

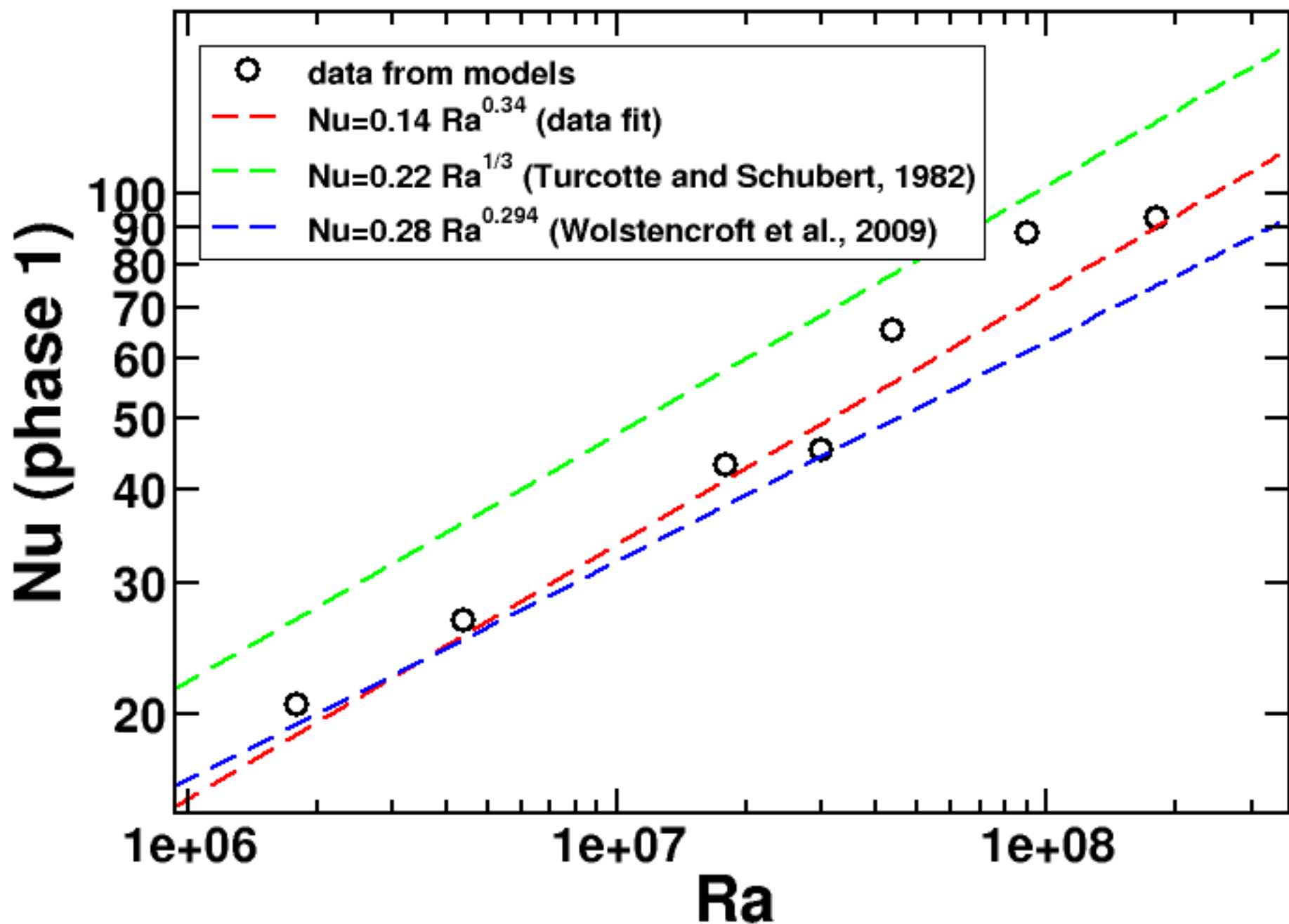


Figure 2.

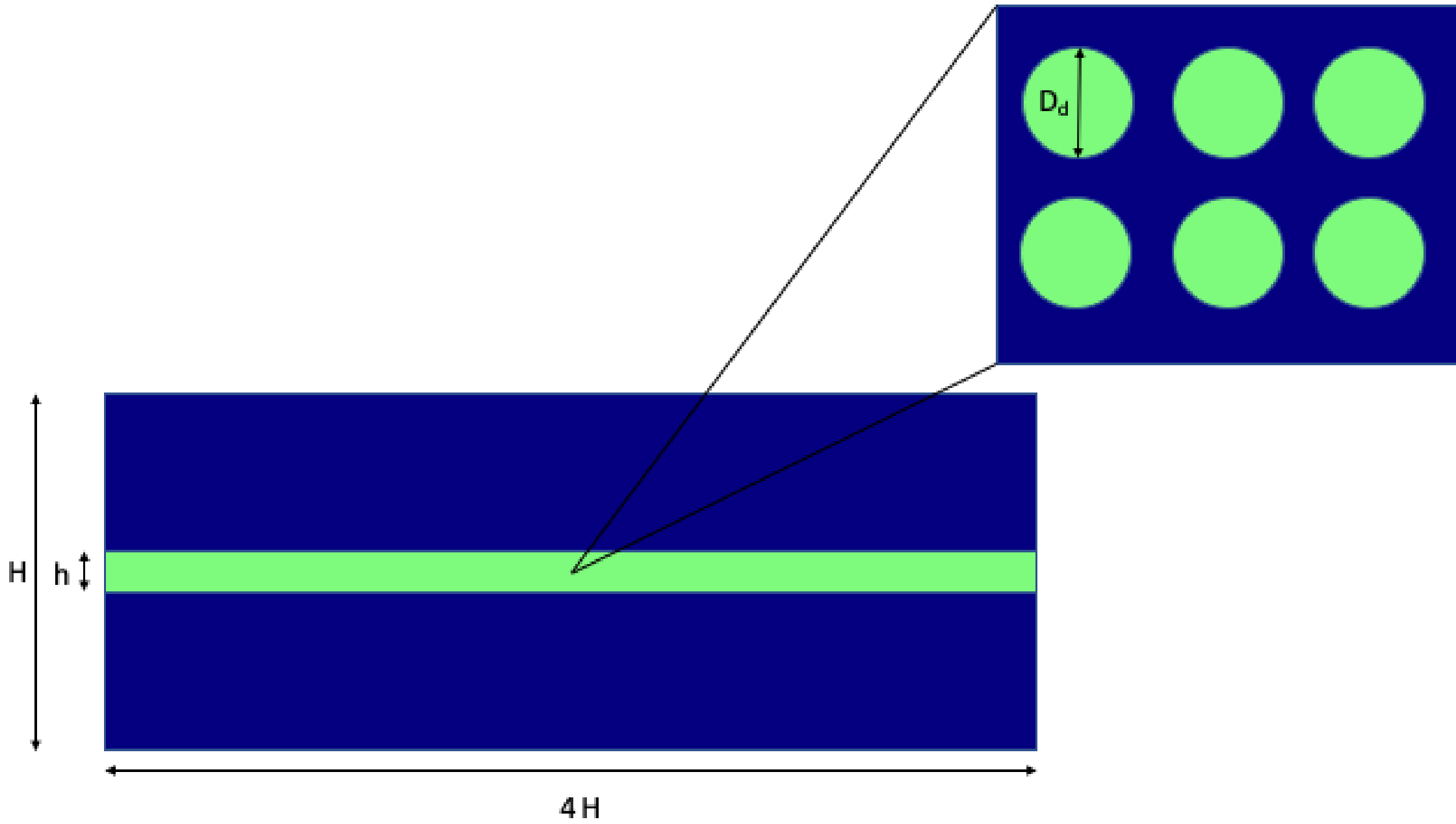


Figure 3.

$\Delta\rho=30 \text{ kg/m}^3$   
 $D_d=10^{-3} \text{ m}$

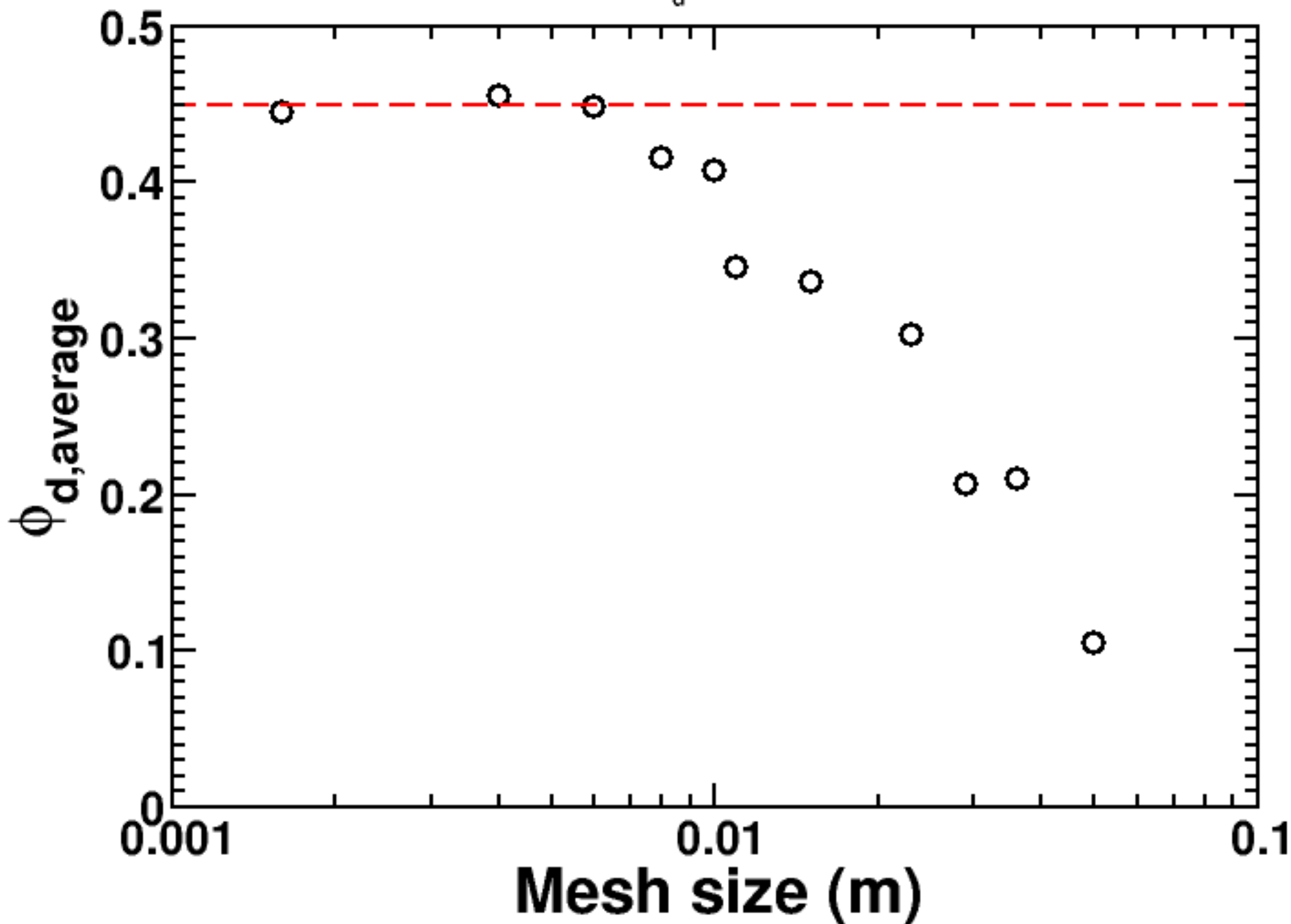


Figure 4.



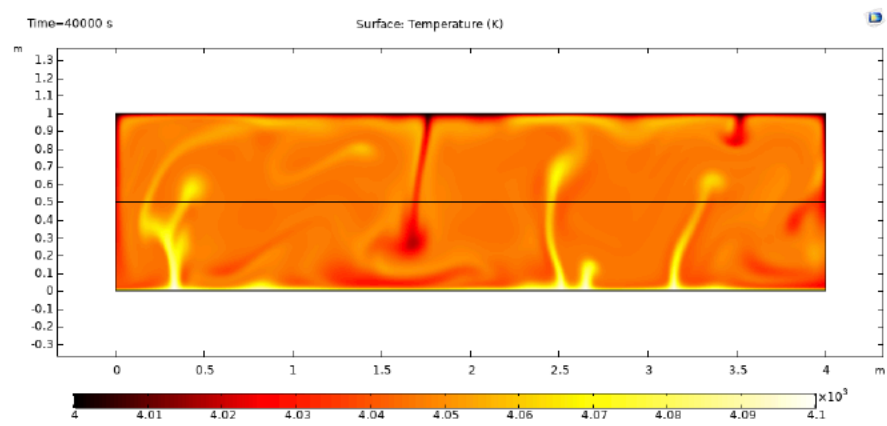
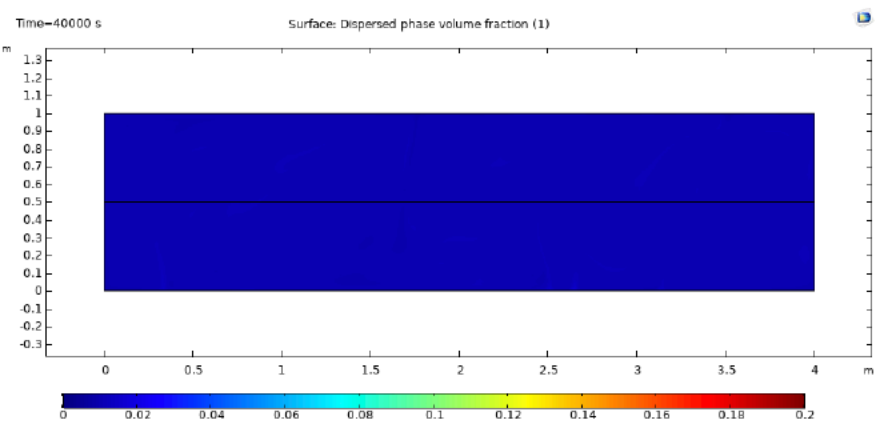
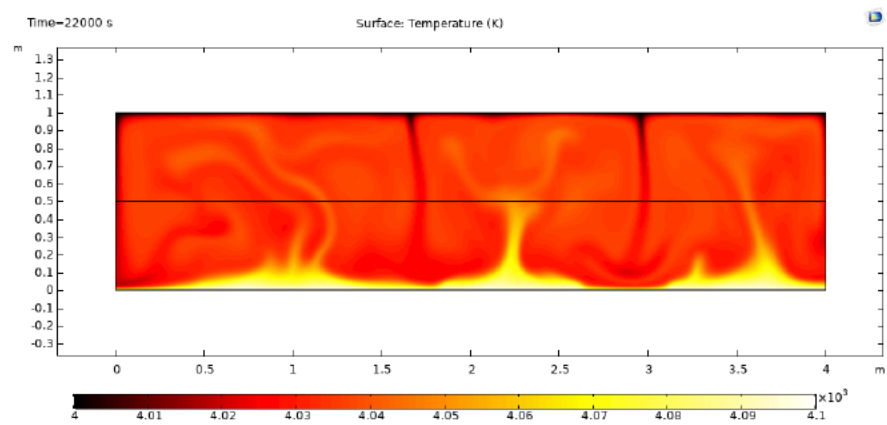
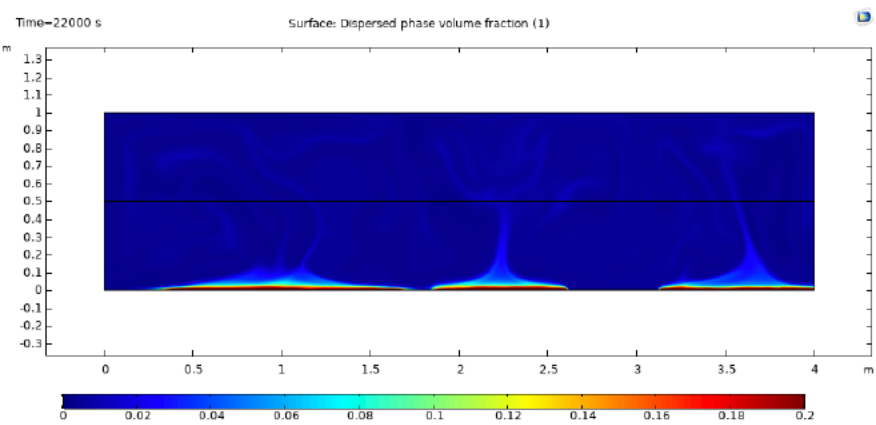
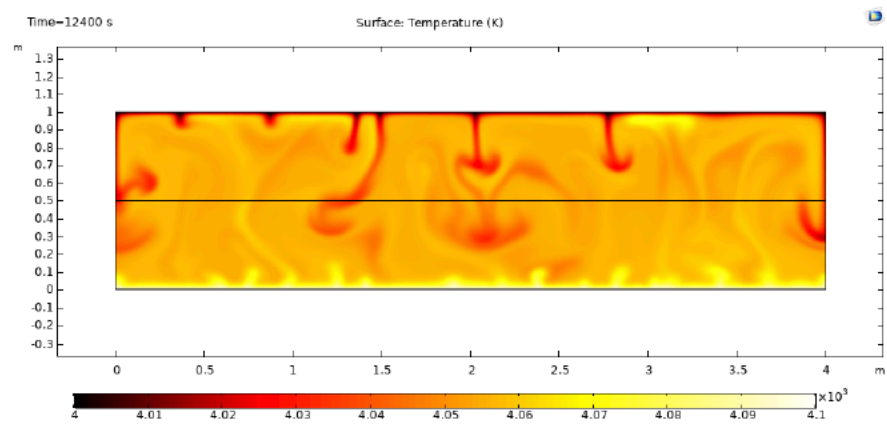
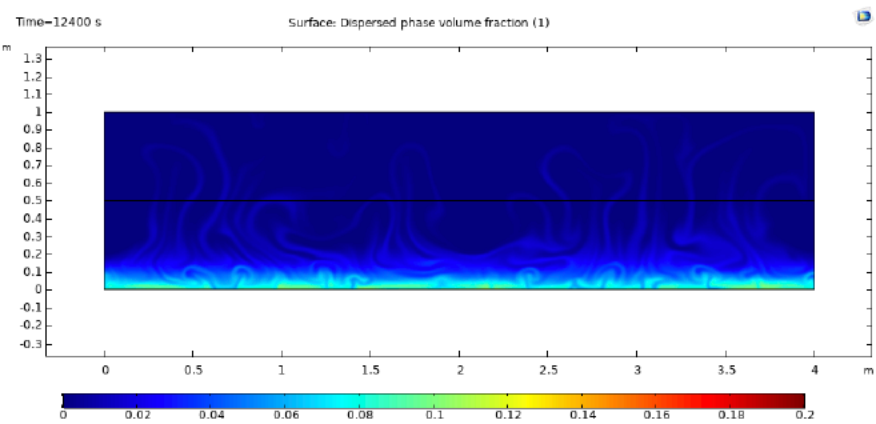
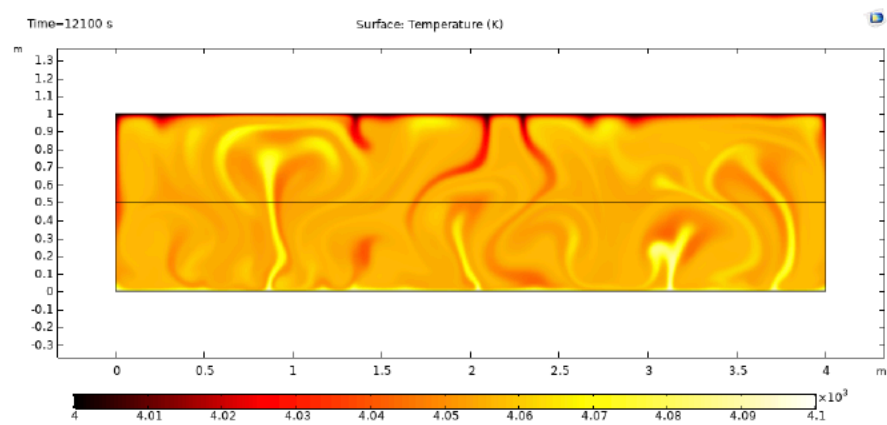
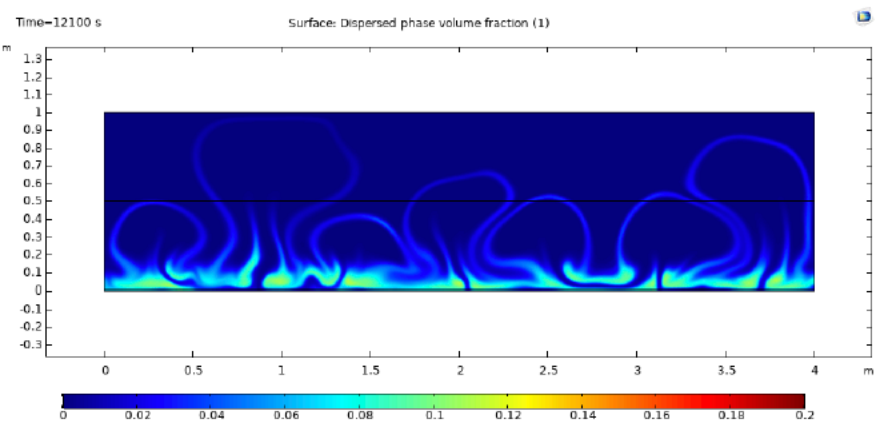
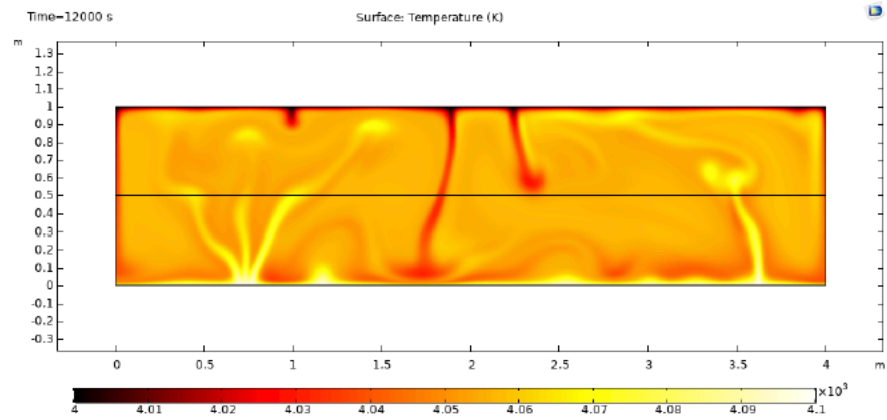
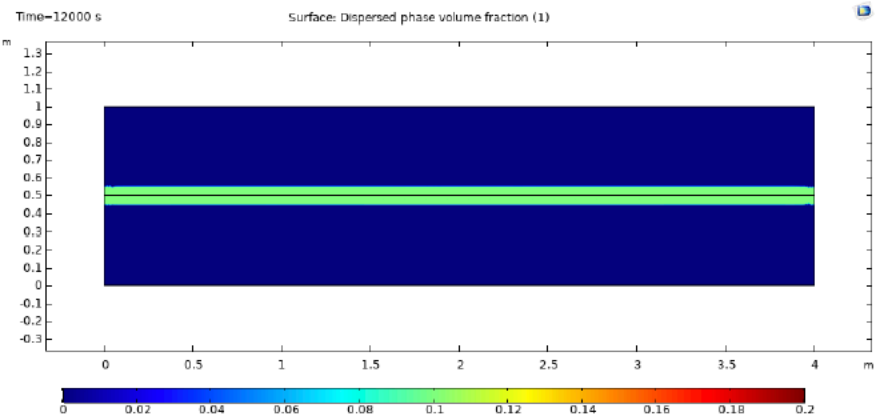


Figure 5.

$\eta_c = 4 \text{ Pa}\cdot\text{s}$

$Dd = 10^{-3} \text{ m}$

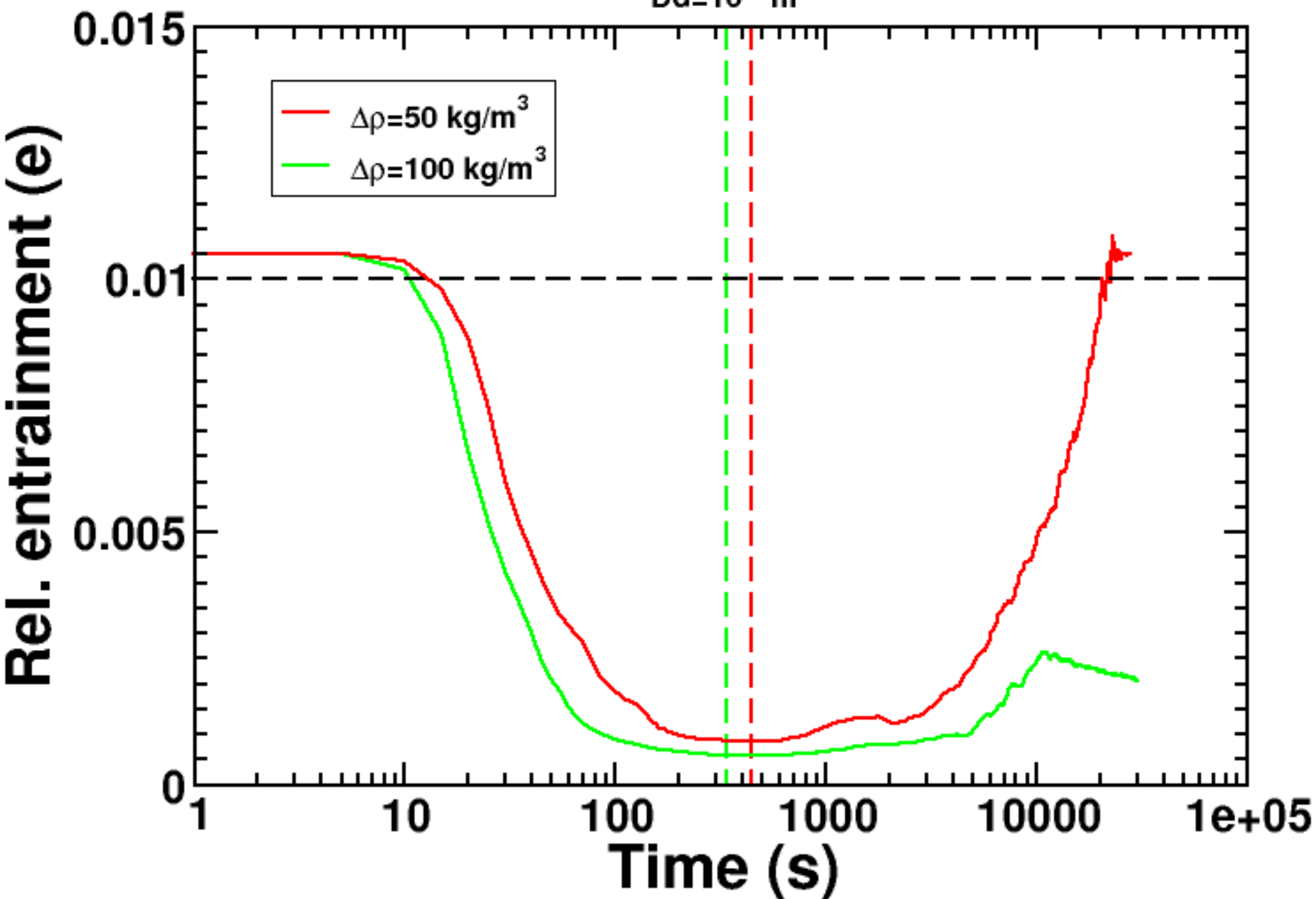


Figure 6.

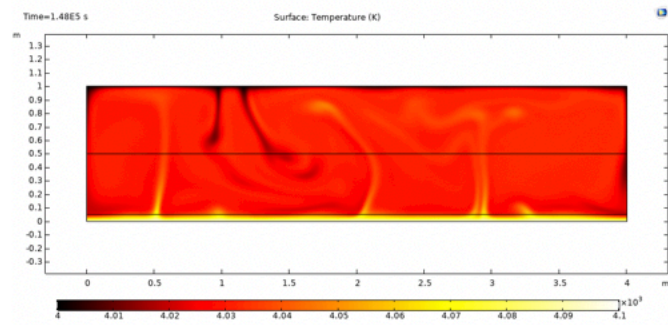
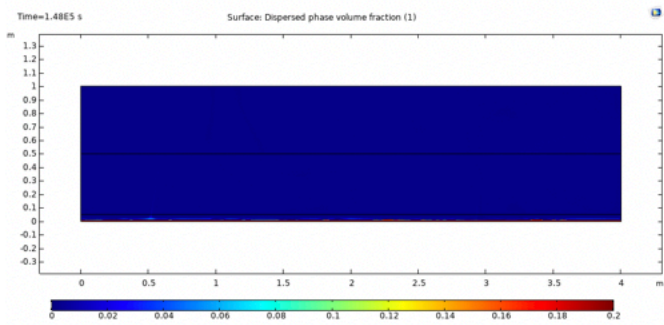
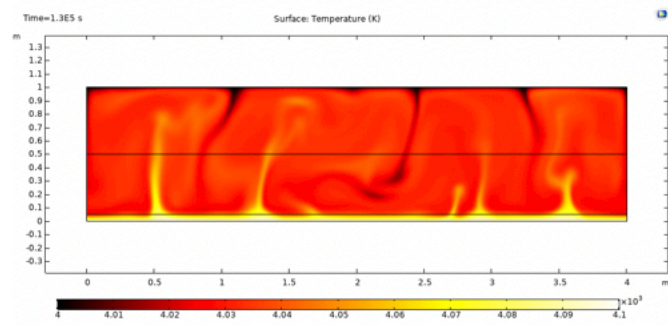
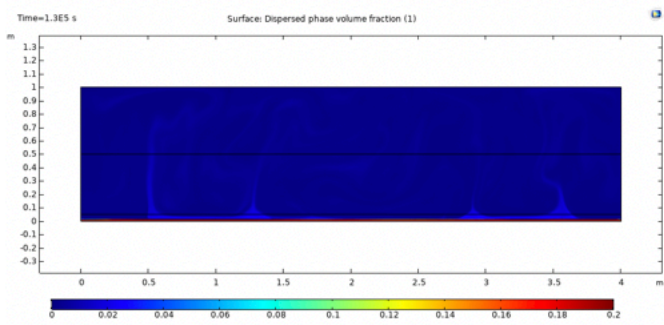
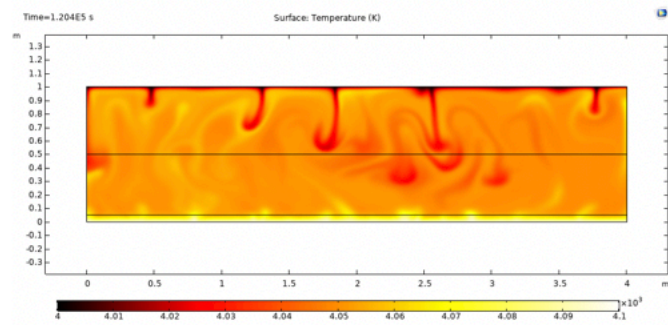
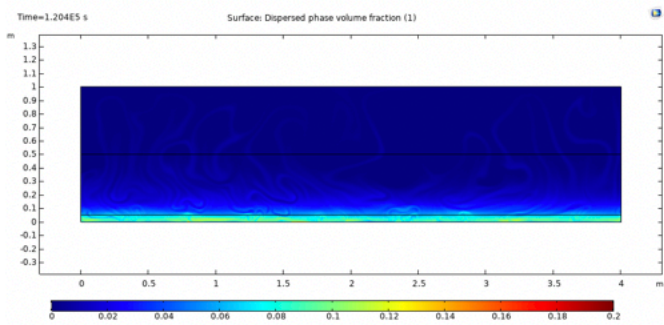
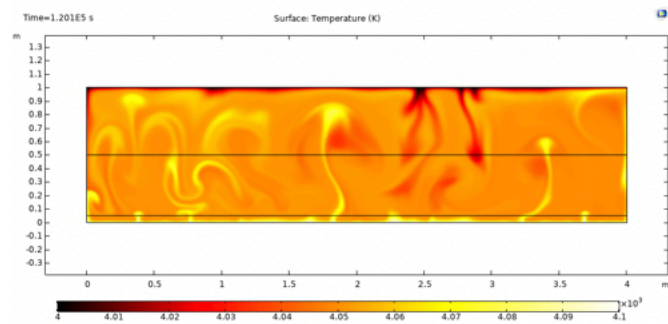
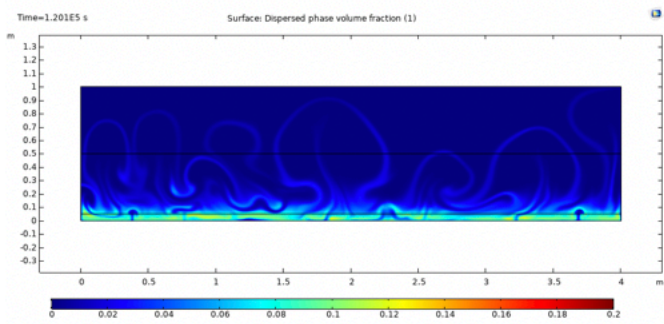
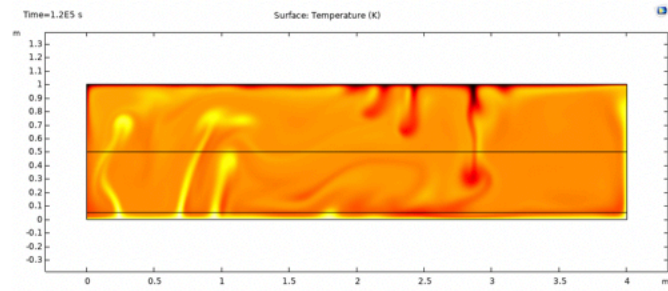
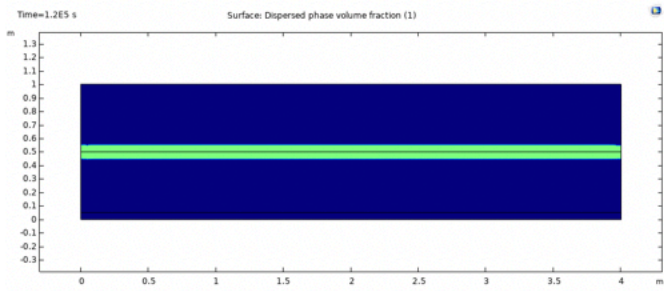


Figure 7.

$\eta_c = 4 \text{ Pa}\cdot\text{s}$

$\Delta\rho = 50 \text{ kg/m}^3$

Rel. entrainment (e)

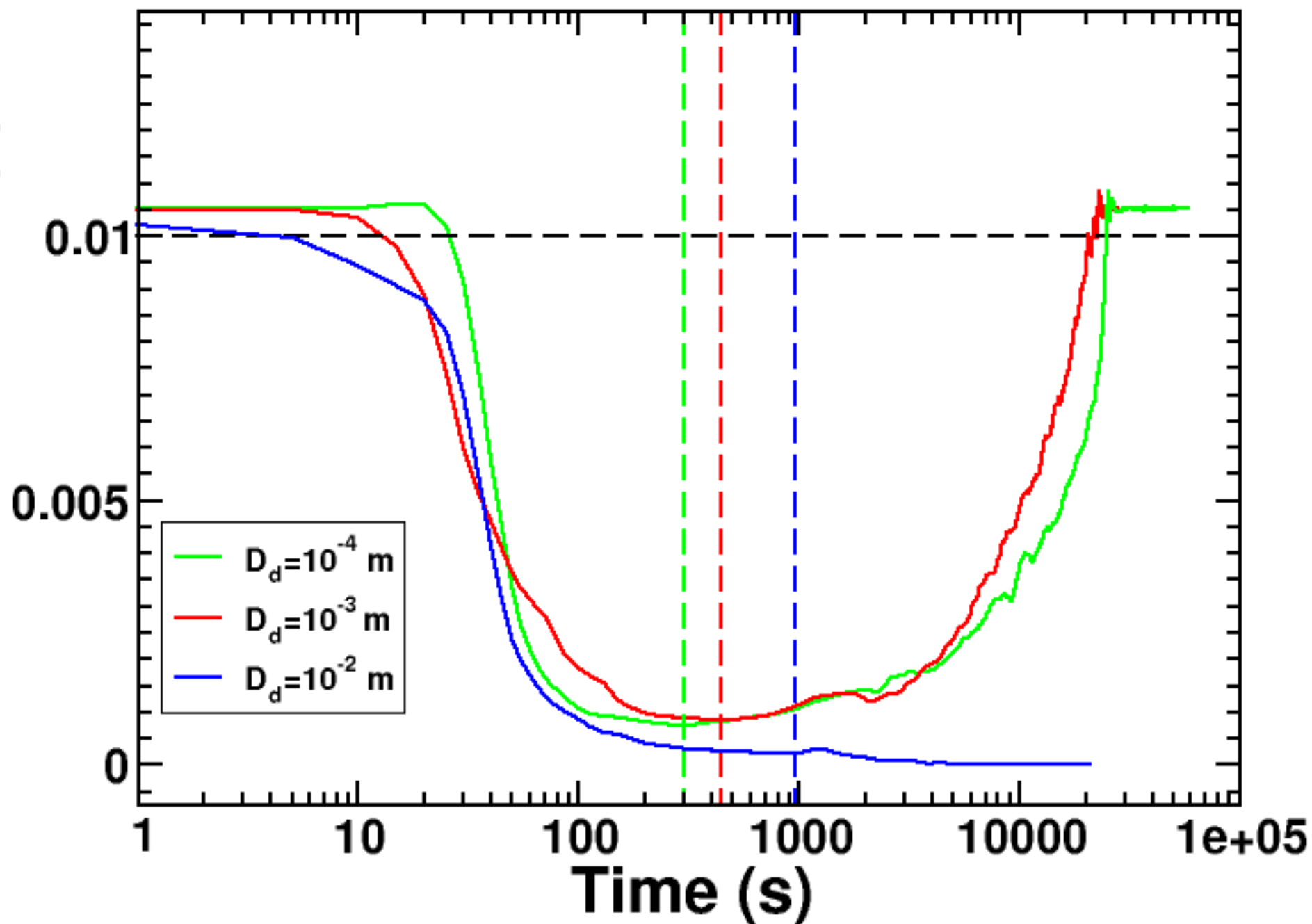


Figure 8.



$$\Delta\rho_c = 50 \text{ kg/m}^3$$
$$D_d = 10^{-3} \text{ m}$$

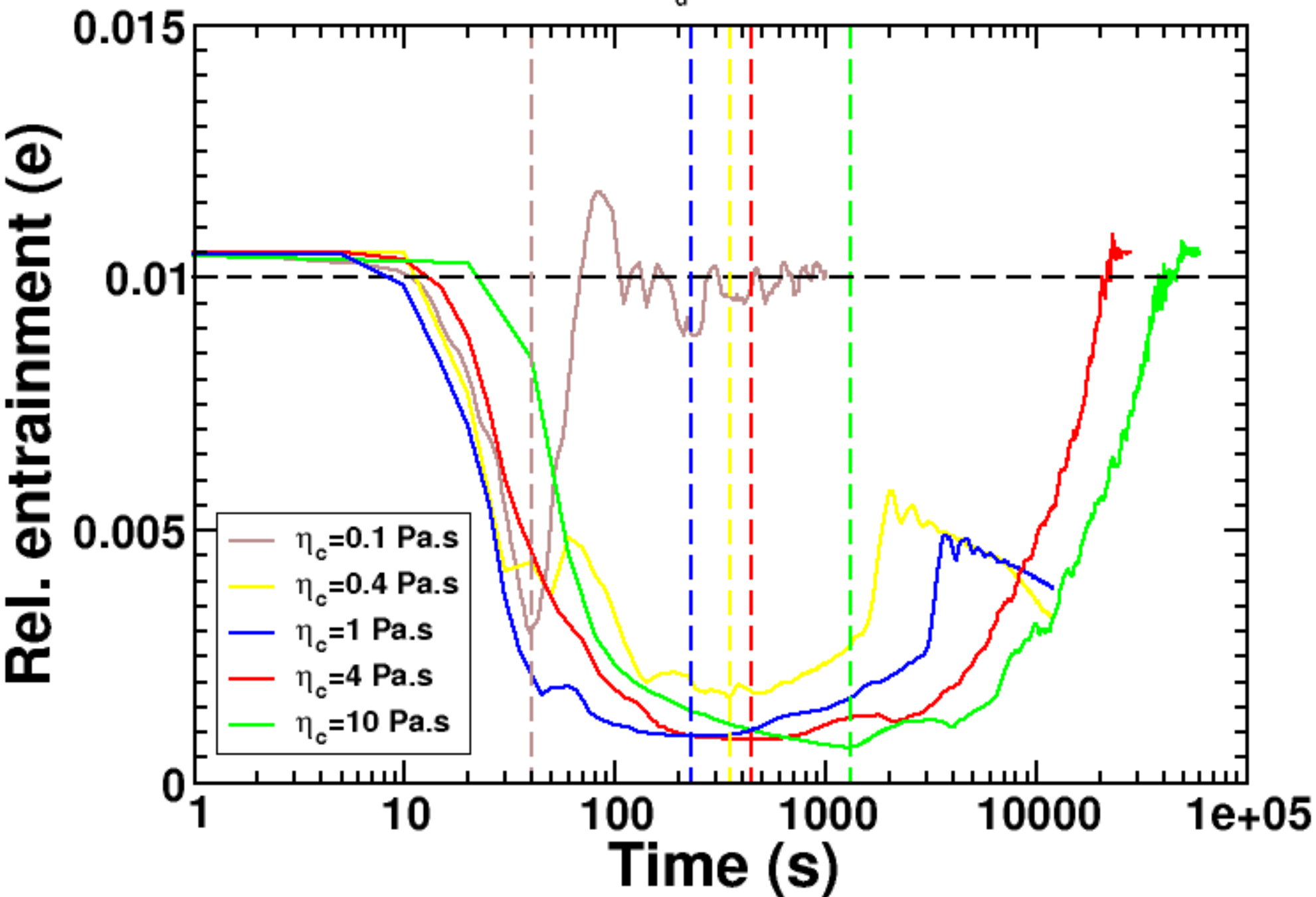


Figure 9.

$$D_d = 10^{-3} \text{ m}$$

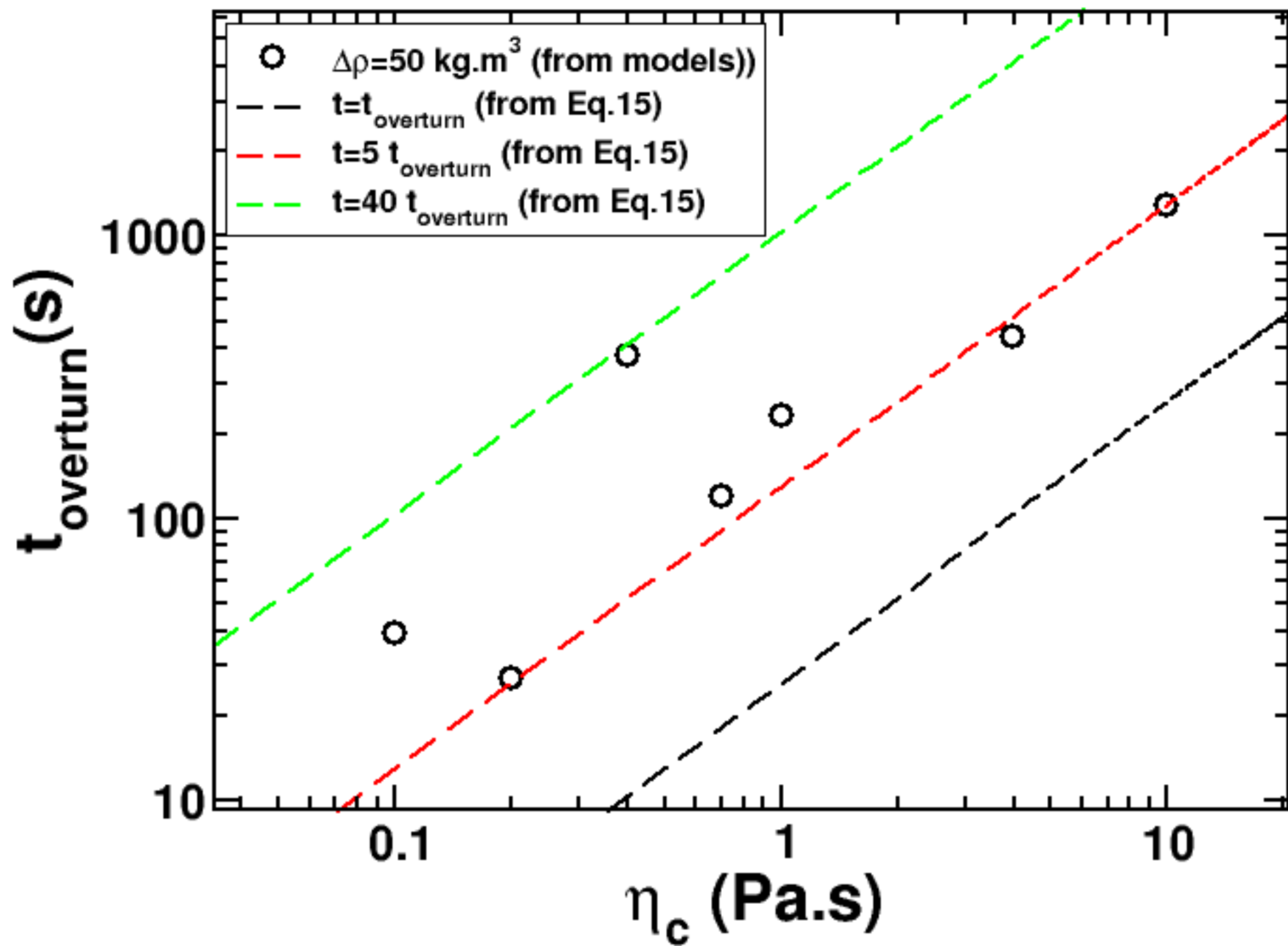


Figure 10.

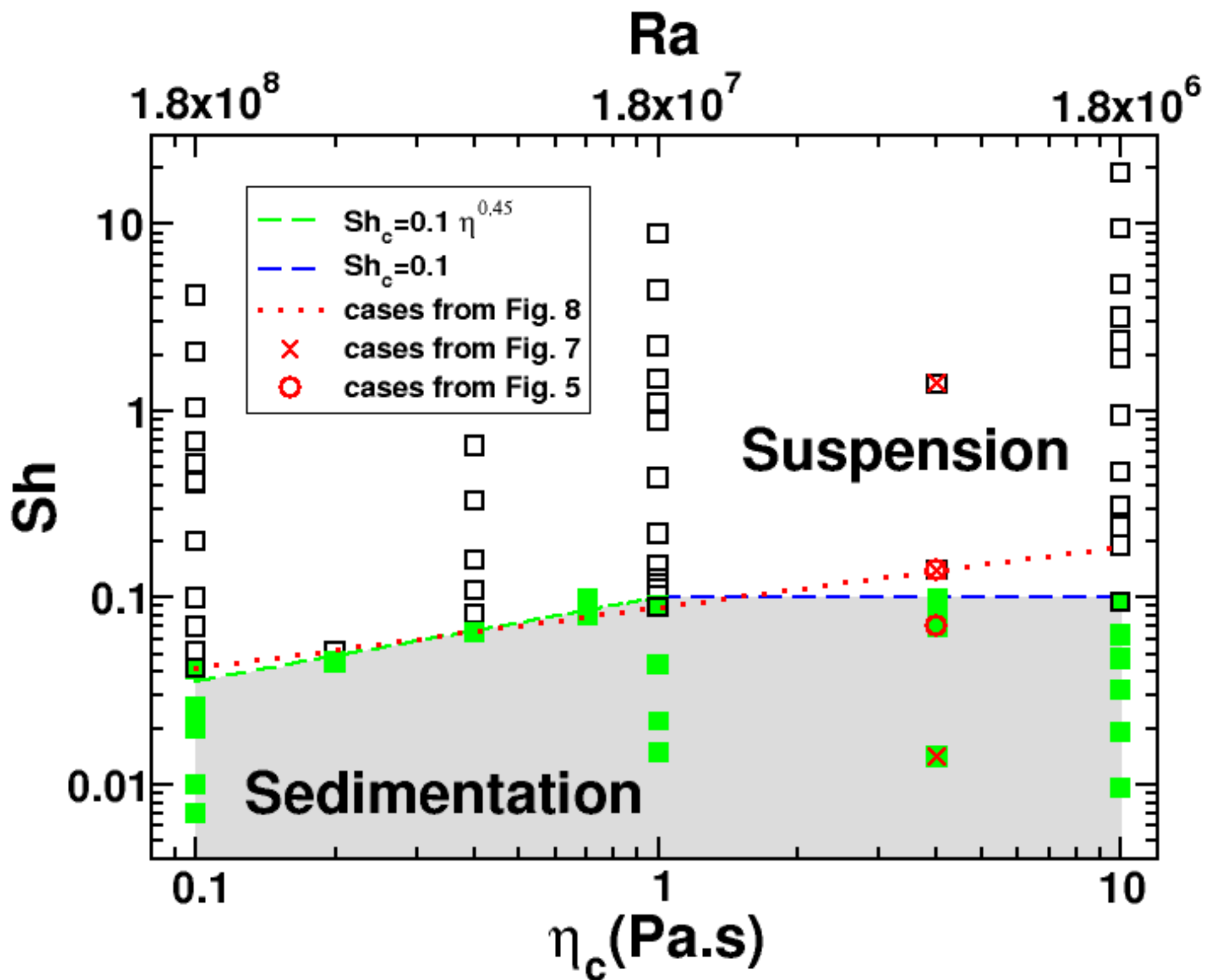


Figure 11.

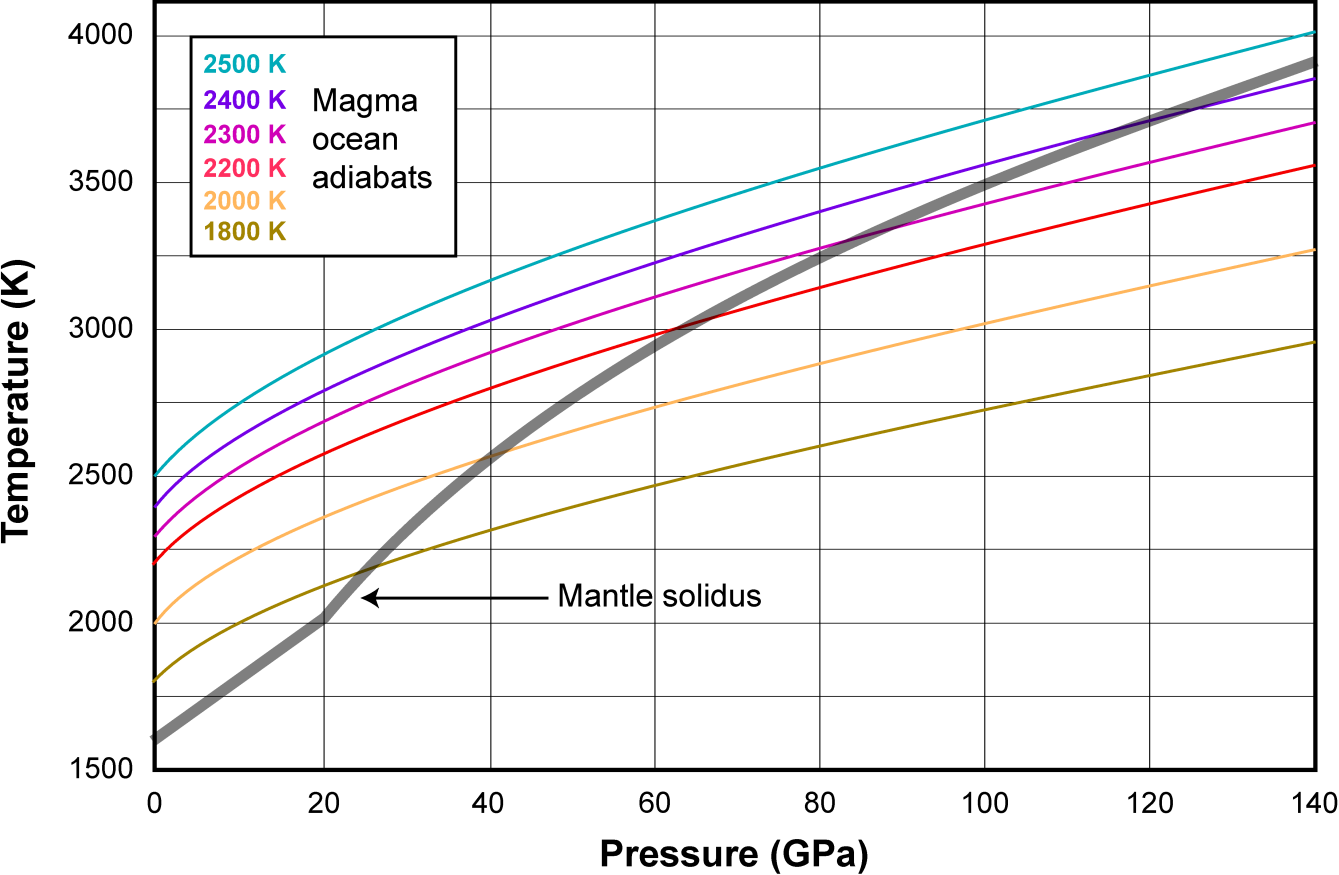


Figure 12.



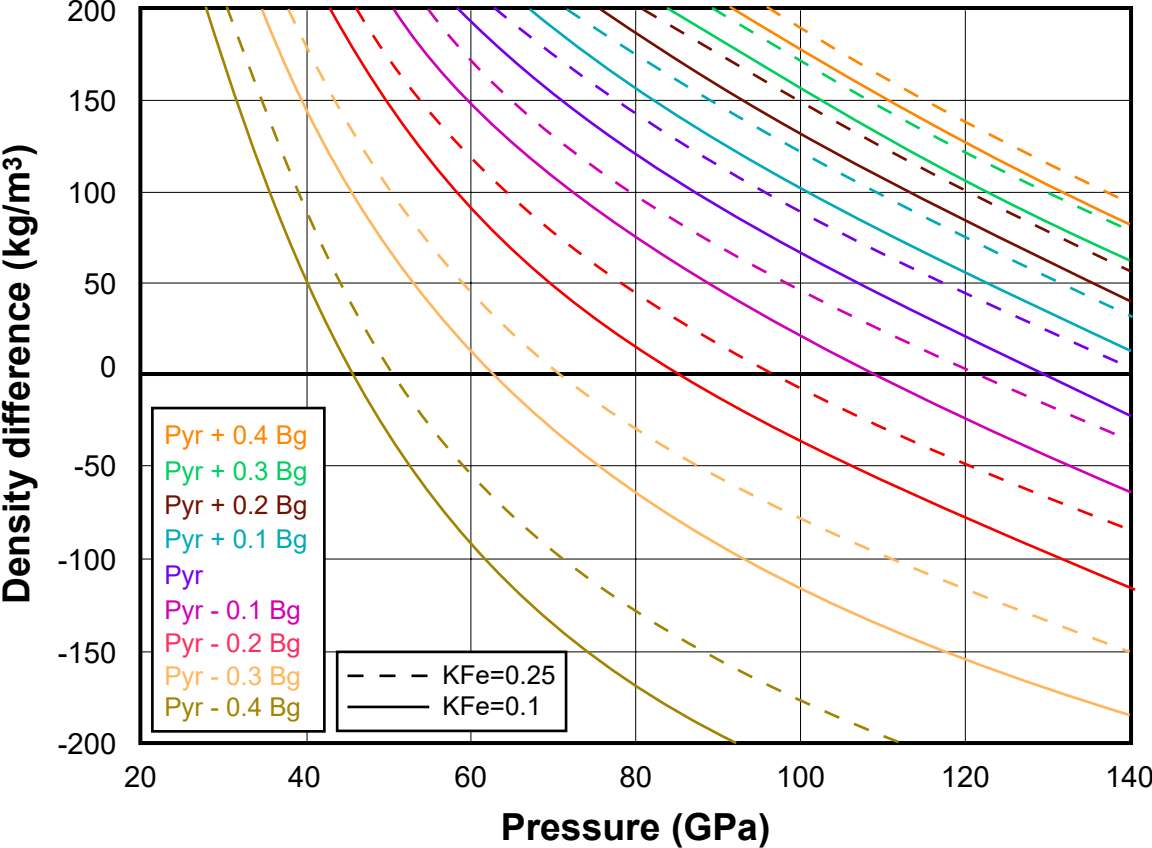


Figure 13.

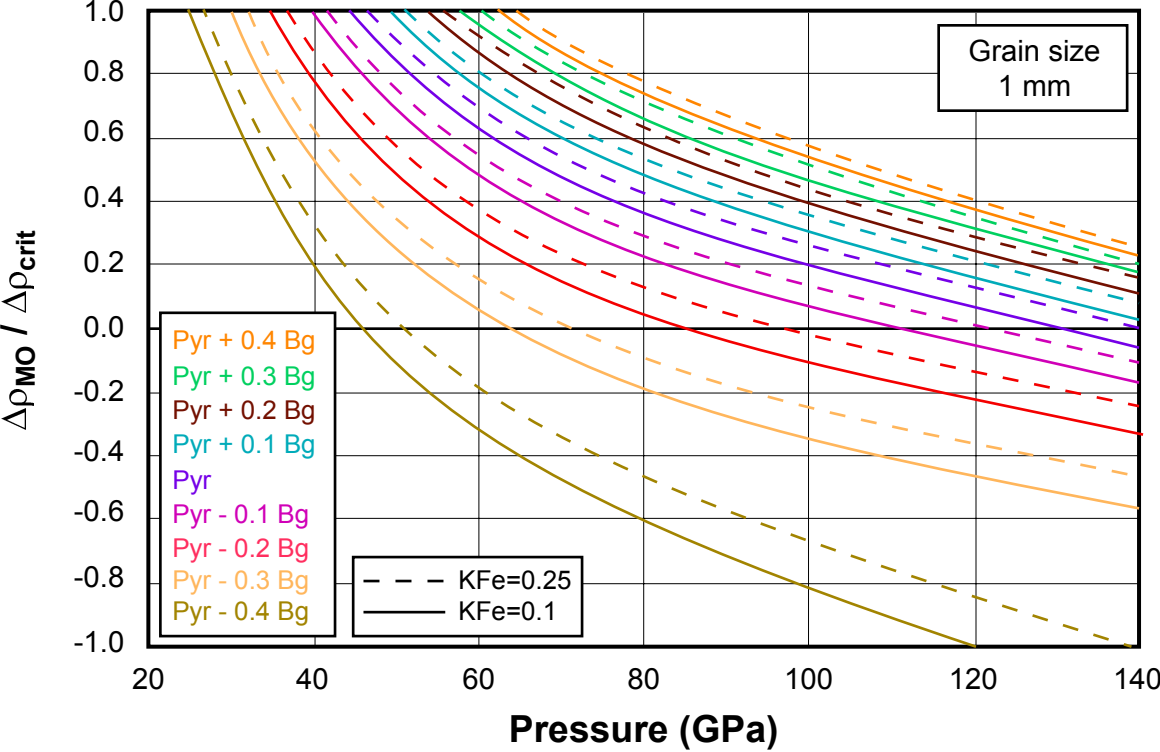


Figure 14.

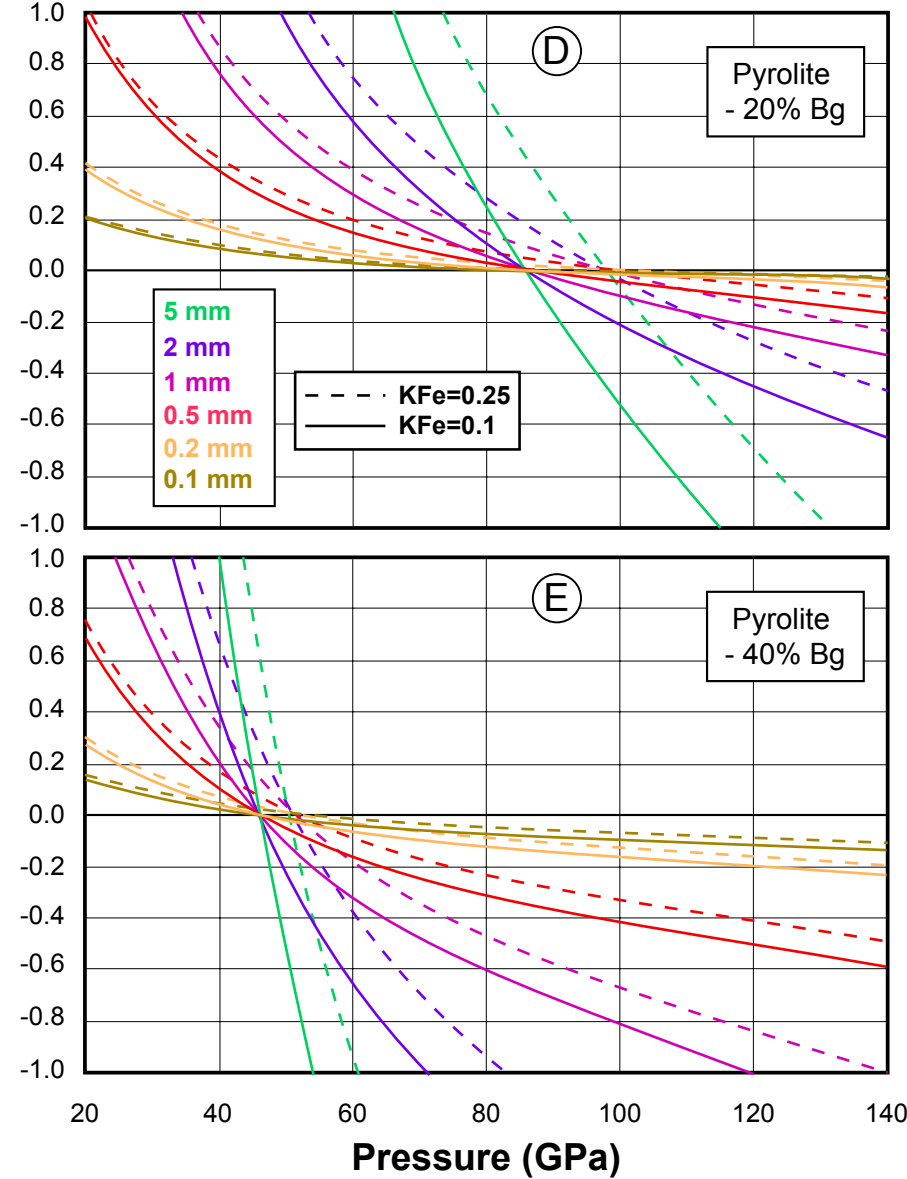
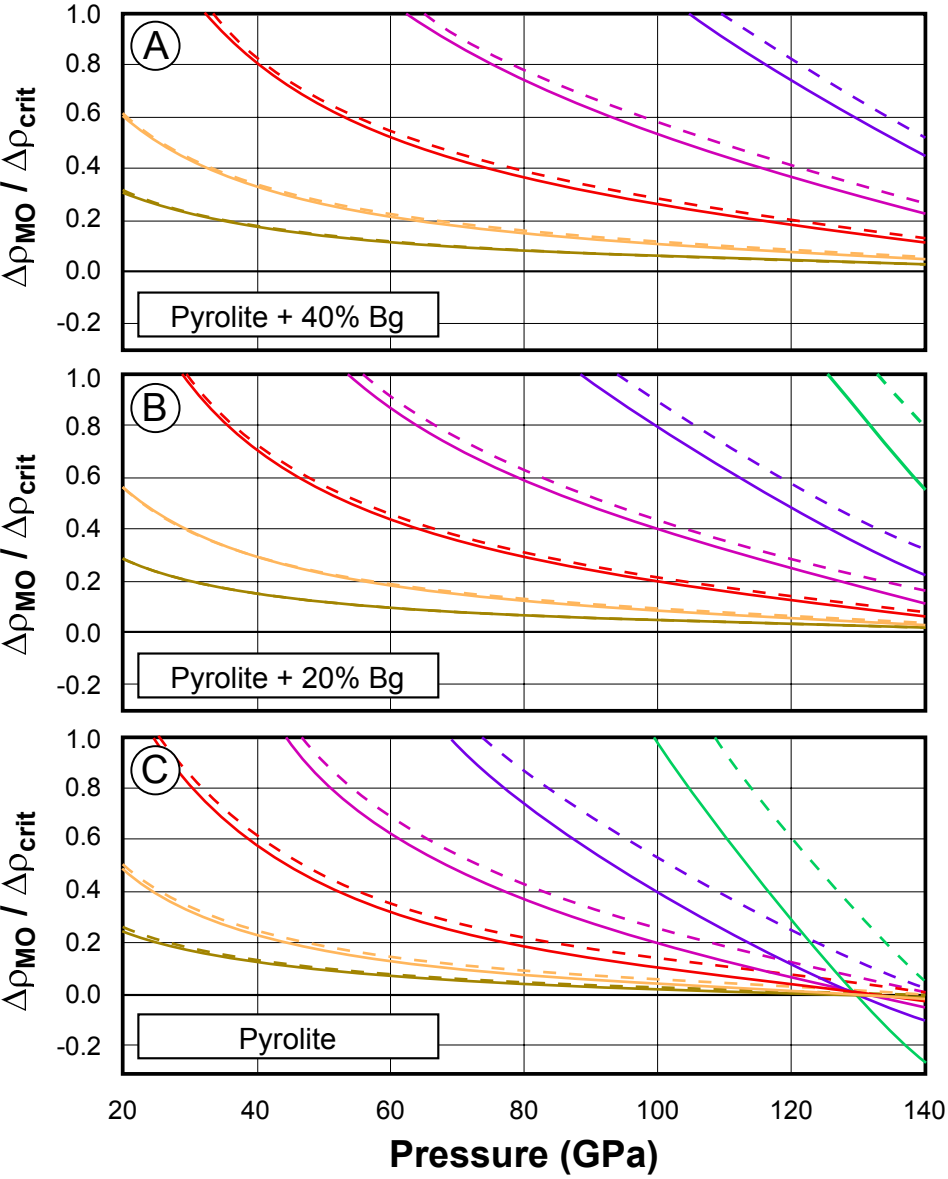


Figure 15.

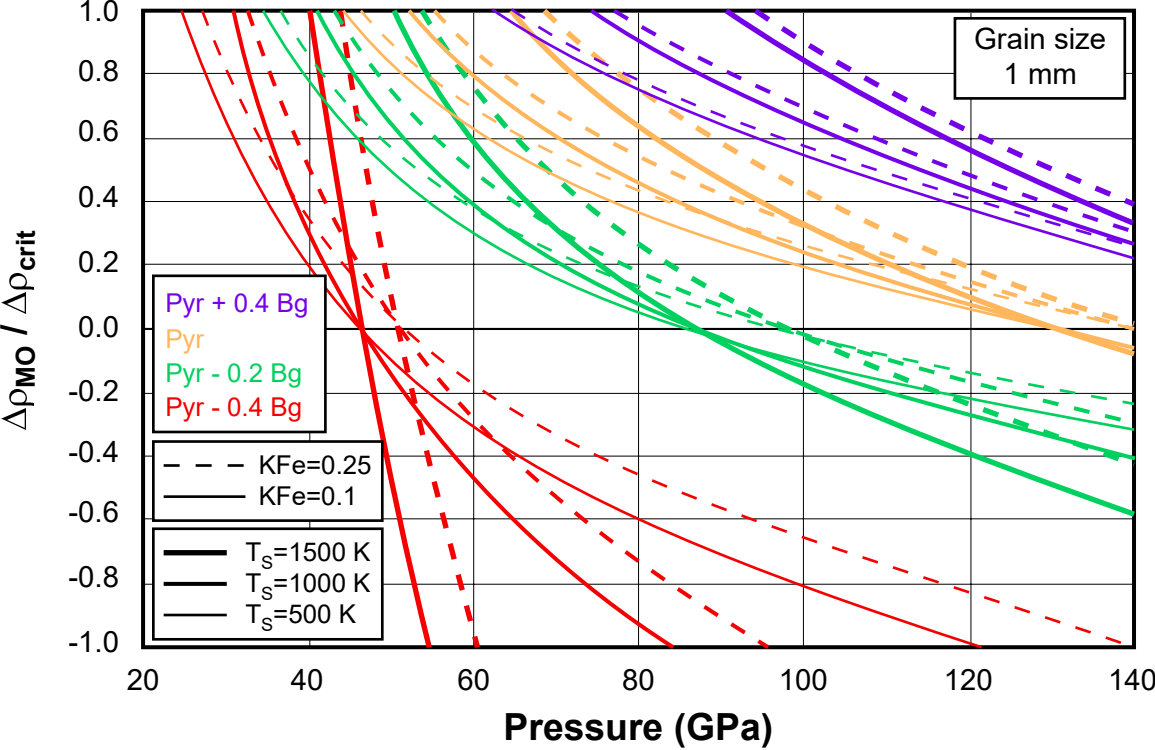


Figure 16.



