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Dynamics and stability of an iron drop falling in a magma ocean

B. Qaddah^{a,b}, J. Monteux^a, V. Clesi^a, M.A. Bouhifd^a, M. Le Bars^b

^a *Université Clermont Auvergne, CNRS, IRD, OPGC, Laboratoire Magmas et Volcans,
F-63000 Clermont-Ferrand, France*

^b *CNRS, Aix Marseille Univ, Centrale Marseille, IRPHE, Marseille, France.
Corresponding author: qaddah@irphe.univ-mrs.fr*

Abstract

The latest stages of planetary accretion involved large impacts between differentiated bodies, hence large scale melting events. Consequently, the iron brought by the impactors sank within a deep magma ocean, before reaching the proto-core. Yet the fluid dynamics of this process remains poorly known. Here, we report numerical simulations of the sinking dynamics of an initially spherical liquid iron drop within a molten silicate phase, up to its possible fragmentation. We consider a 2D cylindrical axisymmetric geometry. We vary the viscosity of the molten silicates in the range of 0.05 Pa.s to 100 Pa.s and the initial radius of the iron drop in the range of 1mm to 350 mm. Hence, we investigate Reynolds number in the range of [0.027 - 85600] and Weber number in the range of [0.073 - 7480]. Our numerical model constrains the morphology, dynamics and stability of the iron drop as a function of the dimensionless Weber and Reynolds numbers as well as of the viscosity ratio between the molten silicates and the liquid iron drop. In particular, we show that the maximal stable drop radius and the critical Weber number are monotonically increasing functions of the magma ocean viscosity. The momentum boundary layer thickness depends mainly on the drop radius and slightly on the magma ocean viscosity. Increasing the viscosity of the silicate phase prevents oscillations of the iron phase and limits the exchange surface. Oppositely, increasing the initial radius of the iron drop enhances its

28 deformation and increases its relative exchange surface. Above the critical We-
29 ber number, we confirm that the fragmentation of the liquid iron occurs within
30 a falling distance equal to 3.5-8 times the drop initial radius in the explored
31 range of moderate Weber number, and we describe a variety of fragmentation
32 regimes. Consequences for Earth's formation models are briefly assessed.

33 *Keywords:* Core formation, fluid dynamics, numerical modeling, metal drop,
34 magma ocean.

35 **1. Introduction**

36 The Earth core formation is a complex process which remains actively de-
37 bated theoretically, experimentally, and numerically (e.g. Stevenson, 1990; Tonks
38 and Melosh, 1992; Chambers, 2004; O'Brien et al., 2006; Wood et al., 2006;
39 Morbidelli et al., 2012; Deguen et al., 2014; Wacheul et al., 2014; Bouhifd et al.,
40 2017). The core formation is highly dependent on accretion as both processes
41 are contemporaneous (Kleine et al., 2002; Touboul et al., 2007). In the latest
42 stages of planetary accretion, giant impacts have occurred [Fig. 1], leading for
43 instance to the formation of the Moon following the collision between a large
44 differentiated body of Mars size and the proto-Earth (Hartmann and Davis,
45 1975). The enormous amount of kinetic energy brought in by these collisions
46 (Tonks and Melosh, 1992; Monteux et al., 2007; Samuel, 2012), the decay of
47 short-lived radio-elements (^{26}Al and ^{60}Fe) causing radioactive heating (Walter
48 and Tronnes, 2004), and the heat dissipation from the conversion of potential
49 energy (Monteux et al., 2009; Samuel, 2012) probably led to the formation of
50 deep magma oceans (Tonks and Melosh, 1992). Following the impact, the liquid
51 iron from the impactor core spread and then sank into this less dense magma
52 ocean as an immiscible fluid, leading to thermo-chemical exchanges between the
53 two phases, before merging with the proto-core. This dynamical process may
54 involve deformation of the initial drops coming from the primary breakup at

55 impact, and possibly their breakup into even smaller droplets [Fig. 1] (Samuel,
56 2012).

57 Three scenarios have been proposed to characterise the motion of liquid iron
58 within the magma ocean and the thermo-chemical equilibration between the two
59 phases. In the first scenario, i.e. the so-called iron rain model (Stevenson, 1990;
60 Karato and Murthy, 1997; Rubie et al., 2003), it is suggested that an impactor's
61 core with a diameter of [10 – 100] km immediately fragments into small droplets
62 with a single characteristic diameter of the order of 1cm, corresponding to the
63 capillary size. All droplets descend independently towards the bottom of the
64 magma ocean at the same velocity and without any further change in shape,
65 leading to an efficient chemical equilibration at a distance of less than 200m
66 within the magma ocean. In contrast, Dahl and Stevenson (2010) proposed a
67 theoretical model where the large liquid iron impactor's core does not break
68 up into the magma ocean if its initial size is large enough; it is only eroded
69 by Rayleigh-Taylor and Kelvin-Helmholtz instabilities. Such a core formation
70 episode would be far from thermo-chemical equilibrium between the impactor's
71 core and the magma ocean. More recently, Deguen et al. (2011, 2014) used
72 fluid dynamics experiments to show that a large core always breaks and forms
73 a cloud of droplets with different sizes. But before doing so, it first evolves from
74 its initial state as a turbulent thermal with strong entrainment and mixing,
75 leading to rapid equilibration even before fragmentation.

76 In these previous studies, the influence of the viscosity ratio between the
77 molten silicates and the liquid iron is neglected. Wacheul et al. (2014) developed
78 analog experiments using gallium to mimic the liquid iron and a mixture of
79 water and glycerol to mimic molten silicates. They found that the value of the
80 viscosity ratio is very important and changes significantly the flow morphology.
81 Later on, Wacheul and Le Bars (2018) validated the turbulent thermal model

82 proposed by Deguen et al. (2014) using global temperature measurements of
83 the liquid metal equilibration. However, numerous questions remain regarding
84 the local dynamics at the scale of one drop, including: What is the maximum
85 stable size of a drop as a function of the viscosity ratio? How is the exchange
86 surface between iron drops and molten silicates influenced by the viscosity ratio?
87 What is the size of the dynamical boundary layer across which the thermal and
88 chemical exchanges occur? Answering those questions is fundamental for a
89 better estimate of the equilibration length in planets, hence for relevant models
90 of planet initial thermochemical state.

91 Several works have already investigated the dynamics of a buoyant bubble
92 or drop in a viscous environment. For instance, a seminal experimental study
93 of rising bubbles of hydrogen in aqueous sugar solutions is reported by Bhaga
94 and Weber (1981) to determine the shape of the bubble, its terminal velocity,
95 the geometry of its wake, and the flow streamline around it. Several experimen-
96 tal investigations of drop breakup in gas-liquid and liquid-liquid systems are
97 reviewed by Pilch and Erdman (1987). An axisymmetric numerical model of a
98 secondary breakup of a spherical liquid drop falling from rest due to gravity in
99 another immiscible liquid is presented in Han and Tryggvason (1999) for dif-
100 ferent density and viscosity ratios, showing large drop deformation and various
101 breakup modes. Another axisymmetric numerical investigation of the evolution
102 of a large bubble rising by buoyancy in the presence of both capillary and vis-
103 cous effects was carried out by Bonometti and Magnaudet (2006), in particular
104 to determine the transition from a spherical cap to a toroidal shape. The influ-
105 ence of viscosity and density ratios is investigated systematically by Ohta et al.
106 (2009, 2010, 2014); Ohta and Sussman (2012). Finally, the first systematics on
107 the asymmetric motion and the fragmentation modes of a bubble of gas rising in
108 a liquid using three-dimensional numerical simulations are reported in Tripathi

109 et al. (2015). However, previous works on the effects of viscosity contrast were
110 motivated by industrial applications mainly, apart from 2 cases in Ichikawa
111 et al. (2010) exploring the relative dynamical changes for viscosity ratios 0.1
112 and 10 between iron and a magma ocean. In the context of the core formation,
113 the viscosity of the magma ocean strongly depends on its evolving temperature
114 and pressure (Karki and Stixrude, 2010). Hence, the viscosity contrast between
115 the metallic and silicate phases can differ by several orders of magnitude. We
116 thus propose here to constrain the influence of the viscosity contrast between
117 the metallic phase and the magma ocean focusing on the sinking of an unique
118 iron droplet. We also investigate the influence of the droplet radius and derive
119 scaling laws to characterise this fluid dynamics.

120 The study is organised as follows. Section 2 introduces the physical and nu-
121 merical model, including the governing equations, the relevant non-dimensional
122 parameters, the numerical model description, and our computational domain
123 and mesh. Section 3 then presents our main numerical results including sys-
124 tematic studies of the drag coefficient, fragmentation modes, characteristic time
125 and distance before breakup, and maximum stable radius before breakup. In
126 Section 4, we discuss possible planetary applications, focusing on the poten-
127 tial efficiency of thermo-chemical exchanges around the drop which depends on
128 the boundary layer thickness and the exchange surface between iron drop and
129 molten silicates. Conclusions and future works are detailed in the final Section
130 5.

131 **2. Physical and numerical model**

132 *2.1. Governing equations*

133 We consider the sinking dynamics of an initially spherical iron drop, falling
134 in a less dense and more viscous fluid under the action of gravity. We assume

135 that both the liquid iron drop and the surrounding molten silicates behave as
 136 Newtonian, incompressible, and immiscible fluids with uniform surface tension,
 137 and constant density and viscosity within each fluid. We note here that we do
 138 not consider the thermo-chemical exchanges that may occur between the two
 139 phases. This point will be the subject of a separated study. Hence, the fluid
 140 dynamics is governed by the Navier-Stokes equations to characterize:

141 1. the conservation of mass

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

142 2. the conservation of momentum

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \cdot [-P\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \rho \mathbf{g} + \mathbf{F}_{st} \quad (2)$$

143 with \mathbf{u} the fluid velocity vector (m/s), ρ the fluid density (kg/m³), μ
 144 the fluid viscosity (Pa.s), t the time (s), P the fluid pressure (Pa), \mathbf{g} the
 145 gravitational acceleration (m/s²), \mathbf{F}_{st} the surface tension force (N/m³)
 146 and \mathbf{I} the identity matrix.

147 We monitor the interface between the liquid iron drop and the molten sili-
 148 cates using the Level Set method, an Eulerian and implicit method frequently
 149 used in multiphase flow problems (e.g. Luo et al., 2006). It consists in defining
 150 a level set function ϕ , equal to 1 in iron and 0 in the surrounding silicates, and
 151 rapidly changing through the interface, whose position is determined by the
 152 isocontour $\phi = 0.5$. The equation governing the transport and reinitialization
 153 of ϕ is :

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left[\epsilon \nabla \phi - \phi(1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right] \quad (3)$$

154 with γ (m/s) and ϵ (m) the reinitialization parameters. ϵ determines the thick-

155 ness of the layer around the interface, and is typically chosen equal to half the
 156 size of the characteristic mesh in the region explored by the interface. γ de-
 157 termines the amount of reinitialization: a suitable value for γ is the maximum
 158 velocity magnitude experienced in the model.

159 The density and dynamical viscosity are evaluated using the level set func-
 160 tion:

$$\rho = \rho_s + (\rho_d - \rho_s)\phi \quad (4)$$

161

$$\mu = \mu_s + (\mu_d - \mu_s)\phi \quad (5)$$

162 where subscripts “s” and “d” stand for the molten silicates and the liquid iron
 163 drop respectively.

164 The surface tension force is determined by :

$$\mathbf{F}_{st} = \nabla \cdot \mathbf{T} = \nabla \cdot (\sigma[\mathbf{I} + (-\mathbf{n}\mathbf{n}^T)]\delta) \quad (6)$$

165 with σ (N/m) the surface tension coefficient, \mathbf{I} the identity matrix, \mathbf{n} the in-
 166 terface normal unit vector, and δ the Dirac delta function, nonzero only at the
 167 fluid interface. The interface normal unit vector is calculated as

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}. \quad (7)$$

168 The level set parameter ϕ is also used to approximate the delta function by
 169 a smooth function (Hu et al., 2014) defined by

$$\delta = 6 |\phi(1 - \phi)| |\nabla\phi|. \quad (8)$$

170 *2.2. Physical and non-dimensional parameters*

171 According to the Buckingham II theorem, in our study, there are 6 dimen-
172 sionless numbers based on the control parameters (see Figures 1 and 2). One
173 could for instance choose the two aspect ratios related to the drop vs. the com-
174 putational domain sizes, the density ratio, the viscosity ratio, and then define *a*
175 *priori* Weber and Reynolds numbers based on the Newton theoretical velocity
176 (see e.g. Wacheul et al., 2014). A complete dynamical study would then necessi-
177 tate to explore the influence of those 4 later parameters in a computational box
178 sufficiently large such that boundary conditions do not influence the dynamics.
179 Here, we are interested in determining the dynamics of metal drops sinking into
180 a magma ocean: we thus vary only the drop radius and the magma ocean viscos-
181 ity, which are the main variables in the geophysical situation of interest, while
182 we keep all the other dimensioned parameters fixed at their expected geophysical
183 values (see Table 1).

184 In each simulation, starting from rest, the drop accelerates until reaching
185 a constant terminal velocity, possibly with small oscillations around it. We
186 monitor this mean terminal velocity V for each case. We end up our simulations
187 when either the drop reaches a stable regime before the bottom of the domain
188 or the drop fragments. In the later case the axisymmetric approximation is
189 not relevant anymore. Each run is thus characterised by the 4 dimensionless
190 numbers:

- 191 • the Reynolds number compares inertia and viscous effects : $Re = \frac{\rho_s V D}{\mu_s}$,
192 with $D = 2R$ the drop initial diameter (R is the initial radius). The
193 Reynolds number determines the falling drop dynamical regime : $Re < 1$
194 implies a Stokes regime where the viscous effects dominate; $Re = 1 - 500$
195 implies an intermediate regime where both viscous effects and inertial
196 forces are important; and $Re > 500$ implies a Newtonian regime where

197 the inertial forces are dominant (see Samuel, 2012).

- 198 • the Weber number measures the relative importance of inertia over sur-
199 face tension: $We = \frac{\rho_s V^2 D}{\sigma}$. It controls and governs the deformation and
200 breakup of the drop (Pilch and Erdman, 1987). Indeed inertia forces aim
201 at deforming and fragmenting the iron drop, while the surface tension force
202 prevents it from deformation and disruption. When $We \gg 1$, the inertia
203 forces dominate leading to strong deformation and rapid fragmentation
204 (e.g. Wacheul et al., 2014).

- 205 • the viscosity ratio is defined as the ratio of the silicates viscosity over the
206 iron drop viscosity: $R_\mu = \frac{\mu_s}{\mu_d}$. The viscosity of liquid iron weakly depends
207 on pressure and $\sim 5 \times 10^{-3}$ Pa.s at both inner core boundary pressure
208 conditions (Poirier, 1988) and at the Earth surface (Assael et al., 2006).
209 Oppositely, the magma ocean viscosity varies between 10^{-4} and 100 Pa.s
210 depending on the thermal and dynamic conditions (Karki and Stixrude,
211 2010; Rubie et al., 2003; Samuel, 2012). In our model, we fix the viscosity
212 of the metallic phase and the viscosity contrast ranges between 10 and
213 20000.

- 214 • the density ratio compares the iron drop density over the silicates density:
215 $R_\rho = \frac{\rho_d}{\rho_s}$. The densities of liquid iron and molten silicates depend on the
216 temperature and pressure conditions (Assael et al., 2006; de Wijs et al.,
217 1998; Samuel, 2012). In our models, for simplicity, we fix $\rho_d = 7500$
218 kg.m^{-3} and $\rho_s = 3500 \text{ kg.m}^{-3}$. As a consequence, in this study, the
219 density ratio is constant and equals to 2.14.

220 After a large collision involving two differentiated protoplanets, the core
221 of the impactor is first fragmented in large scale iron structures (Kendall and
222 Melosh, 2016). In the magma ocean, these structures overcome a second frag-

223 mentation resulting in the formation of a cloud of droplets with typical size
 224 ranging between a few millimetres to several centimetres (Deguen et al., 2014;
 225 Wacheul et al., 2014). In our study, we characterize the dynamics of a droplet
 226 in the iron cloud and determine the influence of the viscosity contrast on this
 227 droplet. For that, we vary the initial radius of the drop from 1 to 350 mm,
 228 exploring a large range of expected sizes in the iron rain cloud.

229 All the parameters used in this paper are listed in Table 1.

Table 1: Symbol definitions and values of the physical and non-dimensional parameters used in this study. Reynolds and Weber numbers are defined *a posteriori* using the relevant terminal velocity, measured in each run.

	Symbol	Value or range
Silicates density	ρ_s	3500 kg/m ³
Iron drop density	ρ_d	7500 kg/m ³
Density ratio	R_ρ	2.14
Iron drop viscosity	μ_d	0.005 Pa.s
Magma ocean viscosity	μ_s	0.05 - 100 Pa.s
Viscosity ratio	R_μ	10 - 20000
Initial drop radius	R	1 - 350 mm
Surface tension coefficient	σ	1 N/m
Reynolds number	Re	0.027 - 85600
Weber number	We	0.073 - 7480

230 2.3. Numerical method

231 In this work, we solve equations (1 - 3) using the COMSOL Multiphysics
 232 software, based on the finite element method. We study a 2D axisymmetric
 233 geometry with no-slip boundary conditions at the lateral boundary and open
 234 boundary conditions at the top and bottom boundaries. To avoid the wall ef-
 235 fects, the computational domain must be large enough. For instance, Bonometti
 236 and Magnaudet (2006) considered a computational domain of $5.5D \times 12.6D$ to
 237 avoid contamination of the results. Their computations are stopped before the
 238 bubble arrives too close to the domain boundary. Ohta et al. (2010) used a

239 computational domain of $4D \times 6D$, and considered a levitating drop with an
 240 entering inflow at the top boundary equal to its terminal velocity. Samuel (2012)
 241 also considered a levitating drop but with a square computational domain of
 242 $5D \times 5D$, and the inflow velocity is self-adjusting at the instantaneous velocity
 243 of the center of mass of the drop. Here, we have checked the convergence of
 244 our results as a function of the domain size, and we do not see any significant
 245 difference once the domain is larger than $4D$ and longer than $75D$. As sketched
 246 in figures 1 and 2, our computational domain is an axisymmetric cylinder of size
 247 $(r \times z) = (6D \times 100D)$.

248 The drop dynamics requires a fine mesh to capture all its details while con-
 249 serving the overall mass of iron. Especially, the level set method has a ten-
 250 dancy to diffuse numerical artifacts on the interface and then gives incorrect
 251 results. Since our computational domain is very large, we need an adaptive
 252 mesh strongly refined in the drop vicinity, which we have implemented manu-
 253 ally. To do so, we divide our domain in several regions, as shown in figure 2.
 254 We mesh the region that the drop crosses over a given time interval with a very
 255 fine mesh of size $h_x = 0.025R$, small enough to capture all the dynamics on
 256 the interface without any significant error or numerical diffusion. We mesh the
 257 region behind the drop with a thin mesh $h_x = 0.07R$ to correctly capture the
 258 physics of the wake, which also influences the dynamics. The mesh around the
 259 drop gradually widens in the radial direction until reaching $h_x = 0.2R$, from
 260 where it remains fixed until the wall. Finally, our mesh in front of the drop in
 261 the vertical direction first increases in an intermediate region to $h_x = 0.07R$, and
 262 then keeps increasing until reaching a very large value $h_x = 5000R$. When the
 263 drop approaches the bottom of the finer mesh region, the simulation is stopped,
 264 the whole pattern is translated, and the simulation is restarted on this new
 265 grid. We have tested this procedure and found that the dynamics of the falling

266 drop doesn't change significantly when using smaller h_x (see Appendix). Also
267 the overall iron mass during the course of each complete computation does not
268 change by more than 0.7%, hence showing good numerical convergence. This
269 method is relatively inexpensive in term of calculation time, and allows for a
270 systematic study, with runs taking from 7 hours to one week on a bi-processor,
271 3.2 – 3.6 GHZ, computer.

Table 2: Non-dimensional parameters for all performed simulations used in this study. In all our simulations, $R_\rho = 2.14$.

<i>Simulation</i>	<i>Re</i>	<i>We</i>	R_μ	$R(mm)$
#1	19.7	0.139	10	1
#2	315	7.09	10	5
#3	372	8.22	10	6
#4	426	9.27	10	7
#5	553	10.9	10	10
#6	1610	37.0	10	25
#7	3280	95.8	10	40
#8	73.9	8.13	50	6
#9	93.0	9.64	50	8
#10	106	11.1	50	9
#11	108	10.4	50	10
#12	202	24.2	50	15
#13	322	37.0	50	25
#14	638	91.0	50	40
#15	1510	290	50	70
#16	14.3	1.82	100	6
#17	35.3	7.43	100	8
#18	44.2	8.74	100	10
#19	51.8	9.58	100	11
#20	66.0	13.5	100	11.5
#21	71.4	15.2	100	12
#22	92.4	20.3	100	15
#23	154	33.9	100	25
#24	314	87.8	100	40
#25	750	287	100	70
#26	11.9	3.35	200	6
#27	19.7	6.90	200	8
#28	25.1	9.02	200	10
#29	30.4	11.0	200	12
#30	36.4	14.6	200	13
#31	38.7	15.3	200	14
#32	42.5	17.2	200	15
#33	76.1	33.1	200	25
#34	146	75.7	200	40
#35	363	268	200	70
#36	637	580	200	100
#37	1.53	1.05	1000	8

<i>Simulation</i>	<i>Re</i>	<i>We</i>	R_μ	<i>R(mm)</i>
#38	2.70	2.61	1000	10
#39	6.49	10.0	1000	15
#40	11.2	22.4	1000	20
#41	15.4	33.9	1000	25
#42	19.7	46.4	1000	30
#43	26.0	68.8	1000	35
#44	28.8	74.3	1000	40
#45	38.5	106	1000	50
#46	52.1	161	1000	60
#47	68.6	240	1000	70
#48	122	530	1000	100
#49	0.027	0.073	20000	15
#50	0.127	0.927	20000	25
#51	0.509	9.27	20000	40
#52	0.952	25.9	20000	50
#53	1.22	38.7	20000	55
#54	1.54	56.6	20000	60
#55	2.27	105	20000	70
#56	5.15	379	20000	100
#57	24.4	26.5	500	20
#58	7.56	42.5	2500	30
#59	8.42	49.5	2500	35
#60	9.82	61.2	2500	40
#61	12.3	84.7	2500	45
#62	2670	636	50	100
#63	24100	1380	10	150
#64	37100	2460	10	200
#65	67800	5480	10	300
#66	85600	7480	10	350
#67	4770	1350	50	150
#68	7360	2420	50	200
#69	13400	5380	50	300
#70	16960	7330	50	350
#71	2380	1350	100	150
#72	3660	2400	100	200
#73	6700	5340	100	300
#74	8430	7290	100	350
#75	1180	1330	200	150
#76	1820	2370	200	200
#77	3360	5360	200	300

<i>Simulation</i>	<i>Re</i>	<i>We</i>	R_μ	<i>R(mm)</i>
#78	4221.35	7273.386	200	350
#79	231	1270.5	1000	150
#80	502.25	3603.643	1000	250
#81	667.8	5309.01	1000	300
#82	837.9	7164.045	1000	350
#83	28.35	17.22	300	15
#84	24.57	19.2	400	18

272 3. Systematic numerical study

273 We performed 84 simulations, whose dimensionless parameters are given in
274 Table 2. In the following sections, we discuss our obtained numerical results
275 in terms of drag coefficient, fragmentation modes, time and distance before
276 breakup, and maximum stable drop radius. A particular attention is paid to
277 the influence of the viscosity contrast between the metallic and silicate phases.
278 The influence of the initial drop shape is shortly addressed at the end of this
279 section; everywhere else, we start from a spherical drop.

280 3.1. Drag coefficient

281 The drag coefficient is a dimensionless number that quantifies the drag or
282 resistance of the sinking drop into the magma ocean. It strongly depends on
283 the viscosity ratio, density ratio, and surface tension, all of which control the
284 interface conditions. In our case where the driving force is buoyancy and the
285 initial geometry is spherical, we classically define the drag coefficient as

$$C_D = \frac{8(\rho_d - \rho_s)gR}{3\rho_s V^2}, \quad (9)$$

286 with V the measured terminal velocity. Below, we first rapidly review the
287 different theoretical models for the drag coefficient, and then compare with our
288 numerical measurements.

289 *3.1.1. For small Reynolds numbers*

290 Several previous studies focused on the analytical determination of the drag
291 coefficient for spherical fluid particles (e.g. Clift and Gauvin, 1970; Hadamard,
292 1911; Mei et al., 1994) and for deformed fluid particles (e.g. Moore, 1965; Darton
293 and Harrison, 1974; Clift et al., 1978; Loth, 2008). For spherical drops, the
294 internal circulation is supposed to prevent forming any wake separation of the
295 external flow. This in turn helps to prevent any change in shape and keeps the
296 droplet spherical. Hadamard (1911) proposed an analytical relation at finite
297 but low Reynolds $Re \ll 1$. An asymptotic solution was derived by Harper
298 and Moore (1968) for intermediate Reynolds numbers but remains limited to
299 $Re < 100$ at finite values of the viscosity ratio. To fill the gap between Harper
300 and Moore (1968) and Hadamard (1911), an empirical mixed Stokes correction
301 factor resulting from the internal circulation was proposed by Mei et al. (1994)
302 in the limit $R_\mu \rightarrow 0$:

$$C_{D_{R_\mu \rightarrow 0}} = \frac{16}{Re} \left[1 + \left[\frac{8}{Re} + \frac{1}{2} \left(1 + \frac{3.315}{\sqrt{Re}} \right) \right]^{-1} \right]. \quad (10)$$

303 *3.1.2. For moderate and large Reynolds numbers*

304 For intermediate but increasing Reynolds numbers ($0.1 < Re < 2000$), the
305 drop begins to distort, leading to changes in the wake from an attached laminar
306 wake (spherical drop), to a separated laminar wake (deformable drop), to an
307 unsteady transitional wake (breakup into droplets) and finally to a turbulent
308 wake (catastrophic breakup) (Loth, 2008). The wake actually depends on the
309 interplay between surface tension and hydrodynamic pressure stresses, hence on
310 We . Davies and Taylor (1950) found a converged value $C_D = \frac{8}{3}$ for gas bubbles
311 in a liquid at infinite Reynolds and Weber numbers. In order to encompass the
312 influence of viscosity and a wide range of small to large Reynolds numbers, an
313 empirical correlation was proposed by Darton and Harrison (1974) and Clift

314 et al. (1978) for infinitely large We :

$$C_{D_{We \rightarrow \infty}} = \frac{8}{3} + \frac{24}{Re} \left(\frac{2 + 3R_\mu}{3 + 3R_\mu} \right). \quad (11)$$

315 To capture the drag in the intermediate range of Re and We values (of inter-
 316 est here), Loth (2008) proposed the following expression by combining Eqs.10
 317 and 11 and adding a functional dependence ($\Delta(C_D)^*$) on We , where $\Delta(C_D)^*$
 318 increases monotonically with Weber number:

$$C_D = C_{D_{We \rightarrow 0}} + \Delta(C_D)^* [C_{D_{We \rightarrow \infty}} - C_{D_{We \rightarrow 0}}] \quad (12)$$

$$\Delta(C_D)^* = \tanh(0.021We^{1.6}). \quad (13)$$

319 Here $C_{D_{We \rightarrow 0}}$ is given by Eq.10, the imposed spherical shape being related to
 320 an infinite surface tension, hence to $We \rightarrow 0$. Experimentally, several investi-
 321 gations partly tackled the relevant limit of a metal drop in a more viscous en-
 322 vironment, including: the fragmentation of liquid mercury drops sinking within
 323 water reported by Patel (1978); Patel and Theofanous (1981), who found a drag
 324 coefficient equal to 2.5 – 3; the fragmentation of gallium drops in water by
 325 Kim et al. (1983), who found that the drag coefficient depends on the Reynolds
 326 number; and the analog model of Wacheul and Le Bars (2018), who reported a
 327 convergence value of the drag coefficient at large Reynolds equal to 3.7 ± 1 .

328 *3.1.3. Results and discussion*

329 We have monitored the velocity V of the sinking metallic drop in our sim-
 330 ulations and obtained the corresponding values for C_D from Eq.9. Figure 3
 331 presents our measured C_D as a function of the Reynolds number for various
 332 viscosity ratios, and the comparison of our results with the analytical solutions

333 of Mei et al. (1994) (Eq. 10) and Loth (2008) (Eq. 12) . For $We < 1$ and
 334 low Reynolds numbers (up to $Re = 20$ depending on R_μ), the droplet remains
 335 spherical and our results agree with the analytical model proposed by Mei et al.
 336 (1994): C_D is inversely proportional to Re and barely depends on the viscos-
 337 ity ratio. When flow separation occurs (i.e. when the Weber number exceeds
 338 unity), this expression is not valid anymore because the drop deforms: it takes
 339 the shape of an ellipsoid, a disc or a cup. This deformation increases the frontal
 340 area and leads to a transient increase of C_D with Re , depending on R_μ . Qual-
 341 itative agreement between our simulations and Eq.12 is satisfactory, but small
 342 quantitative differences exist. This is not surprising, since the empirical formula
 343 Eq.12 was calibrated on gas bubbles rising in a liquid, which are more sensitive
 344 to deformation than the liquid drops studied here. But no equivalent to Eq.12
 345 is yet available for liquid-liquid systems, and one has thus to rely on numerical
 346 results. Finally, for large Re , C_D converges towards a constant value 3.5 ± 0.5 ,
 347 independtly of R_μ . This value is above the analytical estimate of $8/3$, but is
 348 compatible with the results of Wacheul and Le Bars (2018) who found a mean
 349 value of C_D equal to 3.7 ± 1 .

350 3.2. Fragmentation modes

351 The breakup mechanism is very sensitive to the Weber number, as well as to
 352 the viscosity ratio between the metal and the silicates. Two main fragmentation
 353 modes have been documented in previous experimental and numerical studies,
 354 namely the "bag breakup" just above the critical Weber number, and the "shear
 355 breakup" at large Weber number (see the limit cases in Fig. 4) (Krzczkowski,
 356 1980; Pilch and Erdman, 1987; Dai and Faeth, 2001). Several authors have
 357 tackled the description of the different breakup mechanisms in the intermediate
 358 range of Weber number, leading to a complex situation. Examples include
 359 Krzeczkowski (1980), who developed series of experiments for liquid droplets of

360 water, methanol, ethanol, butanol and glycerine in an external air stream, and
 361 documented two breakup modes independent of the viscosity ratio: the "bag-jet"
 362 and the "transition" modes. Pilch and Erdman (1987) introduced two breakup
 363 modes for a single liquid drop within an external gas flow: the "bag-stamen"
 364 mode and the "sheet stripping" mode. Dai and Faeth (2001) used droplets of
 365 water and ethanol and defined a "bag-plume" mode, close to the "bag-jet" and
 366 "bag-stamen", and a "plume-shear" mode, close to the "shear breakup". Cao
 367 et al. (2007) pursued this experimental investigation and presented a new "dual-
 368 bag" breakup mode for $We = 28 - 41$. Recently, 3D numerical simulations
 369 of liquid droplets levitating in a gas flow with a uniform velocity have been
 370 performed by Kékesi et al. (2014), changing the viscosity and density ratios for
 371 a fixed Weber number value ($We = 20$). They identified 5 breakup regimes, as
 372 shown in Fig. 4: "thick rim shear" and "thick rim bag" (both close to "bag
 373 breakup"), "rim shear", "jellyfish shear", and "shear" breakup respectively. In
 374 our study, we use their classification.

375 For each mode of fragmentation, we describe below the temporal evolution of
 376 a typical spherical drop starting from rest at $t = 0$, until its breakup at $t = t_{bk}$.

- 377 • Thick rim shear (Fig. 5): the initial sphere rapidly deforms into a spherical
 378 cap ($t = 0.13s$), then the hydrodynamic pressure force concentrates on
 379 the middle of the drop leading to the formation of a small bag ($t = 0.2s$).
 380 Surface tension then prevents breakup and the drop returns to form a
 381 half-sphere ($t = 0.355s$), before a second oscillation starts. Then, as the
 382 inertial forces and associated pressure are reinforced, the vertical thickness
 383 decreases even more, and a thin film forms near the symmetry axis, with
 384 a thicker rim ($t = 0.55s$). The rim extends radially and drains out the
 385 liquid film ($t = 0.6s$), until a hole occurs at the symmetry axis ($t = 0.62s$).
 386 At this stage, the metal phase actually forms a ring that might persist

387 for a longer time before fragmentation of Rayleigh-Plateau type, to which
 388 we cannot have access with our axisymmetric simulation. Kékesi et al.
 389 (2014) showed in 3D simulations that this last stage is actually rapid, i.e.
 390 a few milliseconds. Note also that thick rim shear seems marginal in the
 391 parameter space explored here, and is replaced rapidly by thick rim bag,
 392 except for cases with the smaller viscosity ratio $R_\mu = 10$ (see Fig. 4).

- 393 • Thick rim bag (Fig. 6): this breakup process is similar to the thick rim
 394 shear, until fragmentation. Then, breakup appears almost simultaneously
 395 in the center of the drop ($t = 0.675\text{s}$) and at the connection between the
 396 film and the rim, forming satellite droplets ($t = 0.68\text{s}$).
- 397 • Rim shear (Fig. 7): again the initiation of the breakup is similar to
 398 the two processes described above, with the formation of a spherical cap
 399 ($t = 0.131\text{s}$), followed by a bag ($t = 0.2\text{s}$), and back ($t = 0.37\text{s}$). Then,
 400 the drop extends in both radial and vertical directions, forming a sheet
 401 ($t = 0.48\text{s}$ and 0.51s) under the action of the strong vorticity in the wake.
 402 Finally, surface tension drains the iron both into the center and into the
 403 rim ($t = 0.57\text{s}$), while the sheet connecting the two thins, and finally
 404 breaks ($t = 0.59\text{s}$).
- 405 • Jellyfish shear (Fig. 8): in this mode, no rim forms. Instead, a thin skirt
 406 forms while iron is mostly localized along the symmetry axis ($t = 0.4\text{s}$ and
 407 $t = 0.45\text{s}$). Oscillations develop in the thin membrane, whose ends fold in
 408 and out. The velocity is concentrated in the wake of the silicates which
 409 accelerates the drop center relative to its membranes, leading to a rapid
 410 fragmentation in the connecting region ($t = 0.51\text{s}$).
- 411 • Shear breakup (Fig. 9): the drop shape deforms first into a spherical
 412 cap ($t = 0.24\text{s}$) and second into a skirt. Then, the rim does not thicken,

413 but folds inside and turns around itself through the action of vorticity,
414 leading to its thinning ($t = 0.4s$). Rapidly, this thin sheet breaks into
415 small droplets ($t = 0.42s$). No oscillations are observed here, and the
416 rapid fragmentation is mainly due to the vorticity in the wake behind the
417 drop that is two to three times larger than the vorticity in the drop.

418 The deformation of the droplet depends on the viscosity of the external
419 flow, the density ratio, the surface tension and the drop size. When Re and
420 We are both small, the drop remains spherical without any deformation, due
421 to the internal circulation within the drop that prevents forming any separated
422 wake. When the hydrodynamic pressure force increases, a separated laminar
423 wake and an external circulation behind the drop occur, leading to shape defor-
424 mation. Increasing the Reynolds number, the drop first deforms to an ellipsoid,
425 and possibly gives rise to oscillations from oblate to prolate shapes. For a vis-
426 cosity ratio less than 100, the drop keeps oscillating until the end of the domain,
427 while for a viscosity ratio greater than 100, the velocity of the drop exceeds the
428 oscillation velocity, leading to rapid damping of the initially excited oscillation.
429 Further increasing the Reynolds number, the drop takes the shape of a spheri-
430 cal cap. And once hydrodynamic pressure overcomes surface tension (i.e. large
431 enough Weber number), one of the five fragmentation modes occurs, depending
432 also on the viscosity ratio. From our systematic study for different viscosity
433 ratios, we built up a fragmentation regime diagram in terms of Reynolds and
434 Weber numbers shown in Fig. 4. For a viscosity ratio $R_\mu = 1000$, we observe
435 only two modes, and drop oscillations are prevented by the high silicates vis-
436 cosity. On the contrary for $R_\mu = 50$, we observe the five different modes and
437 strong drop oscillations. One should also notice that the critical Weber number
438 depends on the viscosity ratio: for $R_\mu = 10$, the breakup begins at $We \approx 9$
439 while for $R_\mu = 1000$, it starts at $We \approx 34$. Systematic estimate of the critical

440 Weber number is shown in Fig. 10. We consider in this figure that fragmen-
 441 tation occurs as soon as the first volume of iron separates from the main drop.
 442 The increase in the viscosity ratio leads to an increase in the critical Weber
 443 number following two empirical scaling laws depending on first-breakup regime.
 444 When the viscosity ratio is rather low (i.e. < 300 typically), the drop fragments
 445 quickly as a thick rim shear after only one or two oscillations along a short drop
 446 path. In this case, critical Weber is defined as a low power law of the viscosity
 447 ratio by the following scaling law

$$We_c = 5.7R_\mu^{0.187}. \quad (14)$$

448 On the other hand, at a viscosity ratio of ~ 300 , a Jellyfish behaviour takes
 449 place, and between $R_\mu = 300$ and $R_\mu = 500$, the drop first breakup becomes slow
 450 and transitions from thick rim shear to Jellyfish. In this region and above, where
 451 shear breakup takes place, the critical Weber number depends more significantly
 452 on the viscosity ratio and is given by the following scalling law

$$We_c = 1.137R_\mu^{0.483}, \quad (15)$$

453 valid at least in the range $R_\mu = [300; 2500]$ explored here.

454 From our simulation #41, we also report a new fragmentation mode illus-
 455 trated in Fig. 11. This mode is initially similar to the jellyfish shear breakup
 456 except that the membrane fold is so important that it finally closes at the back,
 457 encapsulating the silicates within a bubble of iron (Fig. 11, $t = 3.7s$). Then,
 458 the next oscillation of the membrane tears the glued back which breaks from
 459 the center, forming one central droplet and two satellites droplets. Note that
 460 Wacheul et al. (2014) observed in their experiments similar bubbles of metal en-
 461 closing the viscous ambient fluid and exhibiting a lower velocity than pure iron

462 droplets. While being dynamically intriguing, this mode remains very marginal.

463 3.3. Time and distance before breakup

464 After an impact, large drops deform and fragment at a distance and time
465 that depend on the sinking dynamics. We define these time and distance as
466 the breakup time t_{bk} and distance d_{bk} . Deguen et al. (2014) predicted that for
467 large Weber numbers, t_{bk} and d_{bk} reach an asymptotic regime. In this section
468 we test this prediction. From our models, we determine t_{bk} and d_{bk} as the time
469 and location where the first droplet or ligament of iron separates from the main
470 drop. We then define the dimensionless breakup time t_{bk}^* as Pilch and Erdman
471 (1987):

$$t_{bk}^* = \frac{t_{bk}V}{D} \sqrt{\frac{\rho_d}{\rho_s}} \quad (16)$$

472 where the break up time is normalized by the characteristic time of drop breakup
473 by Kelvin-Helmholtz instability. We define the dimensionless breakup distance
474 as:

$$d_{bk}^* = \frac{d_{bk}}{R}. \quad (17)$$

475 Fig. 12 shows the variations of t_{bk}^* as a function of the Weber number
476 for various viscosity ratios. From Fig. 12, we see that t_{bk}^* decreases with the
477 increase of We . We note that, for large We , t_{bk}^* converges towards a constant
478 value ranging between 1 and 1.8. This result is consistent with the result of
479 Pilch and Erdman (1987) who found $t_{bk}^* = 1.25$ for $We > 350$. A dependence
480 on the viscosity ratio is also present, especially at $We \leq 80$, with a tendency
481 for large R_μ to stabilise the drops.

482 The non-dimensionalised breakup distance d_{bk}^* is reported in Fig. 13. It
483 also shows a dependence on the viscosity ratio, especially at low We , and a

484 possible convergence towards an asymptotic value ranging between 2 and 4 at
 485 large We . For comparison, Deguen et al. (2014) found a breakup distance equal
 486 to 6 – 8 times the drop radius for We up to 3000 and $R_\mu = 0.5$. Landeau et al.
 487 (2014) found a value equal to 3.5 – 7.5 times the radius for $25 < We < 1000$
 488 and $0.45 < R_\mu < 1.25$. Hence our results are in correct agreement with those
 489 experimental observations. This is all the more noticeable that Landeau et al.
 490 (2014) observed 3D turbulence in lab experiments at $We > 600$, effects that
 491 are missing from our axisymmetric simulations. Note finally that Wacheul and
 492 Le Bars (2018) found a breakup distance $(13 \pm 2)R$ for $10 < We < 50$ and
 493 $0.4 < R_\mu < 700$, but their breakup criteria actually detected a “significant”
 494 and well-advanced breakup, thus implicitly leading to an overestimation of d_{bk}^*
 495 compared to other results. Figure 13 illustrates the influence of the viscosity
 496 ratio on the breakup distance. For low We , d_{bk}^* ranges between 10 and 80
 497 for the whole range of viscosity ratios used in our study. For large We , d_{bk}^*
 498 ranges between 2 and 4.5. Increasing the viscosity ratio generically increases
 499 the breakup distance and as a consequence, the potential depth of equilibrium
 500 between iron drops and silicates.

501 3.4. Maximum stable drop radius

502 After an impact, the impactor’s iron core disrupts into large scale drops
 503 (Kendall and Melosh, 2016). After this first fragmentation, a second fragmen-
 504 tation occurs within the magma ocean resulting in the formation of a cloud of
 505 droplets (Deguen et al., 2014; Wacheul et al., 2014). At the end of this second
 506 fragmentation, iron droplets reach a maximum stable radius R_{max} . Following
 507 Wacheul et al. (2014) and using the Newtonian velocity scale accounting for the
 508 drag coefficient (Eq.9), R_{max} is simply related to the critical Weber number by

$$R_{max} = \sqrt{We_c \frac{3C_D}{16} \frac{\sigma}{\Delta\rho g}}. \quad (18)$$

509 Numerical data from Fig. 14 show the last drop radius for which deformation
 510 may occur but without fragmentation. According to Fig. 14, the maximal stable
 511 drop radius increases with the magma ocean viscosity. From our numerical data,
 512 we propose a scaling law to determine the maximum stable radius as a power
 513 function of magma ocean viscosity, valid for magma viscosities larger than ~ 0.1
 514 Pa.s up to 100 Pa.s :

$$R_{max} = 0.014\mu_s^{0.32}(m). \quad (19)$$

515 Our results are in agreement with the analytical Eq. 18, confirming the
 516 self-consistency of our numerical results. Fig. 14 also shows the comparison
 517 of our results with the model of Rubie et al. (2003) and the model of Samuel
 518 (2012). Differences come from different values of C_D , where we use our effective
 519 numerical values rather than any theoretical estimation. It should also be noted
 520 that Rubie et al. (2003); Samuel (2012) do not consider the dynamical influence
 521 of the viscosity contrast between metal and silicates in their models.

522 3.5. *The influence of initial conditions*

523 After an impact, the impactor's core is likely fragmented in metallic diapirs
 524 with a large range of shapes (spherical, oblate or prolate) (Kendall and Melosh,
 525 2016). This deformation process is likely to affect the post-impact sinking dy-
 526 namics of the metallic phase as we envision in our study by modifying our initial
 527 shape conditions. Bonometti and Magnaudet (2006) found that their final bub-
 528 ble topology and features vary with the initial shape of the bubble. Without
 529 trying to be exhaustive on this subject that would deserve a dedicated study on
 530 its own, we have thus investigated the behavior of a drop at the critical Weber
 531 number for two viscosity ratios ($R_\mu = 200$ and $R_\mu = 1000$), starting from a
 532 spherical, oblate or prolate form with an ellipticity ranging between 0.59 and
 533 0.82, maintaining the total volume of iron constant. Results for $R_\mu = 1000$ are

534 shown in Fig. 15, reporting a significant sensitivity to initial conditions. For
535 the initial oblate form, the drop does not fragment and converges to a skirt
536 shape. On the contrary, the initial prolate shape disrupts more rapidly than the
537 spherical case, the time and distance before breakup being respectively 27.4%
538 and 28.3% smaller than the corresponding values for the spherical case. The
539 shape is also different, with an increase of the surface in the prolate case of
540 10.9% compared to the spherical case. For the other viscosity ratio $R_\mu = 200$,
541 we find that the fragmentation modes are identical for the three initial condi-
542 tions, but differences on the order of 10% exist in the breakup time, distance
543 before breakup, and surface. Among the three initial cases, the spherical initial
544 condition always leads to a less rapid fragmentation and to a smaller surface.

545 **4. Implications for the metal/silicate exchanges**

546 In the present study, we focus on the dynamics of the two phase flow only,
547 without considering neither the thermal evolution of the metallic droplet nor
548 chemical exchanges that could occur between the metallic and silicate phases.
549 Our results nevertheless enable to constrain two fundamental parameters for
550 thermochemical equilibration, namely the thickness of the boundary layer at
551 the iron / silicates interface, and the surface of the metallic droplet across which
552 thermochemical exchanges are likely to occur. Those two points are addressed
553 below. We then propose some first order estimates of the equilibration of an
554 initially 10 km metallic core sinking and fragmenting within a magma ocean
555 and compare our results with the classical iron-rain model (Rubie et al., 2003).

556 *4.1. Boundary layer thickness*

557 During the sinking of an iron drop, three boundary layers can form at the
558 interface between the metallic and silicate phases: the dynamical, thermal and
559 chemical boundary layers. The thickness of each boundary layer may have a

560 strong influence on the thermo-chemical exchanges. In this study, we focus on
 561 the dynamical boundary layer δ . We thus consider a velocity profile along the
 562 normal to the drop interface at the front of the drop, as shown in Fig. [16]: δ is
 563 defined as the distance from the drop interface to the point where the velocity
 564 is equal to 10% the drop terminal velocity. In the case of a rigid sinking sphere,
 565 the thickness of the boundary layer scales as $Re^{-1/2}$ (Ulvrová et al., 2011). In
 566 our models, the metallic droplet is deformable and three parameters *a priori*
 567 control the flow, hence δ : R_μ , Re and We . Here, we seek a power law for the
 568 boundary layer thickness in terms of the two varied parameters in our study,
 569 namely the drop radius and the magma ocean viscosity.

570 Our numerical results are shown in Fig. 17. A good fit is found with the
 571 empirical scaling law

$$\delta = 1.442R^{0.916}\mu_s^{0.062}(m). \quad (20)$$

572 Hence, the boundary layer thickness depends mainly on the drop radius and
 573 only slightly on the magma ocean viscosity. For a standard viscous boundary
 574 layer in the vicinity of a solid sphere, one would expect a scaling $\propto \mu_s^{0.5}$. This
 575 surprisingly low dependence on the ambient viscosity is probably due to the drop
 576 deformation and to the associated internal circulations and wake. It presumably
 577 affects the equilibration. Note however that Eq. 20 is valid in the frontal section
 578 of the drop, but the boundary layer size is not constant along the drop surface.
 579 Also, the generated wake might encapsulate silicates that are entrained with
 580 the falling iron, as shown in Fig. 18 and observed numerically (Monteux and
 581 Arkani-Hamed (2014)) and experimentally (Fleck et al. (2018)), for an even
 582 more viscous surrounding fluid. This also influences equilibration. Clearly, the
 583 equilibration process is complex, global, and deserves a study on its own.

584 *4.2. Time evolution of the droplet surface*

585 The exchange surface between two fluids qualifies the surface through which
586 thermo-chemical transfers occur. As shown in the figures 5, 6, 7, 8, 9 and
587 11, the spherical drop deforms and oscillates during its sinking. This leads to
588 variations in the potential exchange surface between the liquid iron and the
589 molten silicates.

590 We monitored the surface S of each drop from its initial position until reach-
591 ing a stationary regime or until breakup. We normalized S by the corresponding
592 spherical surface ($S^* = S/(4\pi R^2)$). Fig. 19 shows the evolution of S^* as a func-
593 tion of time for an initial radius $R = 10$ mm. Fig. 19 illustrates the influence
594 of the viscosity contrast R_μ . For $R_\mu = 1000$, the drop remains spherical and
595 its normalised surface is constant ($S^* = 1$). When the magma ocean viscosity
596 decreases, the deformation of the drop becomes significant and the oscillations
597 of the drop lead to oscillations of its surface. For $R_\mu = 100$, the drop deforms
598 and oscillates several times, but the surface tension is large enough to prevent
599 the drop from breaking up, and a steady state is reached after 1.5s. For $R_\mu = 10$
600 and $R_\mu = 50$, the drop surface oscillations are followed by a fragmentation (at
601 0.393s and 0.6s respectively). These large deformation processes significantly
602 increase the droplet surface, which can increase by up to 200% before the frag-
603 mentation. Our results show that the viscosity ratio between the liquid iron
604 and silicate phases strongly influences the shape of the metallic drops. As a
605 consequence, considering a purely spherical drop when calculating the transfers
606 across the exchange surface provides only a lower bound estimate which might
607 be significantly off, especially for $R_\mu < 100$.

608 *4.3. Application to a 10 km metal diapir*

609 In the previous sections, we studied the dynamical properties of sinking
610 droplets as a function of the viscosity ratio between the iron droplet and the

611 magma ocean. We showed that, within an iron cloud, each droplet is associated
612 to a boundary layer thickness and an exchange surface that both depend on the
613 droplet size and viscosity ratio. In our numerical models we do not solve the
614 equations governing the thermo-chemical transfers between the metallic droplets
615 and the magma ocean. However, we can estimate the efficiency of the potential
616 thermo-chemical equilibration by determining the total potential exchange sur-
617 face within a metallic cloud composed of small droplets and resulting from the
618 fragmentation of a 10 km radius metallic diapir, which is the typical lengthscale
619 of iron fragments dispersed after a large impact (Kendall and Melosh, 2016).
620 We consider in these estimations that the 10km metallic diapir is fragmented in
621 a population of small droplets that compose a larger scale metallic cloud sinking
622 through the magma ocean (Deguen et al., 2014).

623 To characterize the size of the droplets within the cloud, we used the analyt-
624 ical law for the distribution of droplets sizes obtained from the fragmentation of
625 a large analog diapir with a viscosity ratio $R_\mu = 50$ derived experimentally by
626 Wacheul et al. (2014). We assume here that this analytical law is valid for any
627 system with the same viscosity ratio once it is normalised by the characteristic
628 radius of the system, i.e. the maximal stable radius R_{max} . The number of drops
629 $n(R)$ for a given radius R resulting from the breakup of a 10 km iron core is
630 then associated to a gamma distribution:

$$n(R) = NR^{k-1}e^{-\frac{R}{\theta}} \quad (21)$$

631 where N is a multiplicative constant determined by volume conservation of
632 iron, k is the shape of the gamma distribution, and θ is the scale of the gamma
633 distribution normalised by R_{max} . Wacheul et al. (2014) explicitly mentioned
634 that the shape and scale might depend on the viscosity ratio. In the absence
635 of any further data, we assume constant values with $\theta = 1.9$ and $k = 2.2$ for

636 viscosity ratios ranging between 10 and 1000. Note that R_{max} is nearly constant
637 in the study of Wacheul et al. (2014) and Eq. 21 is obtained from a snapshot
638 at a given time relatively shortly after the primary breakup, where transient
639 large radius drops are still present. In our study, we have shown that R_{max}
640 is a function of the magma ocean viscosity (Fig. 14). Hence, for each magma
641 ocean viscosity, we use R_{max} from our numerical study (Fig. 14) and determine
642 N by volume conservation from a initially 10 km iron diapir radius. We then
643 compute the number of drops of each size, and their relative surface of exchange
644 normalised by their corresponding spherical surface.

645 We have shown in our numerical models that shape oscillations might in-
646 fluence the surface of the drops (Fig. 19), especially for the largest radii and
647 smallest viscosity ratio. We consider here three models of droplet population
648 within the cloud:

- 649 1. a non oscillating population of droplets with a constant radius for a fixed
650 viscosity corresponding to the classical iron rain scenario (Rubie et al.,
651 2003),
- 652 2. a non oscillating droplet population derived from our models with variable
653 radii where the droplets remain spherical,
- 654 3. an oscillating population derived from our models with variable radii where
655 the droplets deform.

656 Fig. 20 shows the total dimensionless surface within the fragmenting cloud
657 for the three different cases. In all cases, the exchange surface decreases when
658 increasing the magma ocean viscosity because the maximum stable drop radius
659 also increases when increasing the magma ocean viscosity (see Fig. 14). In the
660 iron rain scenario, the population is composed of droplets smaller than in the
661 two cases derived from our models (oscillating and non oscillating) where large
662 drops are allowed in the distribution. Hence the potential exchange surface is

663 larger (up to 60%) in the iron rain scenario and the equilibration should be more
664 efficient. For the population composed of oscillating droplets, the deformation
665 leads to an increase of the surface of the sinking droplets especially for low
666 magma ocean viscosities where R_{max} is smaller than for large magma ocean
667 viscosities. The total exchange surface in the oscillating case is larger than in
668 the non-oscillating case (by 13 to 43 %) but remains smaller than in the iron rain
669 scenario (by 7 to 37 %). For large magma ocean viscosity (i.e. large viscosity
670 contrasts), the droplets do not oscillate and the exchange surface value is close
671 for both oscillating and non oscillating populations. For low magma ocean
672 viscosities (i.e. small viscosity contrasts), the deformations are so important in
673 the oscillating population that the total surface is close to the surface obtained
674 in the iron rain scenario.

675 It is to be noted that large metallic drops (with $R > R_{max}$) are allowed in
676 the populations used to obtain Fig. 20. Such large drops are not stable but
677 are likely to exist during the second phase of the fragmentation following an
678 impact that occurs in the shallow magma ocean (Wacheul et al., 2014). Within
679 a deep magma ocean, transient drops with radii $R > R_{max}$ will fragment in
680 smaller droplets and disappear from the populations used in Fig. 20. We can
681 thus redo our calculation by imposing a cut-off at R_{max} using the values from
682 our numerical models (Fig. 14). Fig. 21 illustrates the total potential exchange
683 surface within a sinking cloud of metallic droplets as a function of the magma
684 ocean viscosity considering the same initial volume as in Fig. 20. Imposing a
685 cut-off at R_{max} generates a population of smaller droplets than in Fig. 20. In
686 the oscillating and non oscillating populations used in Fig. 21 many droplets
687 are even smaller than the maximum stable drop radius of the iron rain model.
688 Hence Fig. 21 shows that the total surface of the metallic droplets for both
689 the oscillating and non oscillating populations is larger than the total surface

690 derived from the iron rain scenario. Still, the non oscillating model will be less
691 efficient for thermo-chemical equilibrium than the oscillating model and large
692 magma ocean viscosities (i.e. large viscosity contrasts) significantly reduce (by
693 a factor 10) the potential exchange surface between the silicate and metallic
694 phases.

695 Results from Figs. 20 and 21 both underline the competition between (1) the
696 deformation processes at the scale of the droplet that enhance the equilibration
697 between the iron and silicate phases and (2) the viscosity contrast that limits
698 the potential exchange surface by allowing large drops. In the shallow part
699 of the magma ocean where large transient metallic drops are likely to exist,
700 the thermo-chemical equilibration will be less efficient than in the deepest part
701 of the magma ocean. However, this conclusion needs to be constrained by
702 implementing thermo-chemical transfers in our dynamical models and using
703 realistic partition coefficients and conductivities that should vary with pressure
704 and temperature.

705 **5. Conclusions and future works**

706 During the late stages of planetary accretion, large impacts between differ-
707 entiated protoplanets have strongly influenced the thermo-chemical state of the
708 future terrestrial planets. Following the impact and the formation of a deep
709 magma ocean, the metallic phase from the impactor has overcome strong de-
710 formation and fragmentation processes before reaching the deepest part of the
711 magma ocean. The dynamics of this fragmentation probably played a key role
712 on the equilibration efficiency between the metallic phase from the impactor
713 and the impacted proto-mantle.

714 We have performed axisymmetric numerical simulations to model the sinking
715 dynamics of an initially spherical liquid iron drop within a molten silicate phase.

716 We have explored a large range of relevant parameters, considering initial drop
717 radii in the range of [1–350] mm resulting from the breakup of an initially larger
718 metallic diapir, and magma ocean viscosities in the range [0.05–100] Pa.s. This
719 large range of viscosity is meant to encompass all relevant geophysical situations,
720 depending on pressure, depth, temperature, composition and impact history.

721 For large Reynolds numbers, we have showed that the drag coefficient for
722 all viscosity ratios converges towards an unique value on the order of 3.5 ± 0.5 .
723 We have found that the maximum stable drop radius increases as a function of
724 the magma ocean viscosity following a power law that scales with $\mu_s^{0.32}$. The
725 corresponding critical Weber number increases as a function of the viscosity
726 ratio following two power laws depending on the breakup regime, that scale
727 with $R_\mu^{0.187}$ and $R_\mu^{0.483}$ for the range of low and large magma ocean viscosity
728 respectively. We have identified five breakup mechanisms depending on the We-
729 ber and Reynolds numbers and on the viscosity ratio between silicates and iron
730 phases. We have also shown that the initial shape of the metallic drop (spheri-
731 cal, prolate or oblate) strongly influences its subsequent dynamics by modifying
732 its final shape before breakup, its potential exchange surface, and the time and
733 distance before breakup. We have emphasized the effect of the viscosity con-
734 trast on the potential exchange surface between the iron phase and the molten
735 surrounding silicates. Indeed, an increase of the viscosity ratio decreases the
736 potential exchange surface between the iron drop and the molten silicates while
737 it increases the time and distance before breakup. We have shown that the
738 dynamical boundary layer thickness increases as a function of the drop radius
739 and the magma ocean viscosity following power law that scales with $R^{0.916}$
740 and $\mu_s^{0.062}$. Finally, we have implemented our numerical results in a first order
741 model to characterise the ability of an initially 10km metallic diapir to exchange
742 with its surrounding environment while fragmenting. Our dynamical model pre-

743 dicts that potential thermo-chemical equilibration within a fragmenting cloud
744 depends on the depth at which the cloud is fragmenting: thermo-chemical equi-
745 libration should be less efficient in the shallowest part of the magma ocean than
746 in the deepest part.

747 The next step is now to implement in our models the resolution of the
748 equations governing the thermo-chemical exchanges between the metallic phase
749 and the magma ocean. The chemical and thermal diffusion of a sinking unde-
750 deformable sphere has been extensively studied in the chemical/heat transfer
751 literature (Levich, 1962; Clift et al., 1978). In their numerical models, Ul-
752 vrová et al. (2011) evaluated time scales of chemical equilibration within an
753 undeformable metallic droplet sinking through a deformable medium. If the
754 exchange dynamics in the case of a sinking sphere is strongly constrained, the
755 dynamics of thermo-chemical equilibration between a deformable droplet and its
756 environment and the influence of the viscosity contrast between the two phases
757 still deserve extensive studies.

758 As shown in our study, the depth of the magma ocean could also influ-
759 ence the fragmentation dynamics. As large transient droplets are more likely
760 in the early fragmentation regime, full thermo-chemical equilibration could be
761 achieved deeper in the magma ocean. The transfer parameters governing the
762 equilibration rate are also pressure/temperature dependent. The viscosity of
763 the molten silicates (Karki and Stixrude, 2010), the partition coefficient of
764 lithophile/siderophile elements (Bouhifd and Jephcoat, 2003) and the thermal
765 conductivity of iron (de Koker et al., 2012) are all affected by pressure changes
766 with depth. An exhaustive study accounting for realistic parameters in the con-
767 text of a deep magma ocean will surely help to constrain the thermo-chemical
768 signature at the end of the core-mantle separation.

769 **Acknowledgements**

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776

777 **6. Appendix: computational resolution and convergence**

778 In order to confirm that our mesh correctly captures the dynamics of the
779 falling drop within the magma ocean and to determine the quality and limits
780 of our numerical model, we performed systematic tests on two representative
781 cases.

782 In the first case, we focus on the dynamics of a strongly oscillating drop
783 that does not converge to a single shape and remains in oscillation (simu-
784 lation #18 in Table 2). This corresponds to a worst case scenario from a
785 numerical point of view. Fig. (22 (left)) shows the normalised boundary
786 layer thickness on the drop radius as a function of different grid sizes $h_x =$
787 $R/15, R/25, R/33.4, R/40, R/50, R/66.7$. We observe a reasonable convergence
788 of the numerical results from $h_x = R/40$, with changes limited to 1.4%. To quan-
789 tify the dynamic difference between $h_x = R/40$ and the finest mesh $h_x = R/66.7$,
790 we calculate the normalised exchange surface as a function of time in Fig. (22
791 (Right)). We note that the first two drop oscillations have the same dynamics;
792 then, differences occur. Yet the dynamical times remain close, and the evolution
793 of the exchange surface is almost the same between the two mesh sizes, with a
794 relative maximum error $\simeq 3.5\%$.

795 In this paper, we are also interested in the fragmentation modes. To confirm
796 that these fragmentation modes don't depend on the mesh size and don't come
797 from any numerical artifact, we calculate an extremely distorted drop which
798 breaks up after a few oscillations in a second test case (simulation #83 in Table
799 2). Fig. (23) shows the final drop shape just after the breakup for the grid sizes
800 $h_x = R/40$ and $h_x = R/66.7$. This figure confirms that from $h_x = R/40$, the
801 fragmentation mode and the final drop shape do not change significantly with
802 the grid resolution.

803 We finally compare the cost (CPU) for one second of simulation of the first
804 test case with different mesh sizes in Table 3. The finest mesh is 4 times more
805 expensive than $h_x = R/40$. The purpose of this article being to perform a
806 systematic study to capture the drop dynamics for a large range of radius and
807 ambient viscosity, we have chosen the mesh size of $h_x = R/40$, which is a good
808 compromise between simulation costs and global dynamical results.

Table 3: Comparison the cost of one simulation for three different grid sizes

<i>Grid size (h_x)</i>	<i>CPU</i>
$R/40$	51h15
$R/50$	121h5
$R/66.7$	205h

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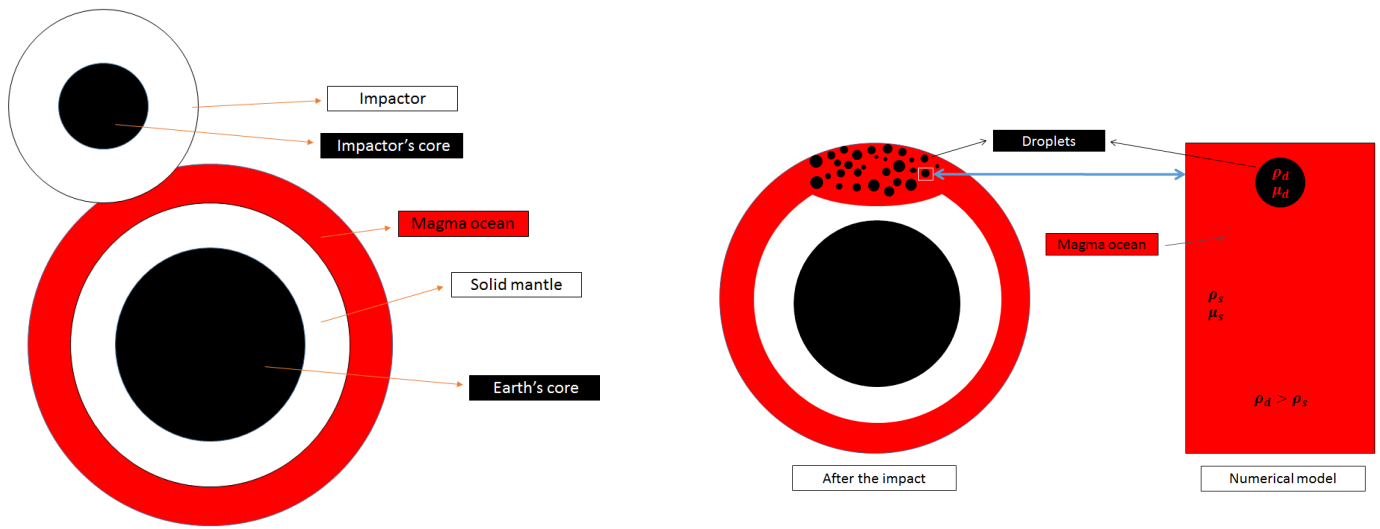


Figure 1: Schematic of the metal/silicate separation during an impact between a differentiated planetesimal and the early Earth with a schematic of our computational domain.

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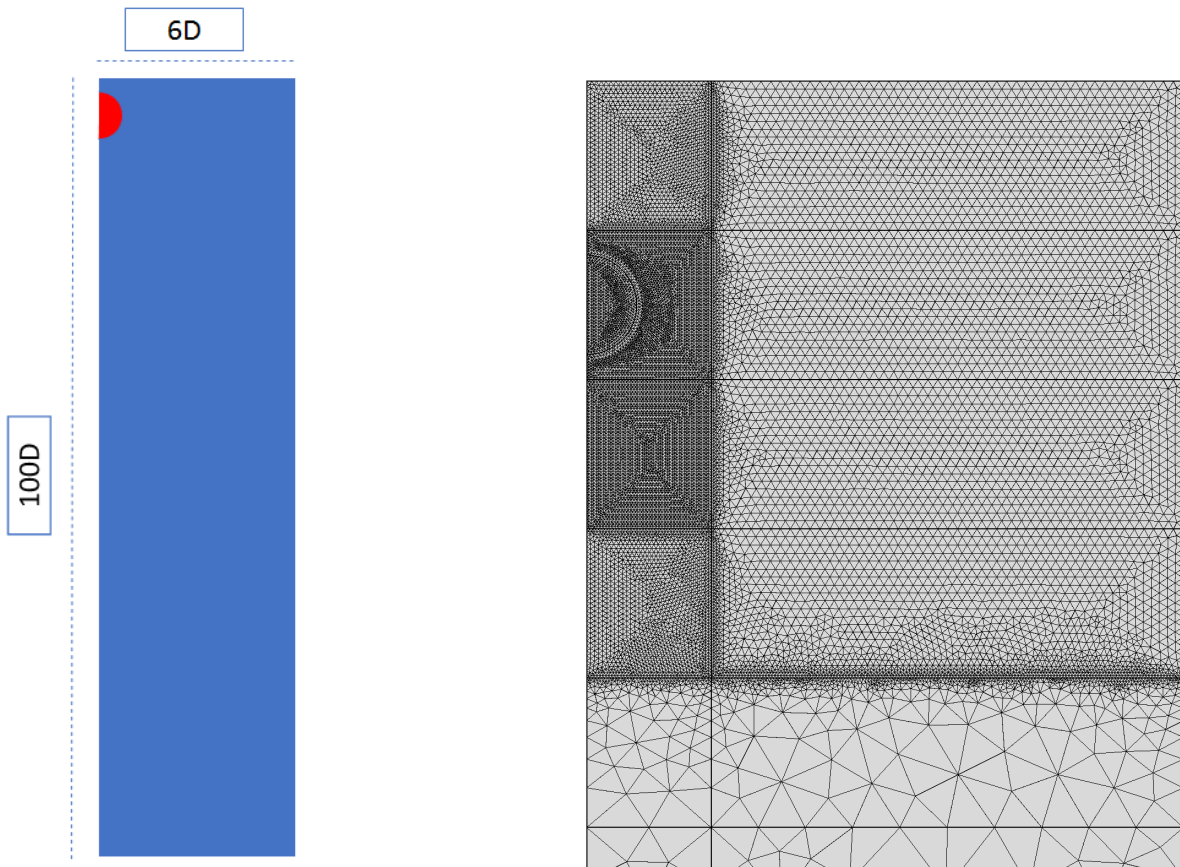


Figure 2: Global view of our geometry with the initial drop at the top (left), and a zoom illustrating our manual method for adaptive mesh (right).

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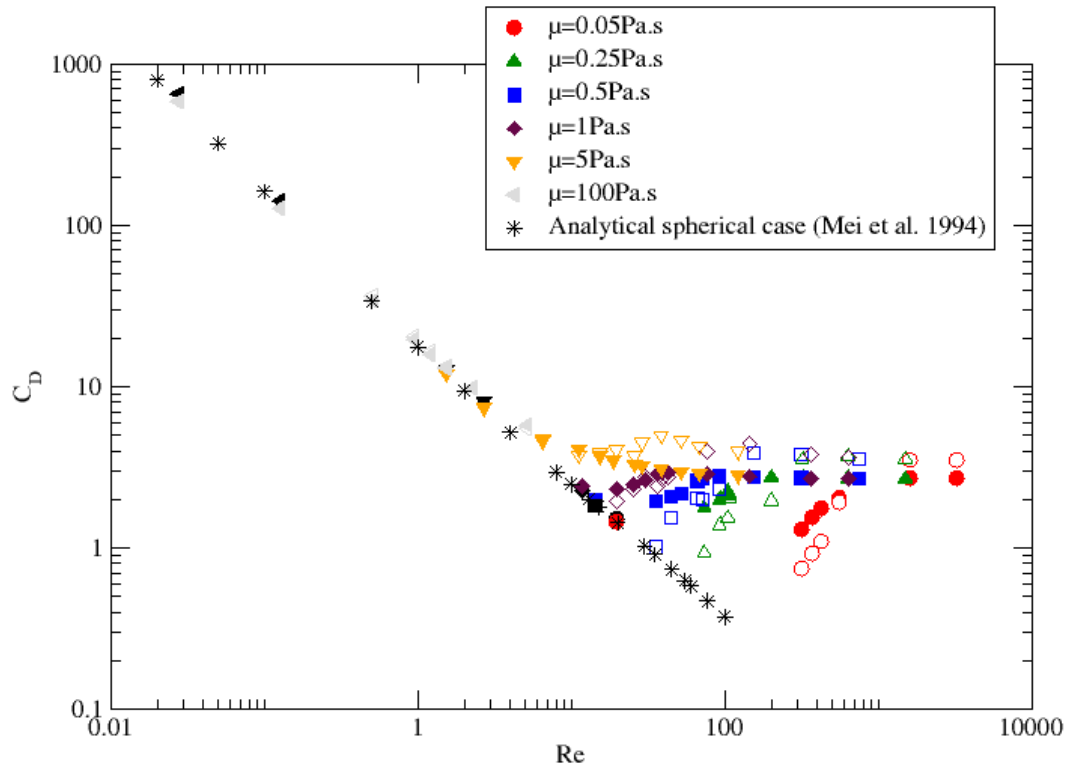


Figure 3: Drag coefficient as a function of the Reynolds number for various values of the silicates viscosity. Filled symbols are the analytical results given by Eq.12, while empty symbols show our numerical results from the first 62 simulations in table 2. Filled black symbols show numerical results for an undeformable sphere $R_\mu = 0$, and black stars are the analytical results from Eq. 10.

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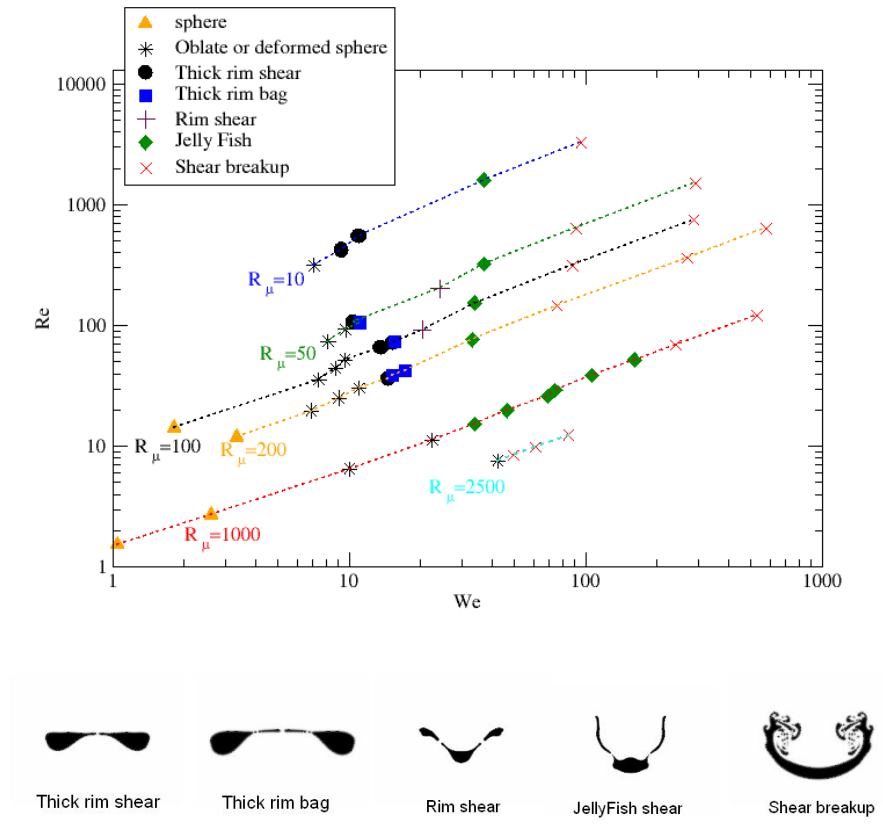


Figure 4: Regime diagram of the fragmentation modes as a function of Re and We numbers for various viscosity ratios: $R_\mu = 10$ (blue dotted line), $R_\mu = 50$ (green dotted line), $R_\mu = 100$ (black dotted line), $R_\mu = 200$ (orange dotted line), $R_\mu = 1000$ (red dotted line), and $R_\mu = 2500$ (turquoise dotted line). Our numerical results come from the first 62 simulations in table 2.

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Figure 5: Deformation and thick rim shear breakup of an iron drop within a magma ocean. In this model, $Re = 36.4$, $We = 14.6$, $R_\mu = 200$ (simulation #30 in Table 2).

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Figure 6: Deformation and thick rim bag breakup of an iron drop within a magma ocean. In this model, $Re = 42.5$, $We = 17.2$, $R_\mu = 200$ (simulation #32 in Table 2).

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Figure 7: Deformation and rim shear breakup of an iron drop within a magma ocean. In this model, $Re = 92.4$, $We = 20.3$, $R_\mu = 100$ (simulation #22 in Table 2).

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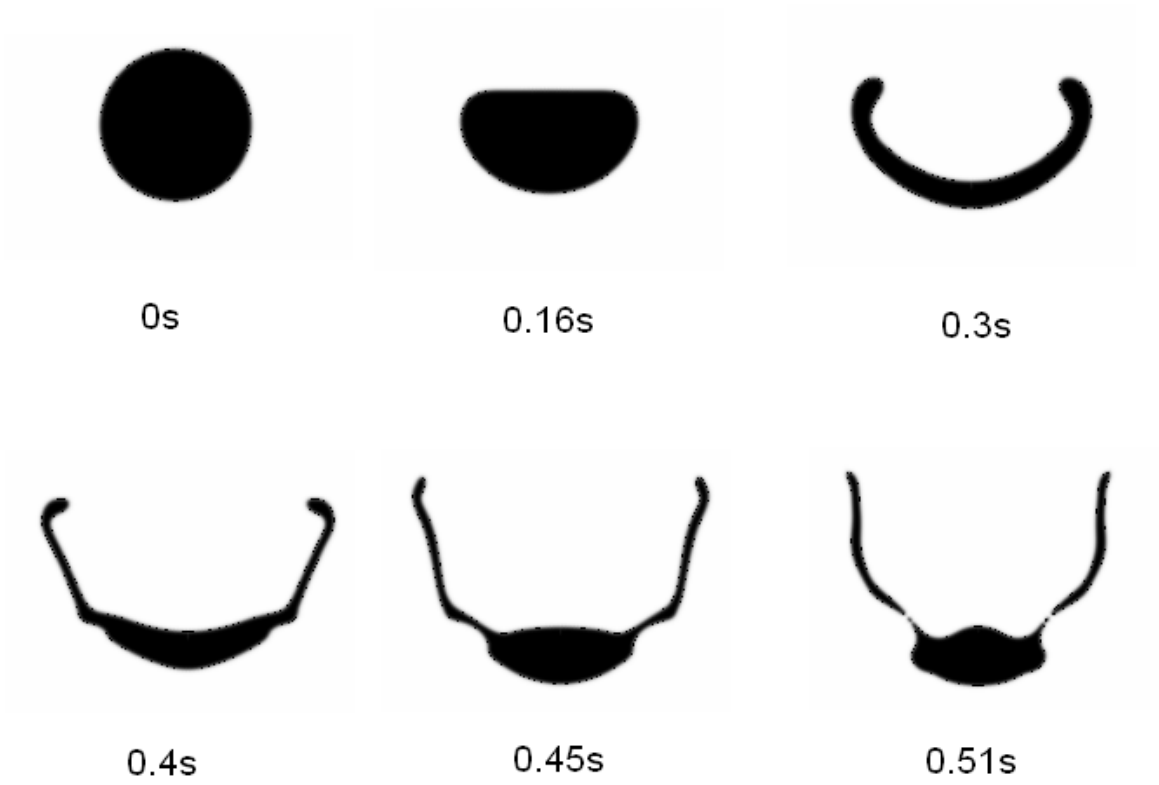


Figure 8: Deformation and jellyfish shear breakup of an iron drop within a magma ocean. In this model, $Re = 76.1$, $We = 33.1$, $R_\mu = 200$ (simulation #33 in Table 2).

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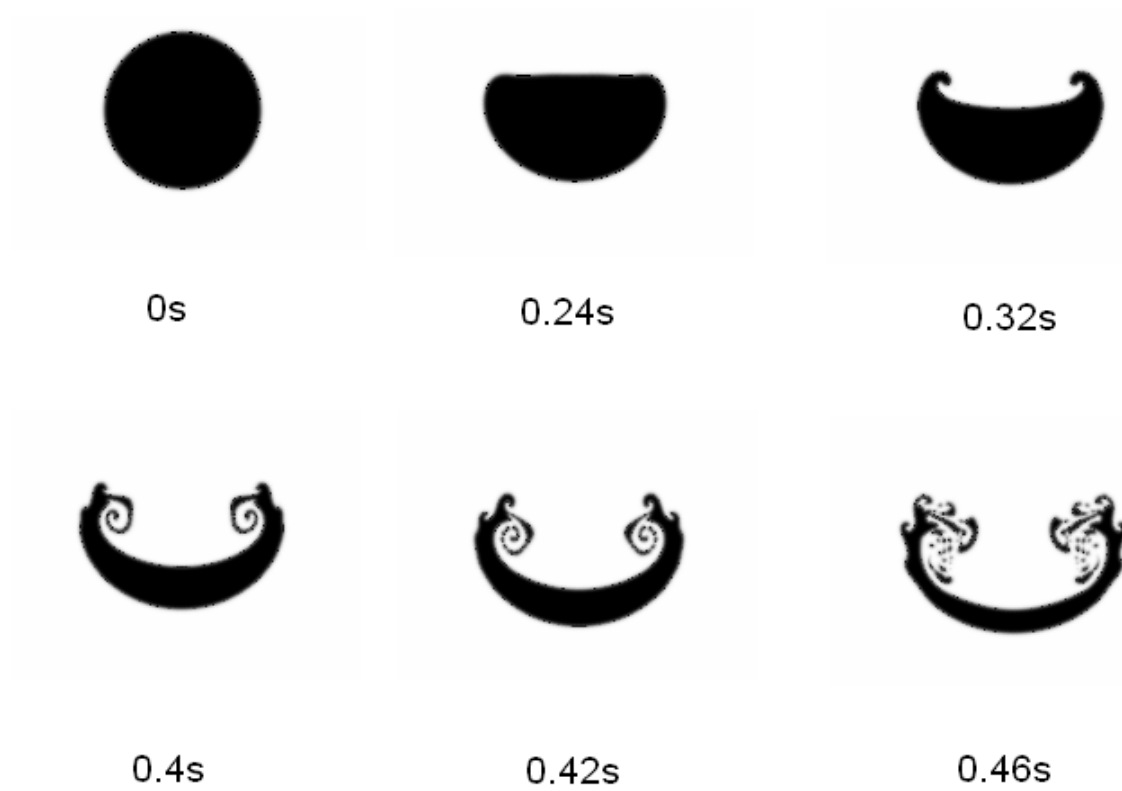


Figure 9: Deformation and shear breakup of an iron drop within a magma ocean. In this model, $Re = 2670$, $We = 636$, $R_\mu = 50$ (simulation #62 in Table 2).

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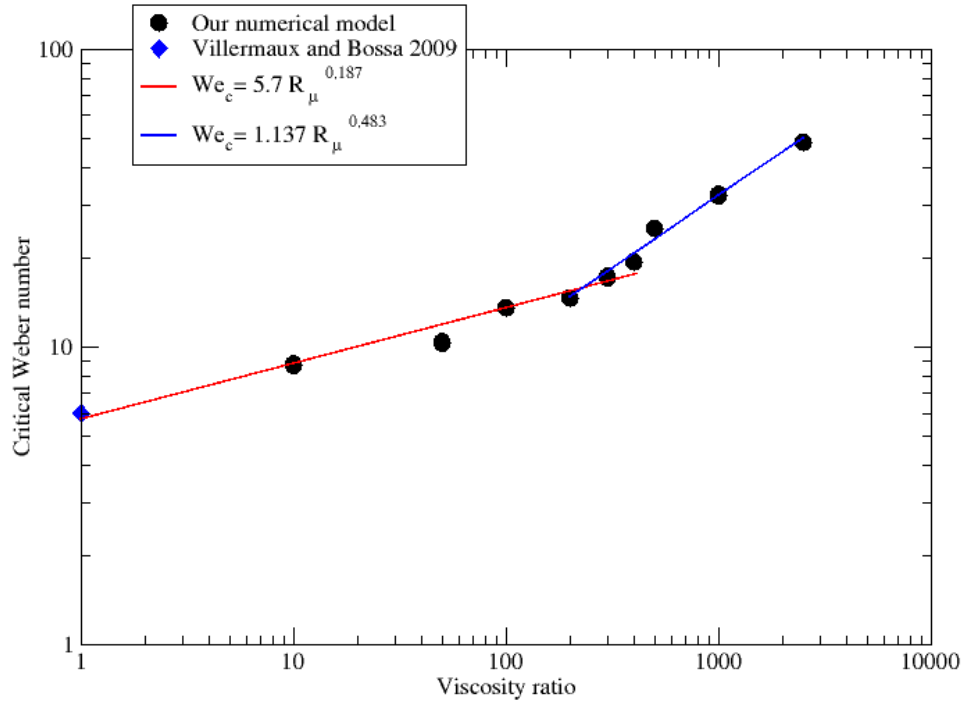


Figure 10: Critical Weber number as a function of the viscosity ratio. The blue diamond is the critical Weber number when the viscosity ratio equal to 1, as obtained by Villermaux and Bossa (2009). The red and blue lines represent the scaling laws derived from our data.

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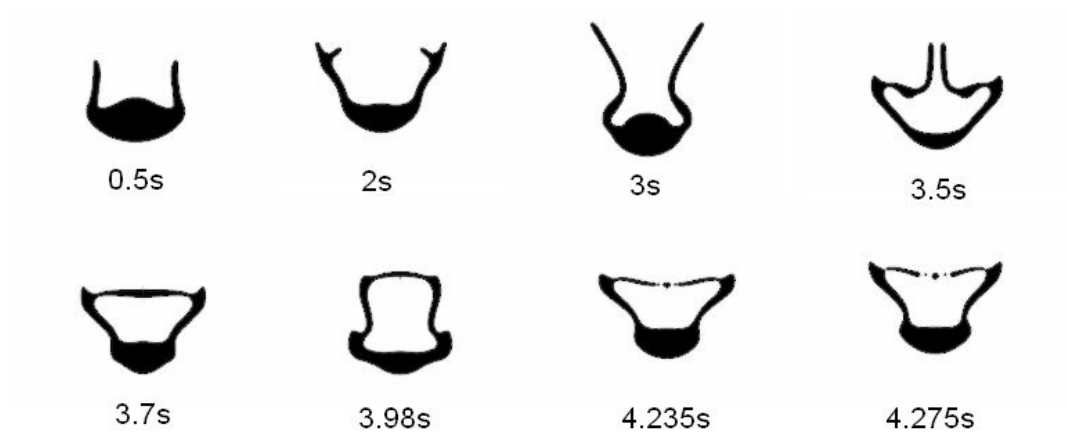


Figure 11: The path of a new fragmentation mode where the iron structure encloses the silicates.

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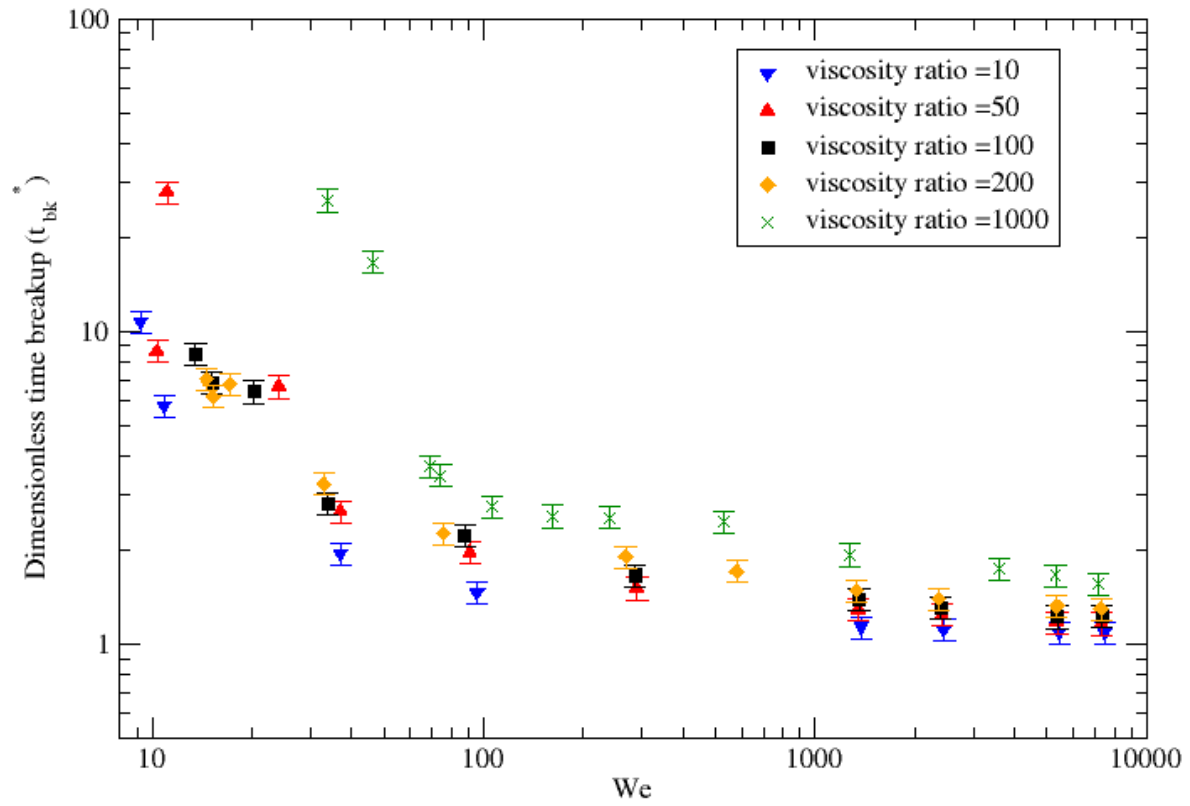


Figure 12: Non-dimensional break-up time as a function of Weber number for viscosity ratios R_μ ranging between 10 and 1000.

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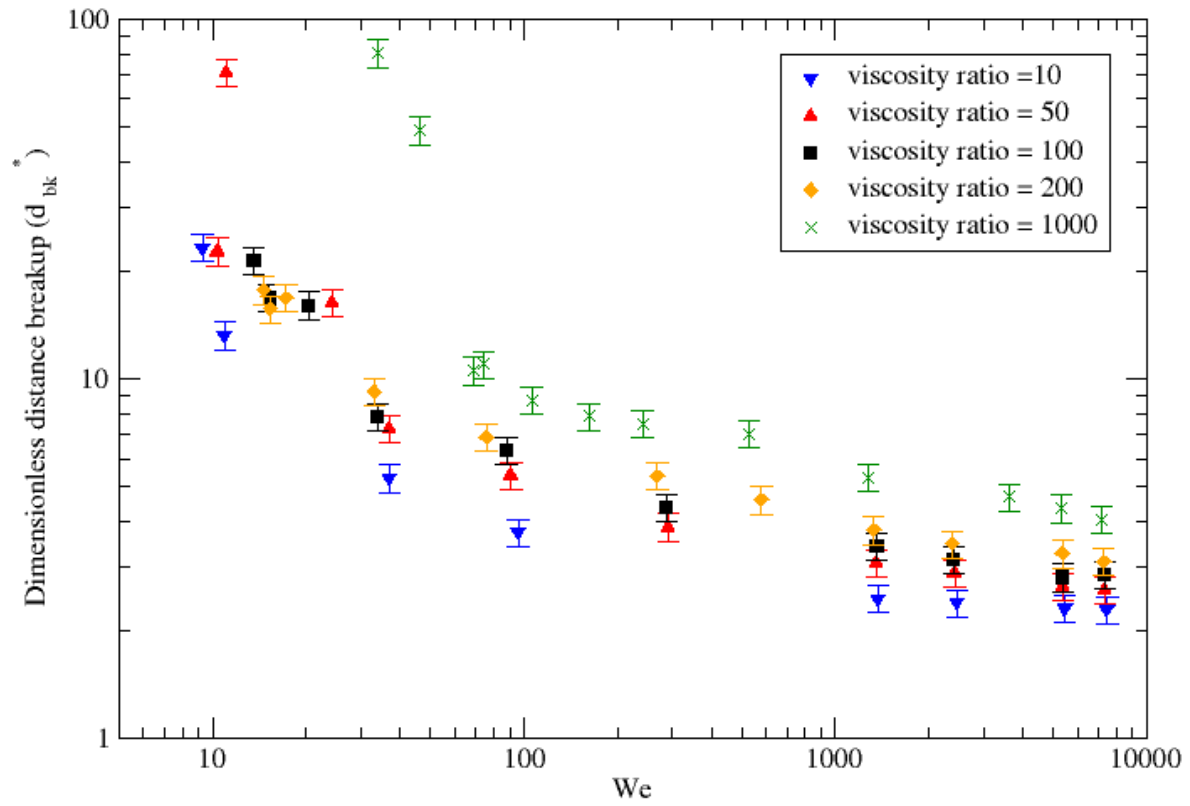


Figure 13: Non-dimensional break-up distance d_{bk}^* as a function of the Weber number for viscosity ratios R_μ ranging between 10 and 1000.

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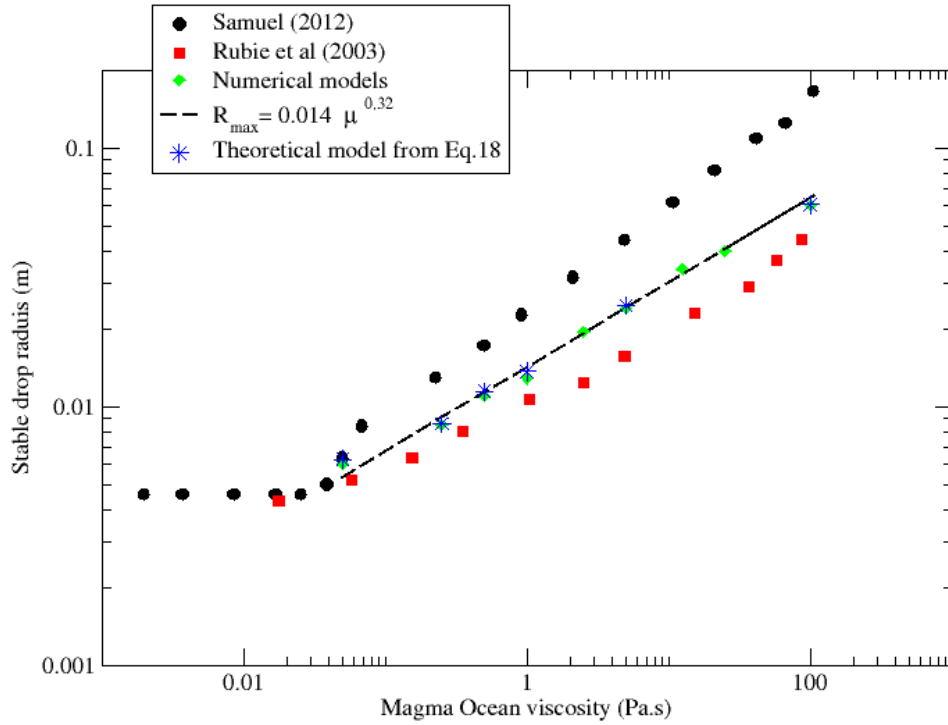


Figure 14: Stable drop radius as a function of plausible magma ocean viscosities. The green diamonds present our numerical results, the red squares correspond to the results of Rubie et al. (2003), the black circles display the results of Samuel (2012), the blue stars correspond to the analytical results of the Eq. 18 and the black dash line presents the scaling law proposed by this study.

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Figure 15: The final shape of the iron droplets for different initial conditions. Spherical case (left), prolate form (middle) and oblate form (right).

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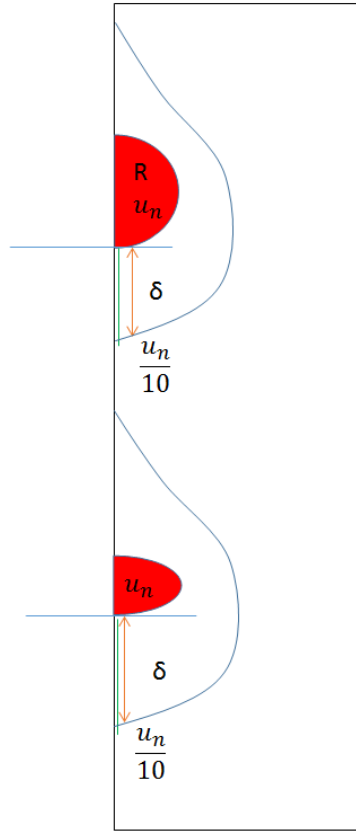


Figure 16: Schematic representation of the geometry used for the determination of the boundary layer thickness δ at the drop surface: spherical case (top) and deformed drop (bottom).

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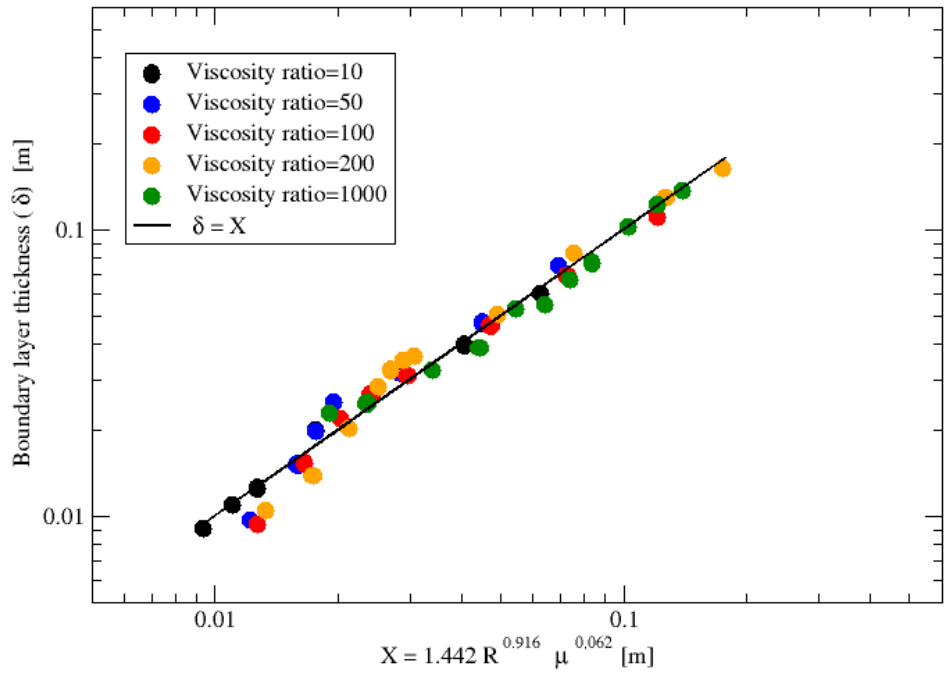


Figure 17: Boundary layer thickness as a function of the varied parameters in this study (drop radius and magma ocean viscosity) for viscosity ratios R_μ ranging between 10 and 1000. Our numerical results come from the first 62 simulations in Table 2).

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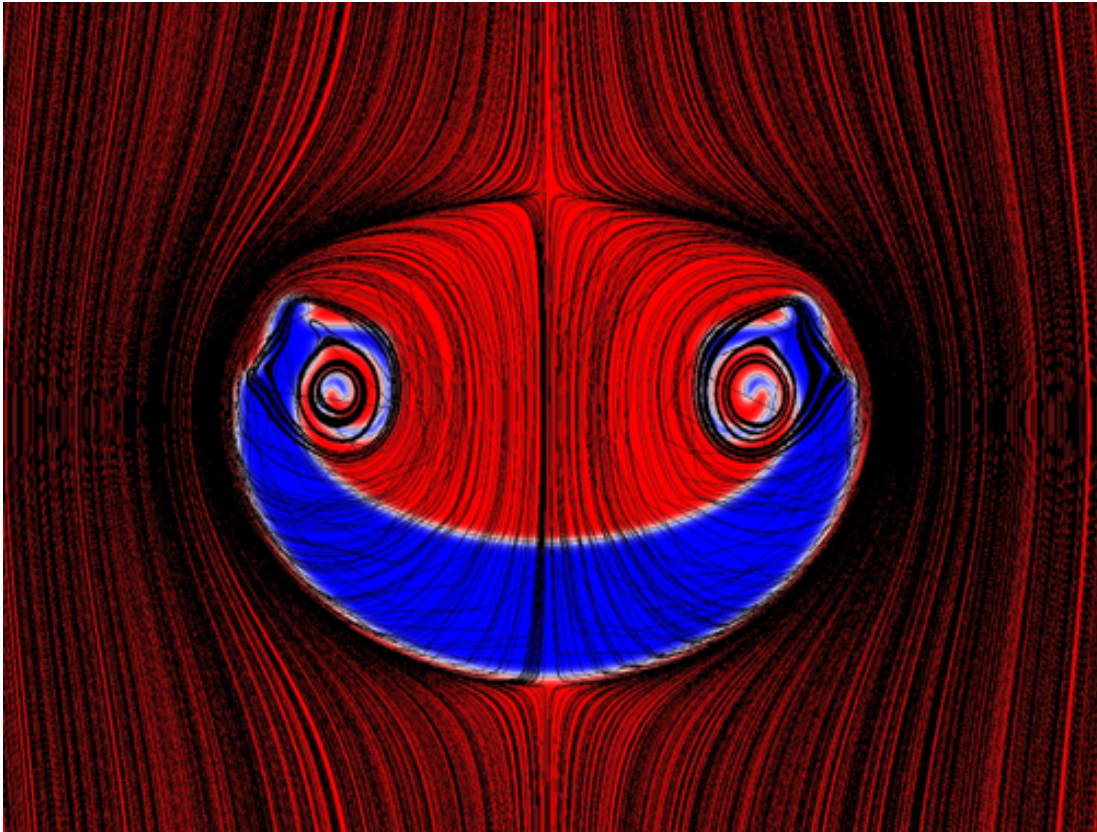


Figure 18: The streamlines around a large drop. In this model, $Re = 2670$, $We = 636$, $R_\mu = 50$ (simulation #62 in Table 2). The black lines are the streamlines, the red region represents the molten silicates and the blue region represents the deformable iron drop.

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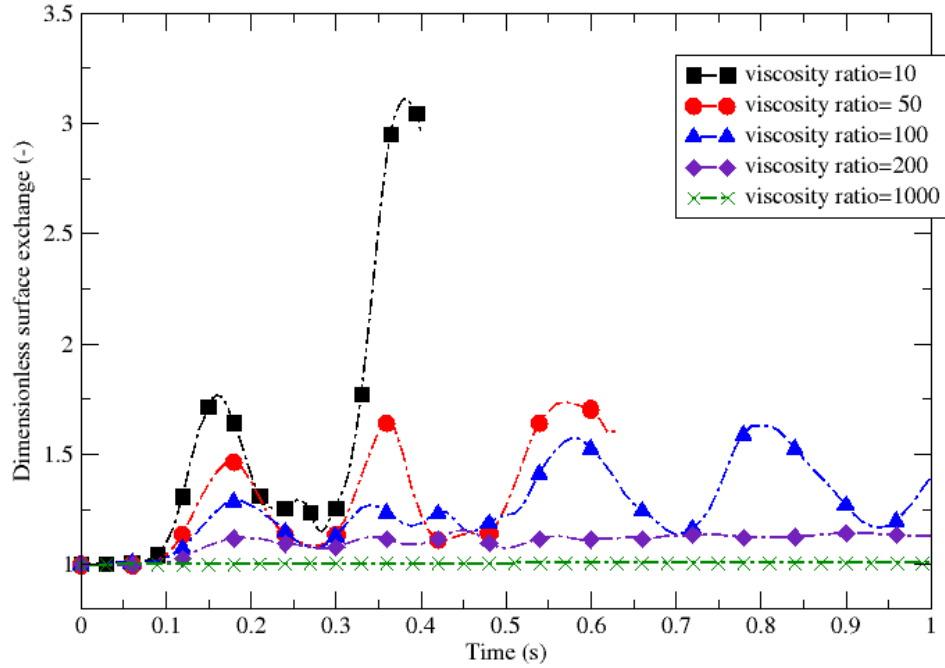


Figure 19: Non-dimensional surface exchange as a function of time for viscosity ratios R_μ ranging between 10 and 1000. Here, we consider a drop of initial radius $R = 10$ mm. For viscosity ratio = 10 (black line), $Re = 553$ and $We = 10.9$. For viscosity ratio = 50 (red line), $Re = 108$ and $We = 10.4$. For viscosity ratio = 100 (blue line), $Re = 44.2$ and $We = 8.74$. For viscosity ratio = 200 (purple line), $Re = 25.1$ and $We = 9.02$. For viscosity ratio = 1000 (green line), $Re = 2.70$ and $We = 2.61$.

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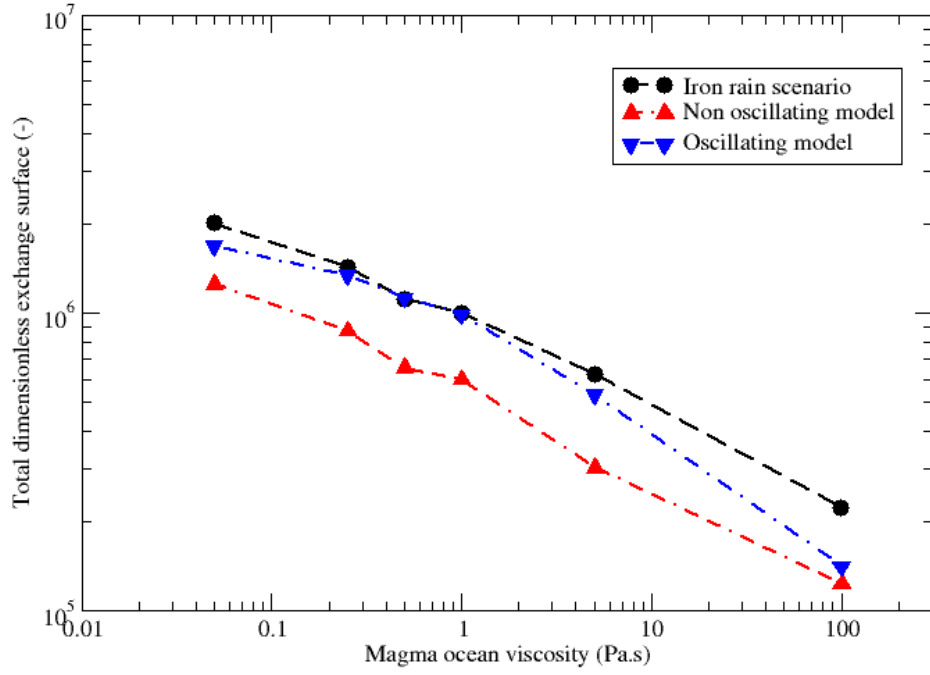


Figure 20: Normalised exchange surface S^* as a function of magma ocean viscosity after the breakup of a 10 km metal diapir. In the sinking droplet population, no cut-off is considered at $R = R_{max}$.

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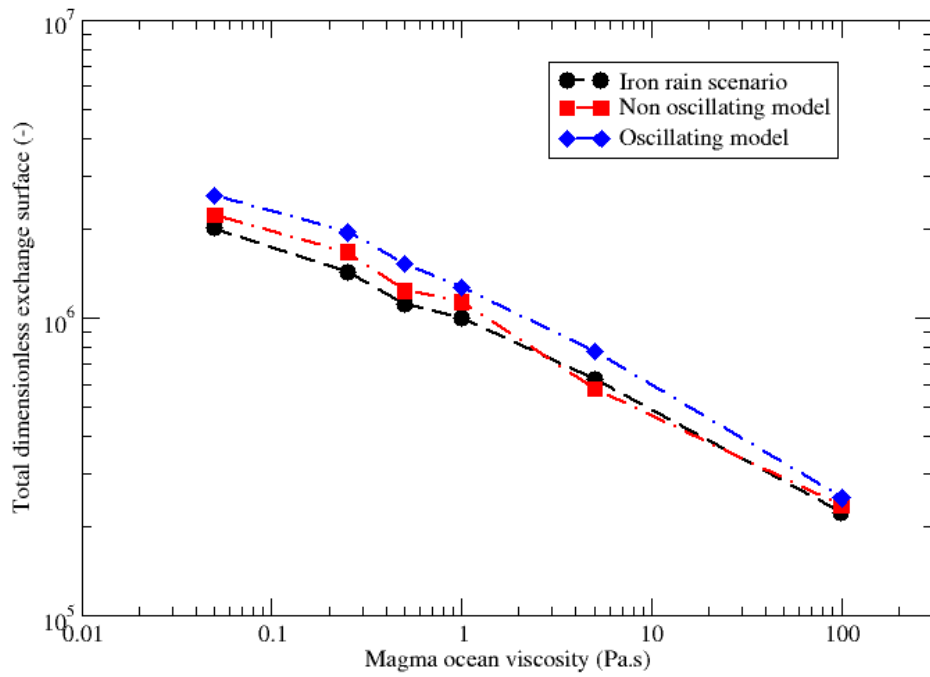


Figure 21: Normalised exchange surface S^* as a function of magma ocean viscosity after the breakup of a 10 km metal diapir. In the sinking droplet population, a cut-off is considered at $R = R_{max}$.

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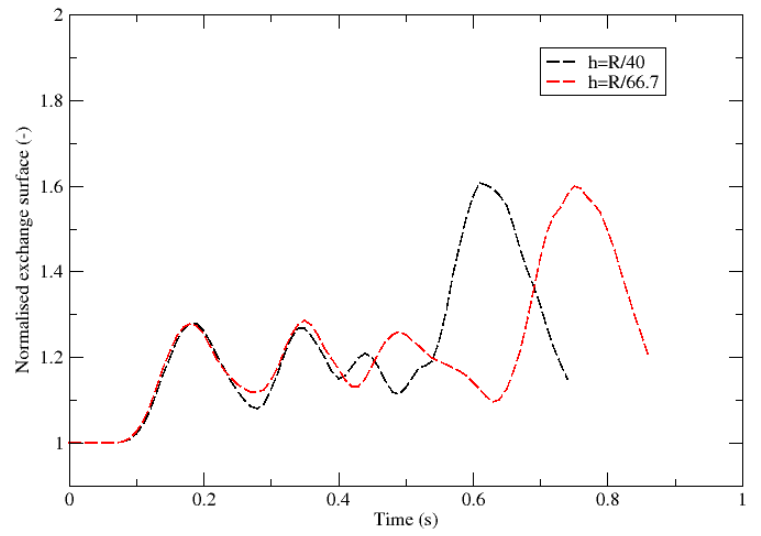
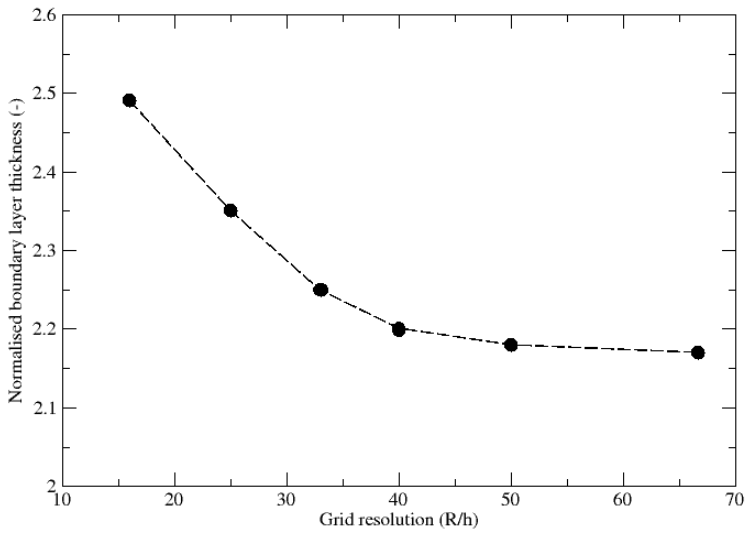


Figure 22: Comparison of different mesh sizes of a strongly oscillating drop (simulation #18 in Table 2). Left: Normalised boundary layer thickness as a function of grid sizes. Right: Normalised exchange surface as a function of time.

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Figure 23: Comparison of the final shape of the fragmented drop for two different mesh sizes. (simulation #83 in Table 2).

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