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# NEW INSIGHTS ON THE FORMATION OF THE TERRESTRIAL PLANETS

by  
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# Abstract

Not only do the sampled terrestrial worlds (Earth, Mars and asteroid 4 Vesta) differ in their nucleosynthetic isotopic compositions of Ca, Ti, Cr and Mo, but in addition the magnitude of these anomalies also appear to correlate with heliocentric distance. These cosmochemistry observations can be used to constrain plausible dynamical mechanisms for planet formation in the inner Solar System. While several studies examining the feeding zones of the terrestrial planets in the framework of the classical and Grand Tack models show that the terrestrial planets are more likely to have formed by the accretion of mostly-local materials with little material mixing in the protoplanetary disc, recent works challenge the ‘traditional’ view that the terrestrial planets formed by collisions of increasingly massive planetesimals by showing that the accretion of cm- to m-sized planetary bodies known as ‘pebbles’ can also reproduce the mass-orbit distribution of the terrestrial planets.

In this thesis, we adopt a two-pronged approach to determine the more plausible formation pathway of the terrestrial planets by combining  $N$ -body simulations with constraints from cosmochemistry data. We apply the pebble accretion model and the depleted disc model to the inner Solar System and study their dynamical outcomes and cosmochemistry implications. For the pebble accretion model study, we modelled the growth of a disc of planetesimals in the terrestrial planet region subjected to a flux of pebbles assumed to originate from the outer Solar System. The simulations were ran for a period of 4 Myr, after which we quantify the amount of mass in pebbles accreted by the inner disc planetesimals. For the depleted disc model study, we simulated the growth of a solid disc in the inner Solar System made up of planetesimals and embryos preferentially concentrated in an annulus within 1 – 1.5 au sans an inward-drifting pebble flux. The simulations were carried out in two phases: the first 5 Myr with a gas disc and the subsequent 150 Myr without. At the end of the simulations, we compute the feeding zones of the terrestrial planet analogues and the formation location of Vesta analogues.

Our results show that pebble accretion, if it occurred, can increase the mass in the solid disc by at least a few times its initial mass with reasonable assumptions that pebbles fragment to smaller-sized grains at the snow line and that gas-disc-induced orbital migration effects are in force. Such a large contribution in mass by pebbles would imply that the isotopic composition of the inner Solar System would be similar to the outer Solar System, where the pebbles are assumed to have originated from. This implication is in contrast to the observed isotopic dichotomy of the Solar System as sampled by known meteorites. The pebble accretion mechanism, however, is capable of generating a compositional gradient in the inner Solar System only if the planetesimals have diameters less than 300 km because of the dependence of pebble accretion efficiency with distance from the Sun.

The terrestrial planets that formed within the framework of the depleted disc model have feeding zones that correlate with their semi-major axis, indicating that they accreted most of their building blocks locally and that there was limited mixing of the solids in the disc. Furthermore, Vesta analogues also originate from regions in the disc close to Vesta’s current orbit. If the isotopic composition of the solids in the inner Solar System was heterogeneous and the isotopes were distributed along a heliocentric gradient, then the results from the depleted disc model imply that Earth, Mars and Vesta can be isotopically distinct.

Based on cosmochemical arguments we conclude that it is unlikely that pebble accretion played a major role in the formation of the terrestrial planets. The terrestrial planets should have formed via the mergers of planetesimals and embryos instead. In addition, there

should have been isotopic gradients in the inner Solar System established before the formation of the planetesimals. The isotopic gradients could have been generated by the accretion of material from the interstellar medium, as suggested by several studies, or that it could be innate to the Solar System.

## **Publications associated with this dissertation**

Parts of this thesis have appeared in the following publications and preprints:

- **Mah, J.**, Brasser, R., 2021. Isotopically distinct terrestrial planets via local accretion. *Icarus* 354, 114052
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# 1 Introduction

Understanding the formation of the terrestrial planets in our Solar System is a continuous endeavour motivated in part by humanity's curiosity of our own origins. How did the Earth form? What made the Earth? Where can we find clues? These seemingly basic questions turn out to be complex puzzles that require contributions from multiple fields such as astronomy, cosmochemistry and planetary science, to name a few. In recent years, researchers from these apparently disparate but complementary fields have taken notice of the developments in each other's fields and started to collaborate towards achieving a more comprehensive model of planet formation. Some of the results of these studies may be negative, appear inconclusive, challenge long-held perceptions and lead to even more questions, but our understanding of planet formation nevertheless increases because of the debate that these results ignited.

In this thesis, we synthesise state-of-the-art knowledge from theories of planet formation and cosmochemistry data and use this information to answer the question of whether the terrestrial planets grew by the accumulation of small (cm-sized) solids or were they the products of mergers between large (km-sized) planetary bodies. We will put forward a proposal to explain cosmochemistry data trends based on the outcomes of our numerical investigations. The thesis consists of two studies, each examining the formation of the terrestrial planets from one of the two aforementioned pathways. We aim to convey the message that utilising a variety of relevant cosmochemistry data can help to distinguish between different planet formation models and point to the direction(s) that future studies could follow in the quest of gaining full understanding of how the terrestrial planets take shape. In the following sections we will review several dynamical models of planet formation, introduce relevant cosmochemistry data used in our work, and outline the motivation and approach of the studies presented in this thesis.

## 1.1 Developments in planet formation theories

Studies to unravel the mysteries surrounding the formation pathways of the terrestrial planets have made considerable advances since the initial proposal by [Safronov \(1969\)](#) on the genesis of planetesimals via the agglomeration of dust particles in the protoplanetary disc. It is commonly accepted in the community that the terrestrial planets formed from collisions among protoplanets (also known as planetary embryos) of increasing size, although, as we will later discuss, this paradigm is starting to be challenged. The Classical model of terrestrial planet formation ([Chambers, 2001](#)) was built upon the results of early analytical derivations (e.g., [Wetherill, 1980](#); [Wetherill and Stewart, 1989](#)) and numerical simulations ([Kokubo and Ida, 1995, 1996, 1998](#)) of the evolution of a self-gravitating solid disc of planetesimals. Several planetesimals in the solid disc will grow much faster than the rest and produce a bimodal population in the disc comprising larger-sized planetary embryos and smaller-sized planetesimals ([Kokubo and Ida, 1998](#)). The embryos continue growing by accreting nearby planetesimals until they exhaust all the planetesimals in their feeding zones, by which time



39 the embryos will collide and merge among themselves to finally form the terrestrial plan-  
40 ets. [Chambers \(2001\)](#) shows that the growth timescales of the terrestrial planets are around  
41 several tens of millions of years.

42 A fundamental shortcoming of the Classical model is that it systematically produces  
43 planets that are several times the mass of Mars around 1.5 au. This shortcoming — termed  
44 as the ‘small Mars problem’ — spurred successive improvisations and refinements to the  
45 Classical model to form the terrestrial planets with the correct masses and orbits. Several  
46 studies found that starting with the gas giants Jupiter and Saturn located near their current  
47 orbits but with orbital eccentricities twice their current value ([Raymond et al., 2009](#)), or that  
48 starting with a narrow ring of material concentrated between 0.7 au and 1.0 au ([Hansen, 2009](#))  
49 are favourable initial conditions to reproduce Mars analogues with the correct mass. These  
50 studies show that rather specific initial conditions are needed to reproduce the masses and  
51 orbits of the terrestrial planets. For example, it was noted by [Raymond et al. \(2009\)](#) that the  
52 high eccentricities required of the gas giants are rather unrealistic, and the means to truncate  
53 the material in the solid disc is lacking (although see [Pierens et al. \(2014\)](#) and [Clement et al.  
54 \(2021\)](#) for the possibility of more eccentric Jupiter and Saturn).

55 In the following years, a radical proposal for the disc truncation mechanism was put  
56 forward. [Walsh et al. \(2011\)](#) presented a scenario wherein Jupiter and Saturn are locked in a  
57 mean-motion resonance (MMR) and migrated through the asteroid belt twice — first inwards,  
58 then outwards — aided by their interactions with the surrounding gas disc. In the process  
59 they concentrated the solid material in the terrestrial region to a narrow annulus. The gas-  
60 driven migration of the gas giants, dubbed as the ‘Grand Tack’, is successful at reproducing  
61 the small mass of Mars because the solid disc is truncated at around Earth’s orbit and this  
62 left the planetesimals in Mars’ region with insufficient material to grow to large sizes. The  
63 Grand Tack model has since been widely studied (e.g., [Jacobson et al., 2014](#); [Jacobson and  
64 Morbidelli, 2014](#); [O’Brien et al., 2014](#); [Jacobson and Walsh, 2015](#); [Brasser et al., 2016](#); [Deienno  
65 et al., 2016](#); [Matsumura et al., 2016](#)) and became well-established over time because it provided  
66 a plausible framework of the evolutionary history of the Solar System in addition to its ability  
67 in explaining the low mass of the asteroid belt and the apparent compositional diversity  
68 among its constituents ([DeMeo and Carry, 2014](#)), which seem to suggest that radial mixing  
69 of solid material occurred in the disc.

70 Despite the successes of the Grand Tack model, there are some studies that scru-  
71 tinised the model and found that the migration of Jupiter with Saturn in tow depends sen-  
72 sitively on the initial conditions of the gas disc. For example, [D’Angelo and Marzari \(2012\)](#)  
73 showed that the outward migration of Jupiter and Saturn to the region beyond 5 au only  
74 works for limited values of gas viscosity, surface density and temperature, and [Zhang and  
75 Zhou \(2010\)](#) showed that the surface density of the gas disc affects the orbital eccentricities  
76 of the gas giants which in turn determines the order of the MMR that they are captured in  
77 and whether the MMR is stable.

78 Alternatives to the Grand Tack scenario as the mechanism to truncate the solid disc  
79 have also been proposed. The works of [Izidoro et al. \(2014, 2015\)](#) and [Raymond and Izidoro  
80 \(2017b\)](#) explored the possibility of reproducing the orbital configuration of the terrestrial  
81 planets and the low mass of the asteroid belt by considering a local mass depletion around  
82 Mars’ orbit and various surface density profiles of the solid disc. The model achieved success  
83 with a very steep solid surface density profile ([Izidoro et al., 2015](#)) and also with the extreme  
84 assumption that the asteroid belt region was initially devoid of solid material ([Raymond and  
85 Izidoro, 2017b](#)). It was, however, not further elaborated nor investigated how the presupposed  
86 distribution of the solids came to be nor whether such steep density gradients are realistic.

87 Another model that was recently found to be capable of reproducing the configu-  
88 ration of the inner Solar System is the early instability model (e.g., [Clement et al., 2018, 2019](#)).  
89 It is the outcome of a sophisticated reinvestigation of the earlier proposed Nice model (e.g.,  
90 [Tsiganis et al., 2005](#)) which is based on the conjecture that a dynamical instability occurred  
91 in the outer Solar System sometime in the history of the Solar System that resulted in the ob-  
92 served dynamical features of the current Solar System after a phase of giant planet scattering  
93 and migration ([Thommes et al., 1999](#)). [Clement et al. \(2018\)](#) found using direct simulations of  
94 both the inner and outer Solar System that a giant planet instability occurring within 10 Myr  
95 from the time of the dispersal of the gas disc is consistent with many currently observed fea-  
96 tures of the Solar System. A follow-up study ([Clement et al., 2019](#)) with simulations including  
97 the effects of collisional fragmentation further revealed that the formation timescale of the  
98 terrestrial planets in the framework of this model are also consistent with the measurements  
99 from radioactive chronometers (e.g., [Touboul et al., 2007](#); [Kleine et al., 2009](#); [Dauphas and](#)  
100 [Pourmand, 2011](#)).

## 101 **1.2 Formation of the terrestrial planets: Planetesimals or** 102 **pebbles?**

103 Until now it seems to be the case that the community is approaching a clearer understanding  
104 of the appropriate initial conditions to form the terrestrial planets with the aid of progres-  
105 sively high-resolution simulations performed on fast computers. The dynamical models that  
106 we have described so far are based on the conventional understanding that the terrestrial  
107 planets evolved to their current size through a series of accretion processes involving increas-  
108 ingly massive planetary bodies. However, there is now an emerging view which postulates  
109 that the growth of the terrestrial planets could in fact be a consequence of the accretion of  
110 small cm-sized bodies called ‘pebbles’ instead, in direct challenge to the traditional view. Al-  
111 though the *pebble accretion* model ([Ormel and Klahr, 2010](#); [Lambrechts and Johansen, 2012](#))  
112 was originally developed to resolve a problem related to the formation of the core of gas  
113 giants, several recent studies ([Levison et al., 2015b](#); [Johansen et al., 2021](#)) have applied this  
114 model to the terrestrial planet region and found positive results that encourage further in-  
115 vestigations on the plausibility of this formation pathway for the terrestrial planets.

116 Pebbles, observed to be abundant in protoplanetary discs (e.g., [Testi et al., 2003](#);  
117 [Wilner et al., 2005](#); [Rodmann et al., 2006](#)), are thought to have formed via the coagulation  
118 of smaller-sized dust particles in the outer regions of the disc ([Lambrechts et al., 2014](#); [Ida](#)  
119 [et al., 2016](#)). They tend to spiral towards the central star under the influence of gas drag  
120 because dynamical friction with the surrounding gas causes them to lose angular momentum  
121 ([Weidenschilling, 1977](#)). During their passage through the protoplanetary disc these pebbles  
122 will encounter planetesimals in the inner Solar System and some of these will have been  
123 accreted onto the planetesimals.

124 The effect of this pebble flux on the formation of the terrestrial planets has been  
125 investigated by [Levison et al. \(2015b\)](#) and by [Johansen et al. \(2021\)](#). By adopting specific  
126 values for the various parameters of the gas disc, [Johansen et al. \(2021\)](#) showed that it is  
127 possible for planetesimals in the inner Solar System to achieve masses close to the current  
128 terrestrial planets within the lifetime of the gas disc. The planetesimals that become the  
129 terrestrial planets are assumed to have formed at different times and migrated to their current  
130 orbits from a distant location. The rapid growth of the terrestrial planets in this model is  
131 made possible by the continuous but gradually diminishing flux of pebbles. The authors  
132 further proposed that the pebbles that were initially accreted onto the terrestrial planets have

133 composition akin to the volatile-depleted non-carbonaceous (NC) meteorites while the later-  
134 accreted pebbles have composition akin to the volatile-rich carbonaceous (CC) meteorites.  
135 The proposal is based on a plausible dynamical evolution pathway of protoplanetary discs  
136 where material in the inner region tend to spread outwards initially due to viscous expansion  
137 but will eventually drift inwards to the central star at a later time. The authors fitted the time  
138 for the compositional change to be 3.8 Myr (presumably after the formation of the Calcium-  
139 Aluminium-rich inclusions (CAI) usually adopted as time zero for the Solar System; e.g.,  
140 [Amelin et al., 2010](#); [Bouvier and Wadhwa, 2010](#); [Connelly et al., 2012](#)) based on the results  
141 of [Schiller et al. \(2018, 2020\)](#) that the fraction of CC in the Earth and Mars could be 42% and  
142 36%, respectively.

143 The composition of the terrestrial planets is an area of active research and stud-  
144 ies adopting different initial conditions and assumptions arrive at different results, although  
145 there is a general agreement among earlier works (e.g., [Lodders, 2000](#); [Fitoussi et al., 2016](#);  
146 [Brasser et al., 2017](#); [Dauphas, 2017](#); [Woo et al., 2018](#)), which we will describe in the next sec-  
147 tion, that the contribution of CC material to the terrestrial planets should be fairly limited.  
148 Based on this assumption, [Levison et al. \(2015b\)](#) investigated the outcome of having the peb-  
149 bles that form the terrestrial planets originate locally from the inner Solar System instead. In  
150 this model, the pebbles contribute to the growth of planetesimals in the inner disc in the first  
151 few Myr but the planetary bodies did not reach the full size of the terrestrial planets. [Levi-  
152 son et al. \(2015b\)](#) find that the planetesimals closer to the central star accrete more pebbles  
153 and grow to larger sizes compared to planetesimals further away because the pebble accre-  
154 tion cross-section has a semi-major axis dependence resulting from their assumptions on the  
155 Stokes number. Mars' smaller size compared to Earth and Venus can therefore be easily re-  
156 produced because it formed from the mergers of smaller-sized planetesimals. It is perhaps  
157 more accurate to describe the contribution of the pebble accretion mechanism in this model  
158 as helping to generate the appropriate initial mass-semi-major axis distribution of planetes-  
159 imals that would naturally reproduce the masses of the terrestrial planets via subsequent  
160 collisions and mergers. However, the model proposed by [Levison et al. \(2015b\)](#) requires a  
161 rather high value for the surface density of the gas disc which raises questions about its  
162 feasibility and plausibility; in addition, they did not include planet migration in their study.

163 The results of these studies examining the formation of the terrestrial planets in  
164 the framework of the pebble accretion model are indeed interesting and they set the stage  
165 for further research in this direction. The work of [Levison et al. \(2015b\)](#) found that pebble  
166 accretion played a supportive role in the early growth stages of planetesimals in the inner  
167 Solar System while [Johansen et al. \(2021\)](#) reported that pebble accretion could potentially  
168 be responsible for the formation of the actual terrestrial planets in one stage. Did pebble  
169 accretion play a role in the formation of the terrestrial planets? If it did, how much mass did  
170 the pebbles contribute? Further studies would benefit from incorporating constraints from  
171 cosmochemistry, as demonstrated in the work of [Johansen et al. \(2021\)](#) (for example) to be  
172 useful. In the following section we will delve into the cosmochemistry data that are helpful  
173 to our work described in this thesis.

## 174 1.3 Cosmochemistry data and trends

### 175 1.3.1 Isotopic dichotomy in the Solar System

176 The bulk isotopic and elemental compositions of a planetary body is the cumulative average  
177 of its constituent building blocks (e.g., [Drake and Righter, 2002](#); [Fitoussi et al., 2016](#); [Dauphas,  
178 2017](#); [Mezger et al., 2020](#)), and is the end-product of the protoplanetary disc region(s) from

179 which the planetary body accreted. The sampled solar system bodies for which we know (or  
 180 infer) the parent bodies are: Earth, Moon, Mars and asteroid 4 Vesta. Known Martian me-  
 181 teorites include the Shergotty, Nakhla and Chassigny (SNC) meteorites, ALH 84001, NWA  
 182 7034, Tissint, Zagami and some more, while Vesta is very likely to be represented by the  
 183 Howardite-Eucrite-Diogenite (HED) class of meteorites (e.g., [McCord et al., 1970](#); [Consol-  
 184 magno and Drake, 1977](#); [Binzel and Xu, 1993](#); [Keil, 2002](#); [McSween et al., 2013](#)). Furthermore,  
 185 asteroids 434 Hungaria and 6 Hebe may also be represented in our meteorite collections  
 186 ([Greenwood et al., 2020](#)) because they could be the parent bodies of the aubrites ([Zellner,  
 187 1975](#); [Zellner et al., 1977](#); [Clark et al., 2004](#); [Čuk et al., 2014](#)) and H chondrites, which are one  
 188 of the components of the ordinary chondrites group ([Gaffey et al., 1993](#); [Gaffey and Gilbert,  
 189 1998](#); [Binzel et al., 2004, 2019](#)), respectively. Collectively, the meteorites representing these  
 190 planetary bodies fall into a larger group known as the non-carbonaceous (NC) group based  
 191 on their bulk isotopic compositions ([Warren, 2011](#)). The constituents of the NC group are  
 192 thought to have originated from the inner Solar System, in contrast to the carbonaceous  
 193 (CC) group which is thought to represent the outer Solar System ([Warren, 2011](#)).

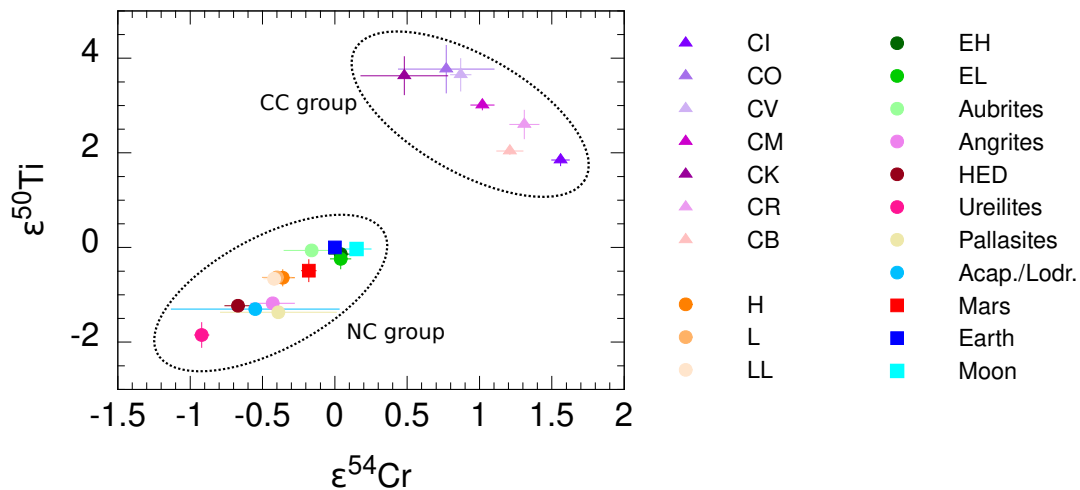


FIGURE 1.1: Measured  $\epsilon^{50}\text{Ti}$  and  $\epsilon^{54}\text{Cr}$  isotopic anomalies of known meteorites normalised to the values for the Earth. The meteorites fall into two distinct groups thought to represent the inner and outer Solar System, suggesting that the material in these two regions were kept separate at least until the formation of the chondrites. Acap. and Lodr. are abbreviations for Acapulcoites and Lodranites, respectively. Data sourced from [Shukolyukov and Lugmair \(2006\)](#); [Trinquier et al. \(2007, 2008, 2009\)](#); [Qin et al. \(2010a,b\)](#); [Yamashita et al. \(2010\)](#); [Larsen et al. \(2011\)](#); [Petit et al. \(2011\)](#); [Zhang et al. \(2011, 2012\)](#); [Yamakawa and Yin \(2014\)](#).

194 The compositional dichotomy of the Solar System is perhaps most obvious from a  
 195 plot of  $\epsilon^{50}\text{Ti}$  versus  $\epsilon^{54}\text{Cr}$ , which are the most neutron-rich stable isotopes of these elements  
 196 (Fig. 1.1). The components of the carbonaceous (or jovian) group are relatively enriched  
 197 in  $\epsilon^{50}\text{Ti}$  and  $\epsilon^{54}\text{Cr}$  while the components of the non-carbonaceous (or terrestrial) group are  
 198 relatively depleted in these isotopes. The clustering of the meteorites into two distinct groups  
 199 is also observed for many other elements with different geochemical characteristics such as  
 200 O, Mo, Ni, Ru and W ([Qin and Carlson, 2016](#); [Kleine et al., 2020](#), and references therein). The  
 201 clear clustering of the meteorites and the dearth of known meteorites plotting in the region  
 202 connecting the two groups led to the notion that the two meteorite reservoirs are separated  
 203 in space and/or time (e.g., [Warren, 2011](#)). A popular proposal for the means to keep the two  
 204 reservoirs separated is the formation and growth of Jupiter ([Kruijer et al., 2017](#)) – proto-  
 205 Jupiter with a mass of about 20 Earth masses ( $M_E$ ) ([Lambrechts et al., 2014](#)) pushes away

206 the gas near its orbit, creating a gap (density deficit) in the protoplanetary disc that traps  
207 inflowing solid material at the outer edge (Morbidelli et al., 2016). Furthermore, Kruijer et al.  
208 (2017) showed using iron meteorites – thought to have formed at an earlier time than the  
209 chondrites (Kruijer et al., 2014) – that the NC and CC reservoirs must have been separated  
210 for at least 4 Myr after the formation of the Solar System. However, the capacity of Jupiter  
211 as the purported ‘barrier’ is challenged by Brassler and Mojzsis (2020) who showed that a  
212 substantial amount of outer Solar System material could have flowed past Jupiter into the  
213 inner Solar System during Jupiter’s growth, ‘contaminating’ the inner Solar System with  
214 outer Solar System material and reducing the isotopic differences between the two regions.  
215 Brassler and Mojzsis (2020) proposed instead that the two reservoirs could be separated by  
216 the presence of ring-like gaps that are innate to the protoplanetary disc. Despite the ongoing  
217 debate, what remains certain is the existence of an early and sustained separation between  
218 the inner and outer regions of the protoplanetary disc.

### 219 1.3.2 Isotopic heterogeneity in the non-carbonaceous chondrite group and 220 the potential building blocks of the terrestrial planets

221 Another observation from Fig. 1.1 is the difference in the isotopic compositions of the Earth,  
222 Mars, HED meteorites, aubrites and H chondrites despite them being part of the same large  
223 NC group. In fact, there are measurable differences in their nucleosynthetic isotope anom-  
224 alies on the scale of parts per  $10^4$  to  $10^6$  for elements such as Ba, Ca, Cr, Fe, Mo, N, Nd, Ni, O, Ru,  
225 Sm, Ti, W, Xe and Zr (see Qin and Carlson, 2016, for an in-depth review). The variations in  
226 these nucleosynthetic isotopes are due to the particular distribution of presolar dust grains in  
227 the Solar protoplanetary disc and are thought to be impervious to planetary processes. The-  
228 ory dictates that no two planetary bodies will exhibit the same isotopic composition unless  
229 they both accreted their building blocks from the same reservoir(s) with the same proportion  
230 of nucleosynthetic isotopes. Therefore, the distinct isotopic compositions of the above plan-  
231 etary bodies suggests that there are differences in the compositions of their building blocks  
232 which would imply formation at various locations throughout the disc (e.g., Carlson et al.,  
233 2018).

234 In particular, the dissimilarity between Earth’s and Mars’ isotopic compositions  
235 has prompted studies to identify the potential building blocks of the terrestrial planets from  
236 known meteorites. In mixing models that use meteorite isotopic compositions as constraints,  
237 chondrites (enstatite chondrites (EC), ordinary chondrites (OC) and carbonaceous chondrites  
238 (CC)) are more commonly employed as the starting point instead of achondrites because the  
239 bulk chemical compositions of the former’s parent bodies are better constrained (Dauphas,  
240 2017). The aim of such mixing model is to compute, using the Monte Carlo method, the  
241 composition of the terrestrial planets as a mixture of chondrites given constraints from the  
242 isotopic anomalies and elemental abundances measured for known chondrites by lowering  
243 the  $\chi^2$  of the fit.

244 For the Earth, the best-fit combination obtained from chondritic mixing models  
245 give 70% EC + 21% H + 5% CV + 4% CI (Lodders, 2000), 91% EC + 7% OC + 2% CC (Dauphas  
246 et al., 2014b), 71% EC + 24% OC + 5% CC (Dauphas, 2017) and 50% angrites + 32% H + 8% CI  
247 + 10% CV (Fitoussi et al., 2016) when achondrites are considered, while dynamical modelling  
248 arrives at 87% EC + 13% OC in the framework of the Grand Tack model (Brasser et al., 2017;  
249 Woo et al., 2018). These results suggest that the dominant building blocks of the Earth are  
250 enstatite chondrites (or, more precisely, parent bodies whose isotopic composition are akin to  
251 enstatite chondrites) with minor contributions from parent bodies isotopically akin to ordi-  
252 nary and carbonaceous chondrites. Earth’s water budget and hydrogen isotope composition  
253 also appears to support an enstatite chondrite source (Piani et al., 2020).

254 This mixing model results for the potential building blocks of the Earth stand in  
 255 contrast to the results for Mars where the models give 85% H + 11% CV + 4% CI based  
 256 on oxygen isotopes (Lodders and Fegley, 1997), 45% EC + 55% OC when taking into ac-  
 257 count chromium, molybdenum, nickel and titanium isotopes (Sanloup et al., 1999; Tang and  
 258 Dauphas, 2014), 68% EC + 32% OC when combining dynamical simulations with the mixing  
 259 model (Brasser et al., 2018), and 55% angrites + 36% H + 9% CI in the special case when achon-  
 260 drites are considered (Fitoussi et al., 2016). These results show that the mixture of building  
 261 material – assuming only chondrites – that went into the Earth is different from that of Mars,  
 262 and furthermore that the mixtures of each planet are dependent on the isotopes considered  
 263 in the model.

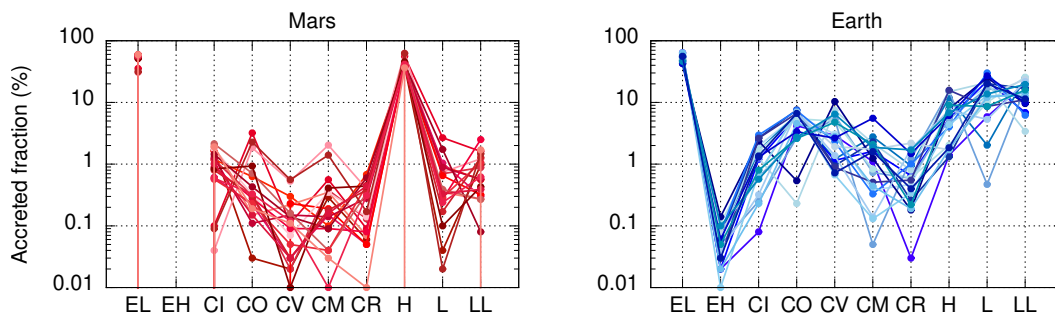


FIGURE 1.2: Contribution of various chondrite group to the composition of Mars and Earth computed from a Monte Carlo mixing model. The model uses meteorite isotopic compositions and elemental abundances as inputs and the isotopic compositions of Earth and Mars (Fitoussi et al., 2016; Dauphas, 2017) as constraints. Shown here are the 20 best-fit combinations (lowest  $\chi^2$ ) from 20 mixing model simulations. The maximum contribution of carbonaceous chondrites to the building blocks of the Earth and Mars is about 10%. Plot taken from Mah and Brasser (2021).

264 We have also carried out our own computations for the composition of the Earth  
 265 and Mars assuming only chondritic meteorites as input. We have expanded on the mixing  
 266 models of Fitoussi et al. (2016), Dauphas (2017) and Brasser et al. (2018) by adding the CM  
 267 and CR meteorite components of the carbonaceous chondrite variety while separating the  
 268 CO and CV into individual components. In addition, we also split up the enstatite chondrites  
 269 and ordinary chondrites – which were taken to be one single component by the previous  
 270 studies – into their respective components. Our mixing model computes the contribution by  
 271 each meteorite component while taking into account the isotopic anomalies in  $\Delta^{17}\text{O}$ ,  $\epsilon^{50}\text{Ti}$ ,  
 272  $\epsilon^{54}\text{Cr}$ ,  $\epsilon^{62}\text{Ni}$  and  $\epsilon^{92}\text{Mo}$  and the respective concentration of these elements. A description of  
 273 the inner workings of our mixing model is given in Appendix A. We show the 20 best-fit  
 274 compositions of the Earth and Mars obtained from 20 mixing model simulations in Fig. 1.2.  
 275 Taking the average from the 20 best-fit outcomes, our mixing model gives  $(52 \pm 6)\%$  EC +  
 276  $(36 \pm 4)\%$  OC +  $(12 \pm 2)\%$  CC for the Earth and  $(53 \pm 9)\%$  EC +  $(45 \pm 8)\%$  OC +  $(2 \pm 1)\%$  CC  
 277 for Mars. The uncertainties are given as one standard deviation of the mean. Our results are  
 278 broadly consistent with those from earlier works where it was found that the contribution  
 279 of EC and OC are roughly equal for Mars with almost no contribution from CC whereas  
 280 EC dominates the composition of the Earth with the maximum contribution of CC capped  
 281 at about 10%. We note that the contribution of EC to Earth is slightly lower in our model  
 282 compared to previous studies and this is likely due to the large uncertainties in the  $\epsilon^{92}\text{Mo}$   
 283 measurement for the meteorites.

284 The results of the mixing model studies give us an estimate of the regions in the  
 285 protoplanetary disc from which the Earth and Mars accreted their building materials. Mars’  
 286 best-fit chondritic mixture suggests that it could have formed near the boundary between the  
 287 EC and OC reservoirs while the Earth could have formed in the EC reservoir and further away

288 from the EC-OC boundary (Woo et al., 2018). The contribution of CC to the building blocks  
 289 of the Earth, however, is open to interpretation. On the one hand, it could be that CC did con-  
 290 tribute to the Earth's making by delivering water and other volatiles, although this became  
 291 disputed by a recent study that reports on the similarity between the deuterium/hydrogen  
 292 (D/H) ratio of EC and the Earth's mantle (Piani et al., 2020). On the other hand, it is also possible  
 293 that the mixing model returns CC as part of the Earth's building blocks simply because  
 294 Earth is an end-member of the non-carbonaceous chondrite group and a mixture of solely  
 295 EC and OC cannot reproduce the isotopic composition of the Earth; this is especially true for  
 296 oxygen.

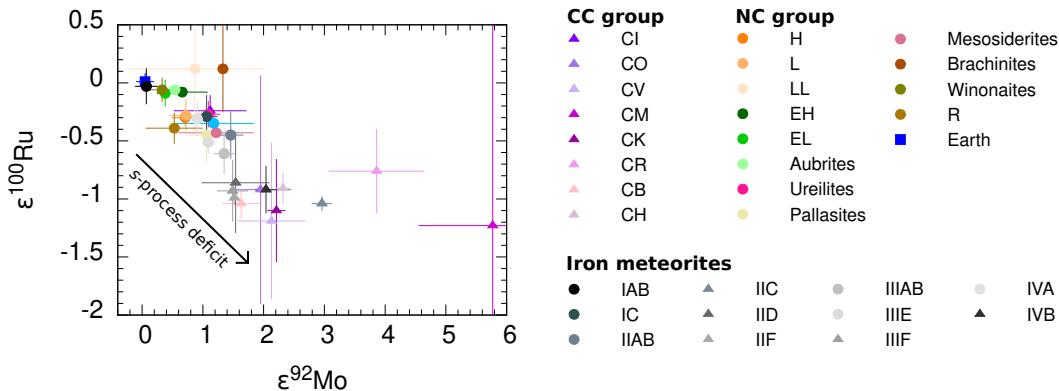


FIGURE 1.3: Measured  $\epsilon^{92}\text{Mo}$  and  $\epsilon^{100}\text{Ru}$  isotopic anomalies of known meteorites normalised to the values for the Earth. All the known meteorites plot to the lower right following a trend of increasing deficit of  $s$ -process isotopes and perhaps also an increasing formation distance from the Sun. The Earth has an end-member composition that prompted proposals that it accreted material from a possibly extant reservoir enriched in  $s$ -process isotopes. Data for  $\epsilon^{92}\text{Mo}$  sourced from Dauphas et al. (2002); Burkhardt et al. (2011, 2012, 2014, 2017); Budde et al. (2016, 2018, 2019); Kruijer et al. (2017); Poole et al. (2017); Render et al. (2017); Worsham et al. (2017, 2019); Bermingham et al. (2018); Hilton et al. (2019); Hopp et al. (2020);  $\epsilon^{100}\text{Ru}$  data are from Chen et al. (2010); Fischer-Gödde et al. (2015); Bermingham and Walker (2017); Burkhardt et al. (2017); Fischer-Gödde and Kleine (2017); Bermingham et al. (2018); Worsham et al. (2019); Hopp et al. (2020).

297 It has been shown (e.g., by Drake and Righter, 2002 and more recently, a review  
 298 by Mezger et al., 2020) that the current repository of known meteorites does not constitute  
 299 the whole picture of the Earth's building blocks. Earth's location as an end-member in plots  
 300 of Ti versus Cr (Fig. 1.1; Trinquier et al., 2009; Warren, 2011) and Ru versus Mo (Fig. 1.3;  
 301 Dauphas et al., 2014a; Fischer-Gödde et al., 2015) could also hint at an additional reservoir  
 302 in the region closer to the Sun than where the ECs are thought to have formed. Fig 1.3  
 303 illustrates the fact that one cannot get the isotopic composition of the Earth by mixing EC,  
 304 OC and CC. This therefore prompted the suggestion of the existence of an additional reservoir  
 305 characterised by an enrichment in  $s$ -process isotopes. The Earth should have accreted some  
 306 material from this reservoir to offset the  $s$ -process deficit signature of the other meteorites  
 307 (Fischer-Gödde and Kleine, 2017; Render et al., 2017). However, meteorite samples from this  
 308  $s$ -process-enriched reservoir have not been found to date and it has been suggested that  
 309 all the material from this reservoir have been accreted into the terrestrial planets (Drake  
 310 and Righter, 2002; Burkhardt et al., 2011, 2016). Indeed, Fischer-Gödde et al. (2020) may  
 311 have found evidence of this reservoir in ancient terrestrial rocks that show positive  $\epsilon^{100}\text{Ru}$   
 312 anomalies, but more measurements are needed to confirm this hypothesis.

313 **1.3.3 Potential isotopic gradients in the inner Solar System and the origins**  
 314 **of the isotopic heterogeneity**

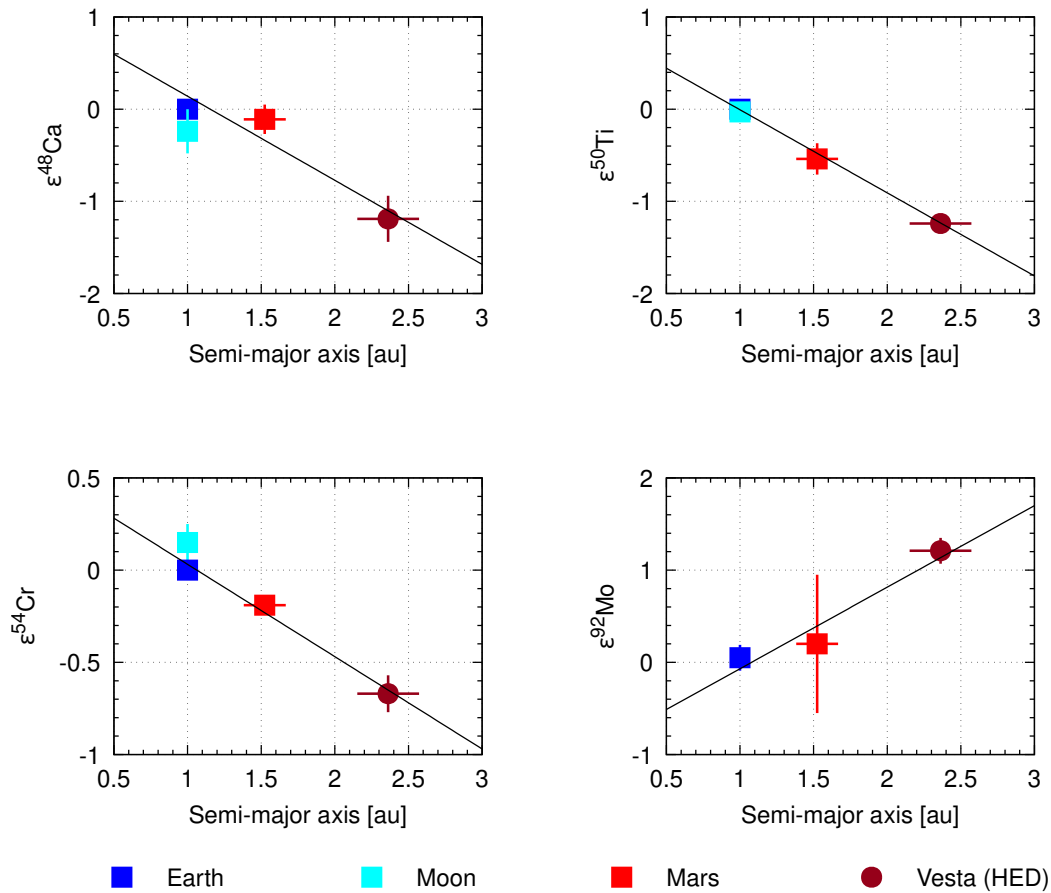


FIGURE 1.4: Calcium, titanium, chromium and molybdenum isotopic anomalies for the Earth, Moon, Mars and Vesta (sampled by the HED meteorites) plotted with respect to the semi-major axes of these planetary bodies. The isotopic compositions of these planetary bodies appear to correlate with their distance from the Sun, hinting at the presence of isotopic gradients in the inner Solar System (e.g., [Trinquier et al., 2009](#); [Yamakawa et al., 2010](#)). Data sourced from the compilation of [Dauphas \(2017\)](#) and references therein. The  $\epsilon^{92}\text{Mo}$  data point for HED is plotted using data for Mesosiderites sourced from [Dauphas et al. \(2002\)](#) because measurements for HED meteorites are unavailable in the literature.

315 Examining the isotopic composition of the Earth with respect to several other dif-  
 316 ferentiated bodies in the inner Solar System could help in understanding the bigger picture  
 317 of how planetary bodies in the inner Solar System formed. Several works (e.g., [Trinquier](#)  
 318 [et al., 2009](#); [Yamakawa et al., 2010](#)) identified an apparent correlation between the isotopic  
 319 anomalies in  $\epsilon^{50}\text{Ti}$  and  $\epsilon^{54}\text{Cr}$  and the semi-major axis of the Earth, Mars and Vesta (HED me-  
 320 teorites). We show in Fig. 1.4 that the reported correlation also exists for  $\epsilon^{48}\text{Ca}$  (e.g., [Schiller](#)  
 321 [et al., 2018](#)) and possibly for  $\epsilon^{92}\text{Mo}$  (e.g., [Burkhardt et al., 2011](#)).

322 The origin of the observed correlations in  $^{50}\text{Ti}$  and  $^{54}\text{Cr}$  favoured by [Yamakawa](#)  
 323 [et al. \(2010\)](#) is that Type 1a supernovae supplied these isotopes to the inner Solar System  
 324 just before the formation of the planetesimals that became the precursors of Earth, Mars  
 325 and Vesta, although the supernova-origin view is still highly debated. The authors argued  
 326 for a short isotope delivery timing because of the rapid homogenisation of nuclides in the  
 327 protoplanetary disc. Results of hydrodynamical simulations show that radionuclides injected  
 328 by supernovae spread out evenly in the protoplanetary disc in  $10^3$  to  $10^6$  years (e.g., [Ouellette](#)



329 [et al., 2009](#), and references therein). The correlated isotopic compositions of the Earth, Mars  
330 and Vesta therefore reflects a potential gradient in the distribution of  $^{50}\text{Ti}$  and  $^{54}\text{Cr}$  isotopes  
331 in the inner protoplanetary disc where there is an increased depletion of these isotopes with  
332 increasing distance from the Sun. Furthermore, the isotopes  $\epsilon^{48}\text{Ca}$ ,  $\epsilon^{50}\text{Ti}$  and  $\epsilon^{54}\text{Cr}$  show the  
333 same trend (Fig. 1.4) because they are thought to share a common origin, i.e., a supernovae  
334 source (e.g., [Hartmann et al., 1985](#); [Woosley, 1997](#); [Wanajo et al., 2013](#)). The trend for  $\epsilon^{92}\text{Mo}$  is  
335 different because Mo isotopes are synthesised via the  $p$ -,  $s$ - and  $r$ - processes (e.g., [Brennecka  
336 et al., 2013](#)).

337 The origin of the observed diversity in the isotopic anomalies of the differentiated  
338 bodies in the inner Solar System is still not well known. It is commonly thought to be the  
339 product of imperfect mixing of dust and gas during the early stages of the Solar System's  
340 formation (e.g., [Birck, 2004](#); [Andreasen and Sharma, 2007](#); [Trinquier et al., 2007](#); [Brennecka  
341 et al., 2013](#)). There have been several proposals to explain how the heterogeneity came about.  
342 The first of these is that the heterogeneity is a 'cosmic chemical memory' that the Solar neb-  
343 ular inherited during its birth in the natal molecular cloud ([Clayton, 1982](#); [Dauphas et al.,  
344 2002](#)) which could have been the shell of a Wolf-Rayet star's wind bubble ([Dwarkadas et al.,  
345 2017](#)). The second group of proposals accounting for the heterogeneity calls for the late ad-  
346 dition of external material from the interstellar medium. It has been suggested that fresh  
347 ejecta from asymptotic giant branch (AGB) stars or supernovae was added late into the Solar  
348 nebula ([Trinquier et al., 2007](#)), or that there was a temporal change in the composition of  
349 infalling material from the molecular cloud, with early infalling material having CC com-  
350 position and later infalling material having NC composition ([Nanne et al., 2019](#)). The third  
351 group of proposals relates the isotopic heterogeneity to physical processes in the Solar nebula  
352 itself. Thermal gradients in the protoplanetary disc could have selectively remove volatile el-  
353 ements, moderately-volatile elements and thermally-unstable presolar silicates in the region  
354 closer to the Sun, creating a compositional gradient with distance from the Sun (e.g., [Trin-  
355 quier et al., 2009](#); [Burkhardt et al., 2012](#); [Ek et al., 2020](#)). Furthermore, thermal processing  
356 could also modify the composition of infalling material from the molecular cloud ([Ek et al.,  
357 2020](#)). Other than thermal gradients in the disc, the outward-then-inward movement of the  
358 water snow line throughout the lifetime of the disc has also been suggested to be the mech-  
359 anism to generate two planetesimal populations with distinct compositions in the inner and  
360 outer Solar System ([Lichtenberg et al., 2021](#)).

361 Recently, there is also a new interpretation of the isotopic data. [Schiller et al. \(2018\)](#)  
362 suggested that the  $\epsilon^{48}\text{Ca}$  isotopic heterogeneity among the Earth, Mars and Vesta is corre-  
363 lated with the masses (and sizes) of these planetary bodies and could reflect instead their  
364 different accretion timescales, i.e., Vesta accreted earliest, followed by Mars and finally, the  
365 Earth. The authors suggest that the correlation is due to a change in the inner Solar System's  
366 composition and that the change could be brought about by the influx of pebbles from the  
367 outer Solar System. Assuming that the initial composition of the planetesimals in the inner  
368 Solar System is initially homogeneous and akin to those of the ureilites (a type of primitive  
369 achondrite with the lowest abundance of  $\epsilon^{48}\text{Ca}$ ), [Schiller et al. \(2018\)](#) showed that the gradual  
370 accretion of CI carbonaceous chondrite-like material from the outer disc over the lifetime of  
371 the gas disc is consistent with the isotopic compositions of Earth, Mars and Vesta. The in-  
372 terpretation that the isotopic heterogeneity among the major inner Solar System bodies is  
373 generated by the introduction of outer Solar System material over time is in contrast with  
374 the interpretations by other authors described in the previous paragraphs that the isotopic  
375 differences present in the major planetary bodies reflect a spatial heterogeneity in the pro-  
376 toplanetary disc. This proposal formed the basis of further investigations by [Johansen et al.  
377 \(2021\)](#) who used semi-analytical simulations to study the feasibility of forming the terrestrial

378 planets via pebble accretion (described earlier in Section 1.2), although they did not perform  
379 a suite of  $N$ -body simulations.

## 380 1.4 Key questions and structure of thesis

381 High-precision isotope data of meteorites made available in the past decade have been grad-  
382 ually adopted by studies seeking to understand how the terrestrial planets formed. The dis-  
383 tinct isotopic compositions of the Earth and Mars have been employed to constrain dynamical  
384 models of planet formation. Previous studies examining the classical model (Chambers, 2001)  
385 found that the feeding zones (region of the protoplanetary disc where a planet sourced most  
386 of its building material) of the terrestrial planets show a correlation with their semi-major  
387 axis (e.g., Raymond et al., 2004; O’Brien et al., 2006; Fisher and Ciesla, 2014; Kaib and Cowan,  
388 2015; Woo et al., 2018). This is because the planets are thought to grow by the accretion of  
389 solid material within their respective feeding zones in the classical model. Consequently,  
390 Earth and Mars’ isotopic differences can be reproduced if the material that these two planets  
391 accreted have different isotopic compositions. However, forming Mars analogues at 1.5 au  
392 with the correct mass is a fundamental shortcoming of this model.

393 Studies examining the Grand Tack model (Walsh et al., 2011) found that the feeding  
394 zones of the terrestrial planets are wide and strongly overlapping with no obvious correlation  
395 with semi-major axis (Brasser et al., 2017; Woo et al., 2018). The main reason for this outcome  
396 is the migration of the gas giants. Jupiter and Saturn’s excursion through the asteroid belt  
397 region excited the orbits of the material in the terrestrial planet region and caused them  
398 to undergo mixing (Carlson et al., 2018). If there was a difference in the composition of the  
399 material in the terrestrial planet region, it is expected that the difference will be homogenised.  
400 The similar feeding zones of the terrestrial planets in the Grand Tack model thus imply that  
401 they should have similar compositions, in contrast with the isotope data. However, there is  
402 still a low but non-zero probability ( $< 5\%$ ) that Mars analogues can have feeding zones that  
403 are distinct to that of the Earth (Brasser et al., 2017; Woo et al., 2018).

404 The terrestrial planet feeding zones computed from the classical and Grand Tack  
405 models suggest that the formation pathway of the terrestrial planets is more likely to fol-  
406 low the classical model, i.e., the planets accreted the majority of their building blocks locally  
407 within their feeding zone with limited mixing of material in the disc. This is backed up by  
408 very recent high-resolution simulations run on graphics cards (Woo et al., 2021). In addition,  
409 the growth of the terrestrial planets should have proceeded via collisions among planetesi-  
410 mals followed by collision among larger-sized planetary embryos. This view is recently chal-  
411 lenged by studies showing that pebble accretion could have contributed (in various extents)  
412 to the formation of the terrestrial planets (Levison et al., 2015b; Johansen et al., 2021). The  
413 contribution from pebble accretion, if found to be substantial, could potentially change our  
414 understanding of planet formation in our Solar System because it is also associated with the  
415 interpretation of the isotope data proposed by Schiller et al. (2018). It is therefore eminent to  
416 conduct further investigations to understand how pebble accretion works in the inner Solar  
417 System.

418 In this thesis, we will study the formation of planetary bodies in the inner Solar  
419 System as a whole. We will use the correlation between isotopic compositions of Earth, Mars  
420 and Vesta and their respective semi-major axis, as well as the distinct compositions of these  
421 planetary bodies as additional constraints to help us understand their formation pathway and  
422 formation location. To this end, we will employ a two-pronged approach. We will examine  
423 two different models of planet formation – the pebble accretion model (Ormel and Klahr,

424 2010; Lambrechts and Johansen, 2012), and the depleted disc model (Izidoro et al., 2014, 2015)  
425 – with the aim of answering the following questions:

- 426 • Did pebble accretion play a role in the inner Solar System?
- 427 • Are the distinct isotopic compositions of the terrestrial planets and Vesta a natural  
428 outcome of the depleted disc model?
- 429 • Did the terrestrial planets primarily form by the accretion of pebbles or planetesimals,  
430 or a mixture of both?

431 The remainder of this thesis is made up of two chapters dedicated to the results  
432 of our studies on the pebble accretion model and the depleted disc model, and one chapter  
433 summarising our work followed by a discussion of potential future investigations. In Chap-  
434 ter 2 we report the results of our examination of the pebble accretion model. We applied  
435 the model to the inner Solar System to study the growth of a disc of planetesimals subjected  
436 to inward-drifting pebbles from the outer Solar System over the lifetime of the gas disc. In  
437 particular, we will quantify the amount of mass increase in the solid disc by the end of this  
438 period. We will also discuss if the pebble accretion mechanism can generate a compositional  
439 gradient in the inner Solar System and if its implications for the composition of the terrestrial  
440 planets are consistent with cosmochemistry data.

441 In Chapter 3 we report the dynamical outcomes of the depleted disc model. We  
442 constructed a solid disc containing both planetary embryos and planetesimals based on the  
443 original model proposed by Izidoro et al. (2014, 2015) but using a more realistic gas disc model  
444 developed by Ida et al. (2016). The solids are preferentially concentrated within 1 au – 1.5 au  
445 to mimic a mass concentration in the terrestrial planet region and a mass depletion beyond  
446 the orbit of Mars. We compute the feeding zones of the terrestrial planets formed in this  
447 model and determine if the distinct isotopic compositions of Earth, Mars and Vesta can be  
448 reproduced naturally.

449 Finally, in Chapter 4 we summarise the outcomes and implications of the two stud-  
450 ies presented in this thesis and discuss possible future directions to take in the quest of gain-  
451 ing a more comprehensive understanding of how the terrestrial planets in our Solar System  
452 formed. Last but not least, the novel points of our studies are: (1) we conduct high-resolution  
453  $N$ -body simulations with a wide range of initial conditions for the gas disc to quantify the  
454 effects of pebble accretion in the inner Solar System, and (2) we are the first to study in detail  
455 the dynamical outcomes and cosmochemistry predictions of the depleted disc model by using  
456 a realistic gas disc model and testing for a variety of initial conditions.

## 2 Role of pebble accretion the inner Solar System

### 2.1 Introduction

In this chapter we study the effects of pebble accretion in the inner Solar System when Jupiter is still growing. We will use  $N$ -body simulations to model the growth of planetesimals in the inner Solar System that are subjected to a flux of pebbles over the course of Jupiter's growth, with the aim of quantifying the amount of mass delivered to the inner disc by pebble accretion. Our motivation stems from the promising results of several previous works, both from the aspects of planetary dynamics and cosmochemistry, that reported the potential of the pebble accretion mechanism (e.g., [Lambrechts and Johansen, 2012](#)) to lay the groundwork for the formation of the terrestrial planets (e.g., [Levison et al., 2015b](#); [Johansen et al., 2021](#)) and its capability of explaining the correlation between the  $\epsilon^{48}\text{Ca}$  isotopic composition and the mass (or size) of the Earth, Mars and Vesta ([Schiller et al., 2018](#)). However, there have also been reports ([Brasser and Mojzsis, 2020](#); [Kleine et al., 2020](#)) challenging the efficiency of Jupiter as a competent barrier in preventing excessive pebbles from entering the inner Solar System and maintaining the isotopic dichotomy. In the following we briefly describe the method and outcome of several previous works that investigated the feasibility of the pebble accretion mechanism in forming the terrestrial planets.

The work of [Levison et al. \(2015b\)](#) employed numerical simulations to study the effect of pebble accretion in the inner Solar System. They subjected a population of planetesimals distributed between 0.7 au and 2.7 au to a flux of inward drifting pebbles that are continuously generated in the same region over a period of 2 Myr. The planetesimals are embedded in a gas disc with an  $r^{-1}$  ( $r$  is the distance to the star) surface density function. Since the pebbles are formed continuously in the inner Solar System, the surface density of the gas was chosen to be about 5 times the minimum mass solar nebula (MMSN; [Hayashi, 1981](#)), a value deemed sufficient to sustain continuous pebble formation in the disc in their simulations. Simulations with sufficient mass to form the terrestrial planets are continued for another 120 Myr. [Levison et al. \(2015b\)](#) found that the small mass of Mars is a natural outcome of their model because the efficiency of planetesimals to grow via pebble accretion decreases with distance from the star. The key assumption of this work is the local formation of pebbles that contributed to the mass of planetesimals that went on to form the terrestrial planets via planetesimal mergers. It is based on observations that show the composition of outer Solar System material to be too distinct to have contributed much to the terrestrial planets as well as the fact that the flux of pebbles necessary to form the giant planets ([Levison et al., 2015a](#)) is too great to form the terrestrial planets. The assumption of local pebble formation over time is, however, rather peculiar and deviates from the more common assumption used in many studies (including ours) that the pebbles originate in the outer Solar System.

[Johansen et al. \(2021\)](#) propose that the planetesimals that went on to become the terrestrial planets (Venus, Earth and Mars) all formed initially near the water snow line, and

496 that these planetesimals subsequently migrated inwards to the current semi-major axis of the  
 497 terrestrial planets while accreting pebbles along the way. The snow line in their disc model  
 498 is initially located between 1.2 au to 2.0 au and migrates inwards with time. The planet  
 499 formation scenario presented in their work is based on good analytical fits of the growth  
 500 track equations of [Johansen et al. \(2019\)](#). The masses of Venus and Mars can be reproduced  
 501 using reasonable values of the disc temperature profile ( $T \propto r^{-3/7}$ ; [Chiang and Goldreich,](#)  
 502 [1997](#)), Stokes number ( $10^{-3} < S < 0.1$ ) and pebble flux. The study assumes that these  
 503 planets' current masses are their masses at the time of gas disc dissipation, and that both  
 504 Venus and Mars grew entirely from pebbles without giant impacts. [Johansen et al. \(2021\)](#)  
 505 state that these planets began forming near 1.6 au and migrated to their current locations,  
 506 and accreted mm-sized pebbles from inside the snow line. For Earth, the maximum mass  
 507 achieved after the end of the pebble accretion phase (when the gas disc has dissipated) is 0.6  
 508 Earth mass ( $M_E$ ). A giant impact with a body of mass  $0.4 M_E$  later in time is suggested so that  
 509 the mass of the Earth can reach its current value, but it is unclear whether the impactor that  
 510 formed the Moon had such a high mass. In their model, the terrestrial planets (Venus, Mars  
 511 and proto-Earth) accreted pebbles of two different compositions in the sequence of (1) non-  
 512 carbonaceous (specifically, ureilite-like) in the first few Myr, followed by (2) carbonaceous  
 513 (specifically, CI-like) until the dissipation of the gas disc. They assume that  $\sim 40\%$  of Earth's  
 514 composition comes from pebbles that originated in the outer Solar System with an assumed  
 515 CI-like isotopic composition ([Schiller et al., 2018, 2020](#)). The low mass of Mars can be achieved  
 516 by assuming that it formed later than the other terrestrial planets. While the suggestion of  
 517 planetesimal formation triggered by snow line passage is not new ([Drażkowska and Alibert,](#)  
 518 [2017](#)), the only manner in which this can result in planetesimals with a different composition  
 519 is if the material that condensed at the snow line to become planetesimals has a different  
 520 composition at a different distance to the Sun, which [Johansen et al. \(2021\)](#) argue occurred  
 521 because of the initial viscous expansion of the disc. Planetesimal formation at a static snow  
 522 line is difficult to reconcile with different isotopic compositions.

523 The major differences between our work and the studies summarised previously lie  
 524 in the gas disc model we adopted (which we describe in Appendix B.1) and the computation  
 525 and underlying assumptions of the value of the Stokes number. In our simulations, we follow  
 526 [Ida et al. \(2016\)](#) and compute the radius and the Stokes number of the pebbles self-consistently  
 527 depending on their location in the disc, and time. In contrast, the Stokes number used in  
 528 the work of [Levison et al. \(2015b\)](#) is fixed while [Johansen et al. \(2021\)](#) assume that it lies in  
 529 a particular range and that the pebbles are mm-sized. Our simulations are in a sense more  
 530 realistic concerning the treatment of pebbles, but the downside is that a longer computational  
 531 time is required and that our gas disc model may be too simplistic.

532 In the next subsection we will describe how pebble accretion works for planetesi-  
 533 mals of different sizes and a minor but important modification to our numerical code that we  
 534 inherited from [Matsumura et al. \(2017\)](#). This is followed by a description of the initial condi-  
 535 tions of our simulations and the simulation outcomes. The content that we will henceforth  
 536 present is currently in preparation for submission to a peer-reviewed journal.

## 537 2.2 Pebble accretion onto planetesimals

### 538 2.2.1 Basic formulation

539 Based on the formulation of [Ormel and Klahr \(2010\)](#) and [Ormel and Kobayashi \(2012\)](#) and  
 540 modified by [Ida et al. \(2016\)](#), the accretion rate of cm-sized pebbles onto a planetesimal of

541 mass  $M$  and located at distance  $r$  from the central star is derived to be

$$\dot{M} = \min \left[ 1, \frac{C\hat{b}^2\sqrt{1+4\mathcal{S}^2}}{4\sqrt{2\pi}\mathcal{S}\hat{h}_{\text{peb}}} \left( 1 + \frac{3\hat{b}}{2\chi\eta} \right) \right] \dot{M}_{\text{F}}, \quad (2.1)$$

542 where  $\dot{M}_{\text{F}}$  is the flux of pebbles through the disc at a specific location from the star; its  
 543 temporal evolution depends on the gas accretion rate onto the central star and the formation  
 544 efficiency of pebbles. We denote using a circumflex the quantities that are scaled by distance  
 545 to the star. The pebble mass flux  $\dot{M}_{\text{F}}$  is one of the key quantities that control the pebble  
 546 accretion rate. For our fiducial disc model it is given by (Ida et al., 2016)

$$\dot{M}_{\text{F}} = 10^{-3}\alpha_3^{-1}\dot{M}_{*8} \left( \frac{L_*}{L_{\odot}} \right)^{2/7} \left( \frac{M_*}{M_{\odot}} \right) \left( \frac{t+t_{\text{off}}}{1 \text{ Myr}} \right)^{-1/3} M_{\text{E}} \text{ yr}^{-1}, \quad (2.2)$$

547 where  $\alpha_3 \equiv \alpha/10^{-3}$ ,  $\alpha$  is the disc viscosity (also see Eq. B.2; Shakura and Sunyaev, 1973),  
 548  $L_*(L_{\odot})$  is the luminosity of the star (Sun),  $M_*(M_{\odot})$  is the mass of the star (Sun) and  $t_{\text{off}}$  is  
 549 the timescale at which the planetesimals are assumed to instantaneously form. The other key  
 550 quantity that influences the pebble accretion rate is the collision impact parameter  $b$ , which  
 551 takes the form

$$b = 2\kappa R_{\text{H}}\mathcal{S}^{1/3} \min \left( \sqrt{\frac{3R_{\text{H}}}{\chi\eta r}}\mathcal{S}^{1/6}, 1 \right), \quad (2.3)$$

552 where  $\kappa$  is the reduction factor accounting for cases where pebbles are weakly coupled to the  
 553 gas resulting in inefficient accretion,  $R_{\text{H}} = r(M/3M_*)^{1/3}$  is the Hill radius of the planetesi-  
 554 mal,  $\mathcal{S}$  is the Stokes number which determines the degree of coupling between the pebbles  
 555 and the gas, and  $\eta$  is the difference between the gas and Keplerian velocity. The terms in the  
 556 parentheses encompass the two possible pebble accretion regimes, namely the Bondi regime  
 557 (left-hand term) where the relative velocity between the planetesimal and a pebble is domi-  
 558 nated by the pebble's drift velocity, and the Hill regime (right-hand term) where the relative  
 559 velocity is dominated by Keplerian shear. The quantity  $\chi$  is a function of the Stokes number  
 560  $\mathcal{S}$ , and is defined as

$$\chi = \frac{\sqrt{1+4\mathcal{S}^2}}{1+\mathcal{S}^2}, \quad (2.4)$$

561 The Stokes number itself is given by

$$\mathcal{S} = \frac{\rho_{\text{peb}}R_{\text{peb}}}{\rho_{\text{g}}h_{\text{g}}} \max \left( 1, \frac{4R_{\text{peb}}}{9\lambda} \right), \quad (2.5)$$

562 where  $\rho_{\text{peb}}$  and  $R_{\text{peb}}$  are the bulk density and the physical radius of a pebble,  $\rho_{\text{g}}$  is the gas  
 563 midplane density,  $h_{\text{g}} = H_{\text{g}}/r$  is the reduced disc scale height, and  $\lambda$  is the mean free path of  
 564 the pebble. The gas midplane density  $\rho_{\text{g}}$  is related to the disc surface density  $\Sigma_{\text{g}}$  and the disc  
 565 scale height  $H_{\text{g}}$  via

$$\rho_{\text{g}} = \frac{\Sigma_{\text{g}}}{\sqrt{2\pi}H_{\text{g}}}, \quad (2.6)$$

566 where  $H_{\text{g}} = c_{\text{s}}/\Omega_{\text{K}} \propto T^{1/2}$  is a function of the disc temperature  $T$ , the sound speed  $c_{\text{s}}$  and the  
 567 Keplerian orbital frequency  $\Omega_{\text{K}} = \sqrt{GM_*/r^3}$ . The pebble mean free path is given by

$$\lambda = \frac{\mu m_{\text{H}}}{\sigma_{\text{H}_2}\rho_{\text{g}}}, \quad (2.7)$$

568 where  $\mu$  is the mean molecular weight of the gas (mostly hydrogen),  $m_{\text{H}}$  is the mass of a hy-  
 569 drogen atom (mostly that of the proton), and  $\sigma_{\text{H}_2}$  is the collisional cross section of a hydrogen

570 molecule. The reduction factor  $\kappa$  is a function of the Stokes number, expressed as (Ormel and  
571 Kobayashi, 2012)

$$\ln \kappa = - \left( \frac{\mathcal{S}}{\mathcal{S}^*} \right)^{0.65}, \quad (2.8)$$

572 where the quantity  $\mathcal{S}^*$  is defined as

$$\mathcal{S}^* = \min \left[ 2, 4\eta^{-3} \frac{M}{M_*} \right]. \quad (2.9)$$

573 The quantity  $\eta$  is the difference between the gas and Keplerian velocities due to the gas  
574 pressure gradient. It is given by

$$\eta = \frac{1}{2} h_g^2 \left| \frac{d \ln P}{d \ln r} \right|. \quad (2.10)$$

575 The remaining quantities in Eq. 2.1 that we have yet to describe are the constant  $C$  that  
576 determines the mode of accretion (whether 2D or 3D) and the pebble scale height  $h_{\text{peb}}$ . These  
577 quantities are expressed as

$$C = \min \left( \sqrt{\frac{8}{\pi}} \frac{h_{\text{peb}}}{b}, 1 \right), \quad (2.11)$$

578 and

$$h_{\text{peb}} = \left( 1 + \frac{\mathcal{S}}{\alpha_t} \right)^{-1/2} h_g, \quad (2.12)$$

579 where  $\alpha_t$  is the gas disc's turbulent viscosity. Pebble accretion begins in 3D mode ( $C \sim$   
580 1) when the planetesimal is of low mass and then transitions into the 2D mode when the  
581 planetesimal grows larger and its Hill radius becomes larger than the scale height of the  
582 pebbles  $h_{\text{peb}}$ .

### 583 2.2.2 Application to small planetesimals

584 According to Ormel and Klahr (2010) pebble accretion causes rapid growth onto planetesi-  
585 mals with diameters of  $\sim 200$  km or greater. To understand how pebble accretion works on  
586 small(er) bodies the question becomes which of the paths in the  $\min()$  statements in Equa-  
587 tions 2.1, 2.3, 2.9 and 2.11 dominate.

588 We mentioned previously that the two key quantities controlling the pebble accre-  
589 tion rate are the global pebble flux  $\dot{M}_F$  and the impact parameter  $b$ . In the following, we will  
590 demonstrate that the reduction factor  $\kappa$  (Eq. 2.8) turns out to be important as well. The quan-  
591 tity  $\mathcal{S}^*$  (Eq. 2.9) sets the boundary between the so-called *settling regime*, in which the cross  
592 section for accretion is very large (Ormel and Kobayashi, 2012), and the *geometric regime*, in  
593 which the cross section is just the surface area of the planetesimal (Ormel and Klahr, 2010).  
594 The two regions are smoothly connected with the parameter  $\kappa$ , whose functional form is a fit  
595 that Ormel and Klahr (2010) obtained from numerical experiments. The critical Stokes num-  
596 ber that separates the settling regime from the geometric regime results in  $\mathcal{S}^* < 2$ . At around  
597 1 au, this translates to a critical planetesimal-to-star mass ratio of  $M/M_* < \frac{1}{2}\eta^3 \lesssim 1.4 \times 10^{-9}$   
598 which corresponds to a diameter of  $D = 1200$  km for a bulk density of  $\rho = 3000 \text{ kg m}^{-3}$   
599 for the planetesimal, assuming nominal disc quantities (see Appendix B.1 for a description  
600 of our disc model). This critical value of  $M/M_*$  has a distance dependence. For example, at  
601 3 au  $\mathcal{S}^* < 2$  when the planetesimal mass is  $M/M_* < 3.5 \times 10^{-9}$ , or equivalent to a diameter  
602 of 1700 km. As such, when a planetesimal at 3 au has a diameter smaller than about twice  
603 that of Ceres, or that it is roughly 1200 km if it is located at 1 au, the quantity  $\mathcal{S}^*$  can become  
604 smaller than 2, meaning that for these cases we are no longer in the settling regime and are

605 instead approaching the geometric regime where the accretion cross section reduces to the  
 606 surface area of the planetesimal. This has important implications with regards to the pebble  
 607 accretion rate and efficiency of planetesimals below a critical diameter at a given semi-major  
 608 axis.

609 In the asteroid belt, the typical value for the pebble Stokes number  $\mathcal{S}$  is 0.1 and  
 610 the quantity  $\mathcal{S}^*$  is often equal to 2 (Ida et al., 2016). For these values, the reduction factor  
 611  $\kappa = 0.87$ . Suppose now that we want to study accretion onto the parent body of the HED  
 612 meteorites, which, despite existing controversies, we here assume to be the asteroid 4 Vesta  
 613 (McCord et al., 1970; Consolmagno and Drake, 1977; Binzel and Xu, 1993; Keil, 2002; McSween  
 614 et al., 2013). Vesta’s diameter is  $D \sim 500$  km and  $M/M_* = 1.3 \times 10^{-10}$ . For our nominal disc  
 615 model at 2.5 au (where Vesta is currently located),  $\eta \sim 3 \times 10^{-3}$  and  $\mathcal{S}^* \sim 0.02$ . If the  
 616 Stokes number is the typical value of 0.1 then  $\kappa = 0.06$ , but if  $\mathcal{S}$  is higher then  $\kappa$  will be  
 617 lower, resulting in a much lower rate of accretion than when the impact parameter is almost  
 618 equal to the Hill radius. Pebble accretion onto the proposed H-chondrite parent body 6 Hebe  
 619 (Gaffey et al., 1993; Gaffey and Gilbert, 1998; Binzel et al., 2004, 2019), with  $D \sim 200$  km  
 620 and  $M/M_* \lesssim 7 \times 10^{-12}$ , is much less efficient yet again because the quantities  $\mathcal{S}^*$  and  $\kappa$   
 621 work out to be  $\lesssim 10^{-3}$  and  $\lesssim 2 \times 10^{-9}$ , respectively. Thus, because of the  $\kappa$  factor, which  
 622 is related to how the pebbles accrete in the settling regime (Ormel and Klahr, 2010; Ormel  
 623 and Kobayashi, 2012), accretion onto small objects with  $D \sim 200$  km could become *extremely*  
 624 *inefficient*. However, the impact parameter  $b$  must always be equal to or greater than the  
 625 radius of the planetesimal for it to be physically meaningful. For a planetesimal with bulk  
 626 density  $\rho = 3000$  kg m $^{-3}$  we have  $R/r_H \sim 5.7 \times 10^{-3}$  so that the relative impact parameter  
 627 in terms of the Hill radius cannot go much below this value. The revised impact parameter  
 628 therefore should read

$$b = \max \left[ 2\kappa r_H \mathcal{S}^{1/3} \min \left( \sqrt{\frac{3r_H}{\chi \eta r}} \mathcal{S}^{1/6}, 1 \right), R \right], \quad (2.13)$$

629 where  $R$  is the radius of the planetesimal. This shows that the accretion rate of pebbles cannot  
 630 become arbitrarily low, but that small planetesimals are still severely disadvantaged in terms  
 631 of their accretion rate over their larger brethren.

### 632 2.2.3 The role of the snow line and fragmentation

633 Morbidelli et al. (2016) suggest that the pebbles lose their volatiles at the snow line and could  
 634 fragment into mm-sized grains akin to chondrules. This fragmentation, if confirmed by me-  
 635 chanical arguments, lowers the Stokes number (Eq. 2.5). The Stokes number can either be  
 636  $\mathcal{S} \propto R_{\text{peb}}$ , called the Epstein regime, or  $\mathcal{S} \propto R_{\text{peb}}^2$ , called the Stokes regime, depending on  
 637 the distance to the star and the properties of the gas disc. The transition between the two  
 638 regimes occurs at (Ida et al., 2016)

$$r_{\text{ES}} = 2.2 \rho_{\text{peb}}^{-7/26} \left( \frac{L_*}{L_\odot} \right)^{-3/13} \left( \frac{M_*}{M_\odot} \right)^{17/26} \left( \frac{\dot{M}_{\text{F4}}^{1/3} \dot{M}_{*8}}{\alpha_3} \right)^{21/52} \text{ au}, \quad (2.14)$$

639 where  $\dot{M}_{\text{F4}} \equiv \frac{\dot{M}_{\text{F}}}{10^{-4} M_{\text{E}} \text{ yr}^{-1}}$ , and  $\dot{M}_{*8} \equiv \frac{\dot{M}_*}{10^{-8} M_\odot \text{ yr}^{-1}}$ . For nominal gas disc temperature and  
 640 surface density at 1 au, the pebble mean free path  $\lambda \sim 2$  cm. Inside the snow line, where  
 641 fragmentation could occur, the pebble radius is assumed to be  $R_{\text{peb}} \sim 1$  mm (Morbidelli et al.,  
 642 2016) and so in this case  $\mathcal{S} \propto R_{\text{peb}}$  because  $R_{\text{peb}} \ll \lambda$  (Eq. 2.5). Assuming a pebble density of  
 643  $\rho_{\text{peb}} = 1000$  kg m $^{-3}$ , the Stokes number at 1 au for nominal disc parameters is approximately  
 644  $\mathcal{S} \sim 0.2$ , but after fragmentation it is lowered to  $\mathcal{S} \sim 10^{-4}$  (Brasser and Mojzsis, 2020).



645 With the reduction of the Stokes number at 1 au from  $S \sim 0.2$  to  $S \sim 10^{-4}$  as  
 646 a consequence of potential fragmentation, pebble accretion only becomes inefficient once  
 647  $S^* \lesssim 2 \times 10^{-5}$ , i.e., when  $M/M_* \lesssim 10^{-14}$ , which corresponds to a planetesimal diameter of  
 648  $D \lesssim 50$  km. This critical diameter is lower than that derived previously for the case where  
 649 fragmentation is not considered (cf.  $D \sim 200$  km). With the inclusion of the fragmentation  
 650 effect the range of planetesimal diameters for which pebble accretion can proceed efficiently  
 651 is wider. However, the accretion rate depends strongly on the Stokes number, and a lower  
 652 Stokes number actually results in a much slower rate of accretion with everything else being  
 653 equal. Nevertheless, due to the debilitating effect of  $\kappa$ , accretion onto small planetesimals  
 654 by fragmented pebbles is still faster than by intact pebbles beyond the snow line. As such,  
 655 if fragmentation occurred, pebble accretion onto planetesimals with a diameter comparable  
 656 to the H-chondrite parent body or smaller can still proceed, albeit with low efficiency, but  
 657 only as long as they remain inside the snow line. In conclusion, the temporal evolution of  
 658 the snow line plays a critical role in the growth rate of planetesimals in the inner disc from  
 659 the inward spiralling pebbles.

#### 660 2.2.4 Analytical computation of pebble accretion rate

661 We combine all of these aspects to show a global accretion map in Fig. 2.1, which is a contour  
 662 plot of  $\log(M_f/M_i)$ , i.e., the final mass of a planetesimal divided by its initial mass. The map  
 663 was created by integrating Eq. 2.1 as a function of time either for at most 4 Myr or until  
 664 the pebble isolation mass (Lambrechts et al., 2014) was reached. The pebble isolation mass  
 665 of a planetary body is the mass above which pebble accretion stops due to the planetary  
 666 body causing perturbations in the disc that halt the flow of pebbles (Lambrechts et al., 2014).  
 667 Each data point on the map is the result of an integration of a single planetesimal at a fixed  
 668 location. We assume the temperature of the gas disc to be 200 K at 1 au. The disc evolution  
 669 that was used follows that outlined in Appendix B.1 and the pebble flux is computed using  
 670 Eq. 2.2.

671 The top row of Fig. 2.1 has  $t_{\text{off}} = 0.1$  Myr, the middle row has  $t_{\text{off}} = 0.5$  Myr and  
 672 the bottom row has  $t_{\text{off}} = 1$  Myr. These three different starting times account for the delay in  
 673 the timing of planetesimal formation in the disc. The left column has fragmentation included  
 674 while the right does not. It is clear that the mass distribution is bimodal: planetesimals either  
 675 grow large or they barely grow at all. This result is mainly dependent on the initial diame-  
 676 ter of the planetesimals, which in turn determines their pebble accretion efficiency. If their  
 677 diameter is below a critical value (which has a slight dependence on disc parameters), then  
 678 they are in the geometric regime and thus accreting pebbles is very inefficient regardless of  
 679 their distance to the Sun (purple region in the left side of all the panels in Fig. 2.1). If they  
 680 are larger than the critical diameter, then they are in the settling regime wherein the pebble  
 681 accretion efficiency is high, and they will thus experience more growth. The planetesimal's  
 682 critical diameter between the geometric and settling regimes depends on the location in the  
 683 disc, the formation time of the planetesimal, whether pebble fragmentation at the snow line  
 684 is assumed, and also very likely the temperature of the disc (although this factor is not in-  
 685 vestigated here).

686 Without fragmentation (right column of Fig. 2.1) only planetesimals with  $M \gtrsim$   
 687  $3 \times 10^{-5} M_E$  ( $D \gtrsim 500$  km) will efficiently accrete pebbles, with a slight dependence on  
 688 their initial location in the disc; everything smaller will barely accrete anything (large purple  
 689 region in the left part of the panels in the right column of Fig. 2.1). Fragmentation, on the  
 690 other hand, allows for the creation of a narrow annulus of large bodies between 0.8 au to at  
 691 most 1.5 au whose exact extent depends on the time of the formation of the planetesimals  
 692 relative to the evolution of the snow line (left column of Fig. 2.1). The snow line does not

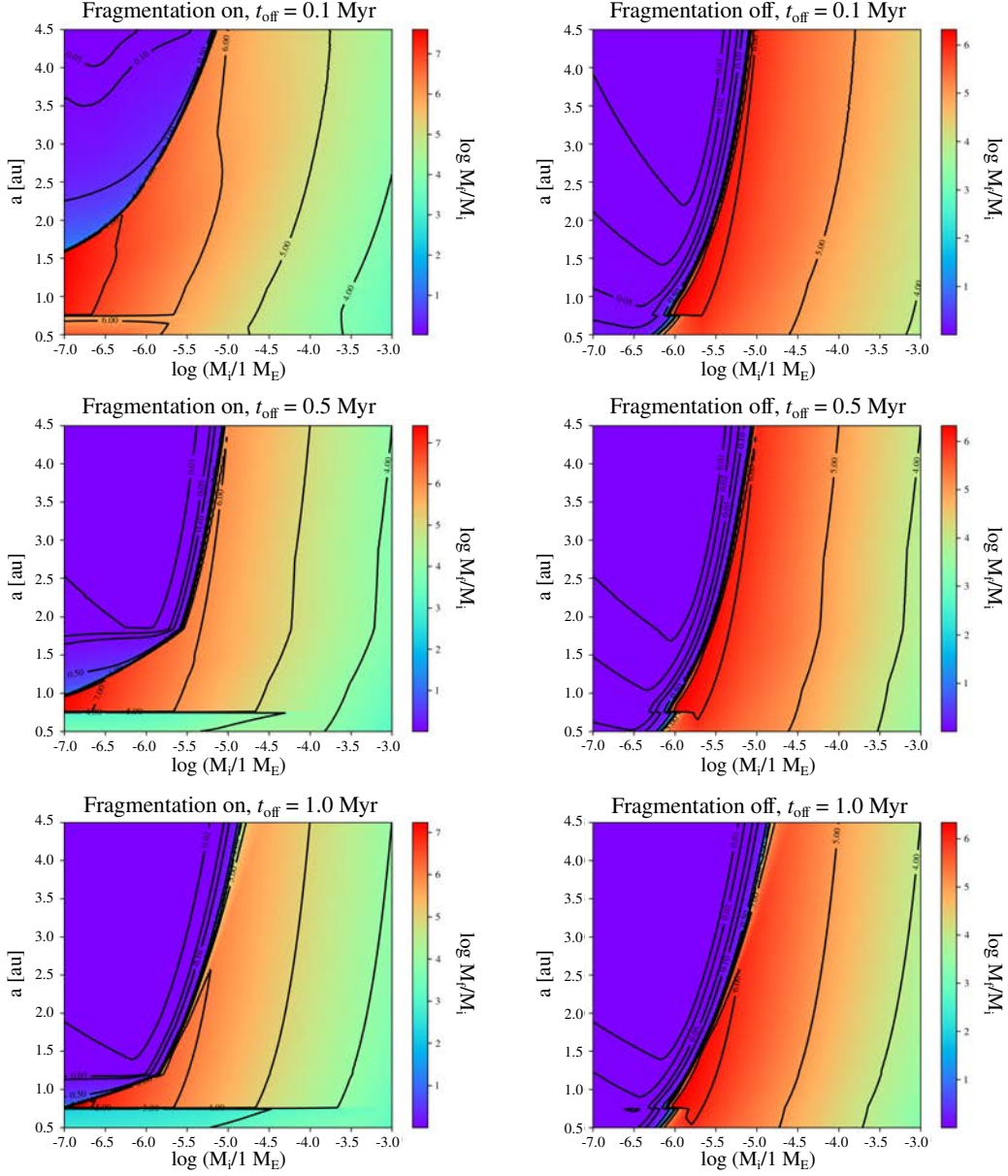


FIGURE 2.1: Contour plot depicting final mass  $M_f$  of planetesimals after a phase of pebble accretion as a function of their initial mass  $M_i$  and semi-major axis, with and without pebble fragmentation at the snow line. The top row assumes all planetesimals form together with the disc at  $t = 0.1$  Myr, the middle row assumes planetesimal formation after 0.5 Myr and the bottom row after 1 Myr. Regardless of our choice of parameters (initial planetesimal size, planetesimal semi-major axis, planetesimal formation timing, inclusion/exclusion of fragmentation effects), pebble accretion onto small planetesimals in the asteroid belt is very inefficient. The planetesimal diameter can be computed from  $\log(D/1 \text{ km}) = \frac{1}{6} \log(M/1 M_E) + 3.597$ , so that  $M/M_E = 10^{-5}$  corresponds to  $D = 580 \text{ km}$ .

reach inside 0.75 au so accretion inside of this distance can be inefficient if planetesimals are predominantly small ( $D \lesssim 300$  km) and formed late ( $t_{\text{off}} \gtrsim 1$  Myr). In our fiducial model the snow line is at 1.2 au when  $t+t_{\text{off}} = 1$  Myr, and it passes 2 au by the time  $t+t_{\text{off}} = 0.44$  Myr, thus substantial pebble accretion in the terrestrial planet region can only occur if planetesimals form very early and/or form large. In the asteroid belt region accretion generally stops really early on, at a time comparable to the formation age of the iron meteorites, and possibly before most chondrule formation ages – typically about 1.5 Myr (Luu et al., 2015) – because of the rapid inward migration of the snow line. Beyond 2 au accretion is generally insubstantial for small planetesimals.

What is further evident in Fig. 2.1 is that more mass is accreted closer to the Sun than farther away (Ida et al., 2016). In other words, pebble accretion creates a gradient in mass per unit distance. Accretion is more efficient closer to the star, everything else being equal, so pebble accretion naturally creates a compositional gradient in the solid part of the inner disc, with the innermost planetesimals near Mars’ orbit being more enriched in outer Solar System (jovian) material than planetesimals in the (outer) asteroid belt.

## 2.3 Methodology of $N$ -body simulations

In essence, we investigate the growth of a disc of planetesimals that is subjected to a flux of inward drifting pebbles ( $\rho_{\text{peb}} = 1000 \text{ kg m}^{-3}$ ,  $R_{\text{peb}} = 10$  cm) originating from a pebble front located in the outer Solar System beyond the orbit of Jupiter (e.g., Lambrechts and Johansen, 2014; Ida et al., 2016) over the lifetime of the gas disc.

### 2.3.1 Gas disc model

We include a gas disc based on the model of Ida et al. (2016) in our simulations, with the detailed prescriptions given in Appendix B.1. The gas disc is a steady accretion disc with a constant value for  $\alpha$  (viscosity parameter; Shakura and Sunyaev, 1973). The temperature of the disc depends on two heating sources, i.e., viscous dissipation or stellar irradiation, which dominate at different regions of the disc. Equations describing the disc temperature profiles Eq. B.4 due to the aforementioned heating sources are obtained from empirical fits to the disc model of Garaud and Lin (2007). The thermal structure of the disc in turn determines the scale height and surface density.

In our simulations, the gas disc dissipates away with time and was photoevaporated away in 500 kyr when the stellar accretion rate  $\dot{M}_* < 10^{-9} M_{\odot} \text{ yr}^{-1}$ . We further include the effects of disc-induced orbital migration and orbital eccentricity damping (Appendix B.2; e.g., Tanaka et al., 2002; Matsumura et al., 2017) and gas envelope accretion for massive bodies (Appendix B.3; Matsumura et al., 2017). We also simulate for the case where orbital migration is excluded.

The starting time  $t_0$  of our simulations is chosen to be 0.4 Myr after the formation of the CAIs. This value of  $t_0$  determines the initial values of the stellar accretion rate  $\dot{M}_*(t = t_0)$  and the initial pebble flux  $\dot{M}_{\text{F}}(t = t_0)$  in the simulation. It also plays a role in computing the subsequent values of  $\dot{M}_*(t)$  and  $\dot{M}_{\text{F}}(t)$  throughout the simulation. In our simulations, the initial stellar accretion rate  $\dot{M}_* = 2.63 \times 10^{-8} M_{\odot} \text{ yr}^{-1}$  and the initial pebble flux  $\dot{M}_{\text{F}} = 10^{-4} M_{\text{E}} \text{ yr}^{-1}$ .

### 2.3.2 Pebble accretion

The pebble accretion formulation we use in this work is based on previous studies that have developed and refined the formulation (e.g., Ormel and Klahr, 2010; Ormel and Kobayashi, 2012; Ida et al., 2016), and studies which applied it to the formation of the giant planets in our Solar System and found success in building the cores of giant planets quick enough to allow gas envelope accretion before the dissipation of the gas (e.g., Lambrechts and Johansen, 2012, 2014). We apply the equations derived by Ida et al. (2016) for the pebble accretion rate at different locations in a steady state accretion disc while taking into account the various properties of the gas disc (e.g., temperature, surface density, scale height). We chose to use this particular pebble accretion formulation for its simplicity and elegance, and because it does not invoke any additional assumptions (such as was done by Levison et al., 2015b; Johansen et al., 2021).

The pebbles are assumed to have originated in the outer regions of the protoplanetary disc where most of the solids (dust) are located (e.g., Youdin and Shu, 2002; Garaud, 2007; Birnstiel et al., 2012). In this region, sub-micron-sized dust grains can grow into pebbles because their growth timescale is much shorter than their migration timescale and the collision rate is low (Birnstiel et al., 2012). Upon reaching a critical size (or a critical Stokes number), the migration timescale becomes comparable to the growth timescale and the pebbles commence their inward migration towards the Sun by virtue of gas drag (Ida et al., 2016). Due to the strong radial dependence of the growth timescale, there will be a location in the disc where dust clumps have just reached pebble size and start to migrate inwards. This is known as the pebble formation front and it moves outwards with time until it reaches the outer edge of the protoplanetary disc (Lambrechts and Johansen, 2014; Ida et al., 2016), after which the pebble flux is severely reduced because all the solids in the disc have been consumed (e.g., Chambers, 2016; Sato et al., 2016).

We implemented the pebble accretion prescriptions of Ida et al. (2016) into the  $N$ -body code based on that presented in Matsumura et al. (2017). We do not directly compute the growth of planetesimals by accretion of physical pebbles, but instead compute their mass increase based on the pebble flux at their respective locations in the disc. Pebble accretion onto planetesimals occurs outside in, that is, planetesimals at the outer edge of our solid disc are the first to encounter the pebbles. They will accrete a fraction of the pebbles, reducing the pebble flux by a factor of  $1 - \dot{M}_p / \dot{M}_F$ . The planetesimals that are next in line will see a reduced pebble flux and the amount of pebbles they can accrete is computed from the reduced pebble flux. Furthermore, when a planetesimal (or more accurately, planetary embryo) reaches its pebble isolation mass  $M_{p,\text{iso}} \sim 1/2(h_g/r)^3 M_*$  we assume that its accretion stops and pebbles are prevented from flowing past its orbit to other planetary bodies residing closer to the Sun. We assume that pebbles were fragmented (or sublimated) into grains of 1 mm when they cross the snow line on their path towards the Sun (Morbidelli et al., 2016). We also study the outcome of excluding this effect.

### 2.3.3 Initial conditions

Our planetesimal disc contains planetary bodies with an initial density of  $\rho = 2500 \text{ kg m}^{-3}$  and diameter  $D$  assigned following a cumulative size-frequency distribution of  $N(> D) \propto D^{-5/2}$  (Fig. 2.2). Their orbital eccentricities  $e$  and orbital inclinations  $I$  are assigned at random from a uniform distribution with intervals  $[0, 0.01)$  and  $[0^\circ, 1^\circ)$ , respectively. The remaining orbital angles (longitude of ascending node  $\Omega$ , argument of periapsis  $\omega$  and mean anomaly  $\mathcal{M}$ ) are assigned values between  $0^\circ$  and  $360^\circ$ , also randomly chosen from a uniform distribution. The semi-major axis of the planetesimals ranges from  $0.5 \text{ au} < a < 2.0 \text{ au}$  and they are

781 distributed according to an  $r^{-1}$  surface density profile. Our choice to limit the outer edge of  
 782 the solid disc to 2 au is guided by the analytical results in Fig. 2.1 and our intent to save com-  
 783 putation time (our simulations contain a fairly large number of planetesimals and they are  
 784 all self-gravitating). Furthermore, planetesimals smaller than  $D \lesssim 500$  km located beyond  
 785 2 au are not expected to grow by much (Fig. 2.1), whereas for bodies with diameter larger  
 786 than 500 km the growth can be substantial (Brasser and Mojzsis, 2020).

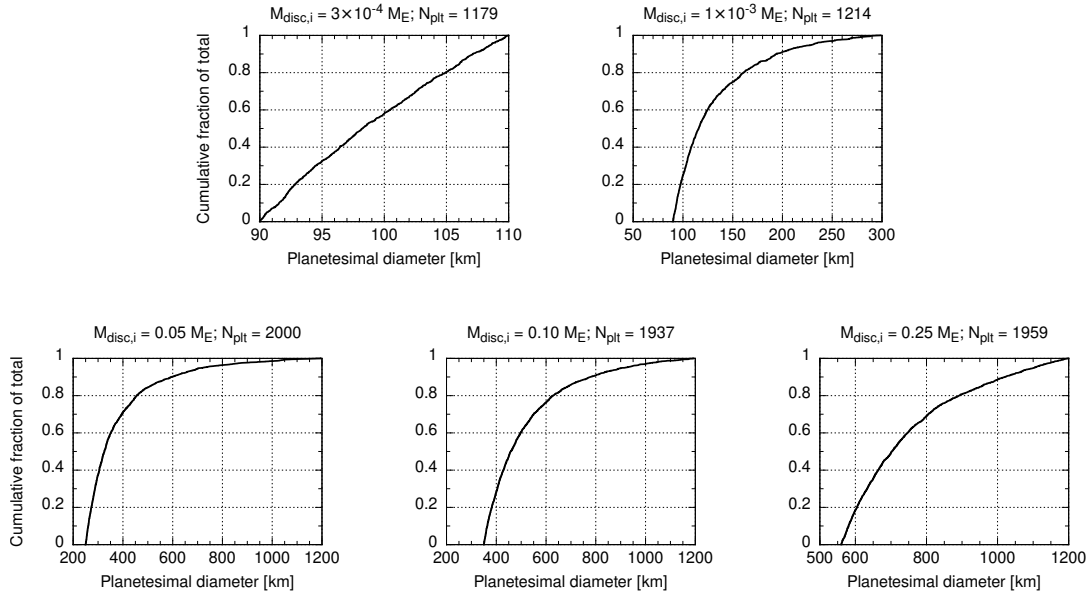


FIGURE 2.2: Cumulative distribution of planetesimal diameter  $D$  for various values of initial solid disc mass  $M_{\text{disc},i}$ .

TABLE 2.1: Initial solid disc mass  $M_{\text{disc},i}$  in units of Earth masses, range of planetesimal diameters  $D$  in each disc, and initial number of planetesimals in each disc  $N_{\text{plt}}$  for the pebble accretion simulations. We repeat the simulations using the same set of initial conditions shown here for different values of initial disc temperature  $T_{1 \text{ au}} = 200$  K, 250 K, and 300 K.

$M_{\text{disc},i} (M_{\text{E}})$	$D$ (km)	$N_{\text{plt}}$
$3 \times 10^{-4}$	90 – 110	$\sim 1200$
$1 \times 10^{-3}$	90 – 300	$\sim 1200$
0.05	250 – 1200	$\sim 2000$
0.10	350 – 1200	$\sim 2000$
0.25	560 – 1200	$\sim 2000$

787 The variables in our simulations are: (1) the initial solid disc mass  $M_{\text{disc},i}$ , (2) the  
 788 range of planetesimal diameters  $D$ , and (3) the initial disc temperature at 1 au ( $T_{1 \text{ au}} = 200$  K,  
 789 250 K, and 300 K) which corresponds to different disc scale heights  $h_{\text{g}}$  and pebble scale heights  
 790  $h_{\text{peb}}$ . The lower mass discs ( $M_{\text{disc},i} = 3 \times 10^{-4} M_{\text{E}}$ ,  $1 \times 10^{-3} M_{\text{E}}$ ) contain  $\sim 1200$  planetesimals  
 791 while the more massive discs contain  $\sim 2000$  planetesimals. All the planetesimals in our  
 792 simulations are self-gravitating, that is, they are able to interact with each other via gravity.  
 793 We summarise the initial conditions in Table 2.1.

794 Our choice of planetesimal diameters are based on the results of previous works.  
 795 The characteristic diameter of early planetesimals that formed via turbulent concentration or  
 796 streaming instability in a Solar-like protoplanetary disc ranges from  $\sim 100$  km up to maybe

1000 km (e.g., Chambers, 2010; Johansen et al., 2014; Klahr and Schreiber, 2020), with a size-frequency distribution that follows a shallow power law  $N(> D) \propto D^{-1.8}$  for diameter, corresponding to  $N(> M) \propto M^{-0.6}$  for mass (e.g., Johansen et al., 2015; Simon et al., 2016; Schäfer et al., 2017; Abod et al., 2019). Models of the collisional evolution of the asteroid belt also suggest that the primordial asteroids were typically 100 km in diameter (Morbidelli et al., 2009). The combined results of these studies suggest that the initial planetesimal population likely consisted of many small planetesimals and a few massive bodies. Vesta could be one of the early-formed massive bodies at the tail end of the distribution.

In addition to the planetesimal disc, following the work of Brasser and Mojzsis (2020) our initial set-up also includes a  $0.01 M_E$  planetary embryo placed at 5.2 au that would eventually become Jupiter. When Jupiter reaches its pebble isolation mass ( $20 M_E$ ; Lambrechts et al., 2014) in about 1 Myr (Kruijer et al., 2017), it starts to open a partial gap in the disc around its orbit that prevents pebbles from beyond its orbit to spiral in towards the Sun, effectively shutting off the pebble flux to the inner Solar System (Lambrechts et al., 2014), although particles with sizes  $\lesssim 100 \mu\text{m}$  are still able to pass through unobstructed (Paardekooper and Mellema, 2006).

We employ the SyMBA  $N$ -body code (Duncan et al., 1998) modified to include a pebble accretion subroutine (described in Section 2.2; Matsumura et al., 2017) and all the additional effects described in this paragraph to carry out our simulations. For each value of  $M_{\text{disc},i}$  we ran one simulation for each permutation of initial conditions (disc temperature  $T_{1 \text{ au}}$ , fragmentation on/off, migration on/off). In total we ran 60 simulations. The simulations were ran for 4 Myr with a time step of 0.01 yr.

We quantify the amount of mass increase in the inner Solar System resulting from the accretion of pebbles by computing the ratio of the final mass of the planetesimal disc versus its initial mass  $M_{\text{disc},f}/M_{\text{disc},i}$ . For the more massive discs ( $M_{\text{disc},i} \geq 0.05 M_E$ ), the larger planetesimals will accrete pebbles efficiently and they can grow to large masses quickly, as we will show in the following section. Therefore, the final disc mass for these cases do not only reflect growth via pebble accretion, but also additional growth due to mergers and gas envelope accretion. However, the additional growth processes from mergers and gas envelope accretion should not affect the cosmochemical outcome and the conclusion of this study.

## 2.4 Results

### 2.4.1 Amount of mass increase in the inner disc

We present the results for the ratio of the final mass in the disc to its initial mass ( $M_{\text{disc},f}/M_{\text{disc},i}$ ) in the region between 0.5 au and 2.0 au plotted with respect to the initial disc mass and the disc temperature in Fig. 2.3. We find that the final mass of the solid disc depends mostly on its initial mass. A higher initial disc mass results in a higher final disc mass because these discs have, on average, a higher number of large planetesimals which are more efficient at accreting pebbles. This result is similar to the outcome of the single-planetesimal computations shown earlier in Fig. 2.1, which illustrates that a planetesimal’s accretion regime abruptly transitions from the less efficient geometric regime to the more efficient settling regime when their masses are above a critical threshold given a specific set of gas disc parameters. We also observe a general inverse correlation between the amount of mass increase and the initial temperature of the gas disc because (1) for hotter discs the scale height is higher and this lowers the pebble accretion efficiency (Ida et al., 2016), and (2) the snow line is on average farther away in hotter discs than in cooler discs.

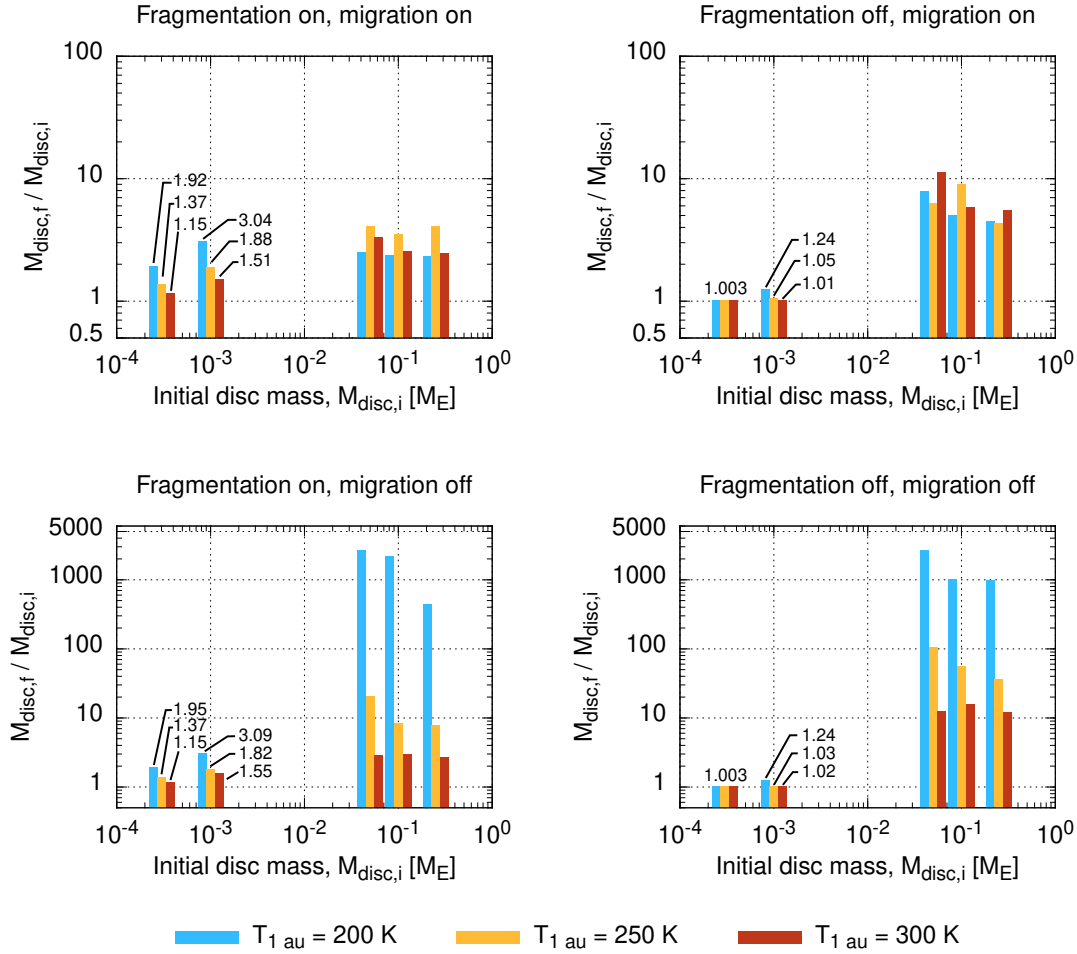


FIGURE 2.3: Ratio of final mass in the disc to its initial mass ( $M_{\text{disc},f}/M_{\text{disc},i}$ ) in the region between 0.5 au and 2.0 au as a result of pebble accretion over a period of 4 Myr since the formation of CAIs, plotted with respect to the initial disc mass and disc temperature. The accretion efficiency depends on the sizes of the planetesimals. Large amounts of mass in the form of pebbles can still be accreted by large planetesimals within 2 au before Jupiter reaches its pebble isolation mass at  $t = 1.5$  Myr.

842 Our results show that the growth of small planetesimals with  $D \lesssim 300$  km located  
 843 between 0.5 au and 2.0 au is very limited as they are not in the settling regime. The final mass  
 844 of the disc is not affected by disc-induced migration effects because these planetesimals do  
 845 not have the opportunity to grow to large sizes for migration to be significant. On the other  
 846 hand, there is an observable difference in the final disc mass due to pebble fragmentation  
 847 effects. If pebble fragmentation at the snow line is taken into consideration, we find that  
 848 the final disc mass is about 1 to 2 times higher and 1.5 to 2.5 times higher respectively for  
 849 discs with initial mass  $M_{\text{disc},i} = 3 \times 10^{-4} M_E$  ( $D \approx 100$  km) and  $M_{\text{disc},i} = 1 \times 10^{-3} M_E$   
 850 ( $90 \text{ km} \leq D \leq 300$  km), compared to the case when fragmentation effects are excluded.  
 851 The numerical  $N$ -body simulations confirm that small planetesimals have difficulty accreting  
 852 pebbles efficiently if the pebbles did not break into smaller sizes at the snow line. The discs  
 853 containing planetesimals with  $D \lesssim 110$  km barely grow at all (just a 0.3% increase) while the  
 854 discs containing planetesimals with  $D \lesssim 300$  km recorded a growth ranging from 1 – 2% for  
 855 hot discs to 24% for cold discs.

856 When planetesimals are larger their growth is affected by both disc-induced migration  
 857 and pebble fragmentation effects. Compared to fragmentation, migration effects exert  
 858 a stronger influence on the final mass in the disc. In the extreme case where migration is

859 excluded, the final solid mass of planetesimals in cold discs can reach a few hundred to a  
 860 few thousand times their initial mass due to gas envelope accretion onto planetary embryos  
 861 (Ikoma et al., 2000). Indeed, the combined effects of a lower gas disc scale height and a closer-  
 862 in snow line results in a high accretion efficiency that allows planetesimals to grow to large  
 863 sizes very quickly with some planetesimals attaining masses sufficient to trigger gas accre-  
 864 tion. For the warm and hot discs the mass increase is a few times to a few tens of times their  
 865 initial mass. When migration effects are included, the final mass in the disc is at most ten  
 866 times its initial mass depending on the disc temperature. This is because large planetesimals  
 867 that formed earlier were continuously removed from the disc: when planetesimals reach a  
 868 certain mass, the angular momentum exchange with the surrounding gas disc results in their  
 869 inward migration towards the disc inner edge (Tanaka et al., 2002) and their eventual loss to  
 870 the Sun. Migration is especially important in cold discs such that the maximum solid disc  
 871 mass (assuming the same initial disc mass) is achieved when the initial gas disc temperature  
 872 is 250 K rather than 200 K. Pebble fragmentation effects, when excluded, generally results in a  
 873 higher final disc mass, roughly a few times higher compared to the case when fragmentation  
 874 was included. The total solid mass in the disc by the end of the simulations for these massive  
 875 discs are in fact higher than what is presented here for  $0.5 \text{ au} < a < 2.0 \text{ au}$  because planetes-  
 876 imals are scattered away from their initial location by their more massive counterparts. The  
 877 planetesimal disc expanded into the region beyond 2.0 au and up to around 3.0 au in the case  
 878 of cold discs (Fig. 2.4 which we discuss next). We chose to compute the final mass between  
 879 0.5 au and 2.0 au to be consistent with the computation for the less massive discs.

880 In Fig. 2.4 we plot, for a selected set of initial conditions, the distribution of solids  
 881 within 3 au at the end of the simulations ( $t = 4 \text{ Myr}$ ). For the lower-mass discs ( $M_{\text{disc},i} \leq$   
 882  $1 \times 10^{-3} M_{\text{E}}$ ) that contain planetesimals with  $D \lesssim 300 \text{ km}$ , we show the results for the  
 883 cases with both fragmentation and migration effects included. The results are similar for the  
 884 cases with fragmentation and/or migration excluded, mainly because the planetesimals do  
 885 not grow to sizes large enough to perturb the orbits of nearby planetesimals. Thus for these  
 886 lower-mass discs, we can clearly see what is happening in the solid disc when the planetesi-  
 887 mals are subjected to the pebble flux. There are several evident trends that we observe. First,  
 888 planetesimals closer to the Sun are more efficient at accreting pebbles and growing larger.  
 889 The trend of inside-out growth is due to the pebble accretion rate having a dependence on  
 890 semi-major axis (Ida et al., 2016). This outcome can also be understood using a more physi-  
 891 cal explanation: planetesimals in the region closer to the Sun see a higher concentration of  
 892 pebbles because the pebbles are confined to an increasingly narrow annulus when they drift  
 893 inwards, which is effectively an increased surface density in the disc, and thus it is easier to  
 894 accrete pebbles in this region. Second, planetesimals in a cold disc experience more growth  
 895 than those in a hot disc. The dependence of planetesimal growth on the temperature of the  
 896 disc can be traced to the disc temperature's effect on the pebble scale height. Pebbles in discs  
 897 with a lower (higher) temperature have lower (higher) scale heights which allows them to be  
 898 accreted more (less) efficiently onto planetesimals. Third, planetesimal growth is dependent  
 899 on their size. We have shown in our analytical computation discussed previously in Sec-  
 900 tion 2.2.4 that pebble accretion is only efficient for planetesimals with  $D \gtrsim 300 \text{ km}$  because  
 901 of their larger accretion cross-section.

902 We show the results of  $M_{\text{disc},i} = 0.1 M_{\text{E}}$  with fragmentation effects included (rows 3  
 903 and 4 of Fig. 2.4) as they are representative of the outcomes for the higher-mass disc ( $M_{\text{disc},i} \geq$   
 904  $0.05 M_{\text{E}}$ ) simulations. Other than the difference in the amount of growth in the disc, there  
 905 are no obvious differences in the mass versus semi-major axis distribution of solids in discs  
 906 with  $M_{\text{disc},i} = 0.05 M_{\text{E}}$  and  $0.25 M_{\text{E}}$ . Compared to the lower-mass discs, we do not see a clear  
 907 inside-out growth trend for the higher-mass discs. This could be due to the discs containing



908 much more larger planetesimals. These large planetesimals tend to grow faster due to their  
909 larger accretion cross-section (and higher accretion efficiency) thus perturbing the orbits of  
910 nearby planetesimals and scattering them to wider orbits. For example, planetesimals are  
911 scattered to 3 au and beyond in the case of a cold disc (with migration effects included)  
912 where planetesimal growth is more efficient. The difference between the simulations with  
913 migration effect included and those that do not is most obviously seen for a cold disc. With  
914 migration included, the most massive planetesimals in the disc is less than  $1 M_E$ . This is  
915 because planetesimals that grew to large sizes earlier migrated towards the Sun and were  
916 removed from the simulation (Fig. 2.5). With migration excluded, planetesimals in a cold  
917 disc can reach masses on the order of  $100 M_E$ , indicating that their core masses have crossed  
918 the threshold for gas envelope accretion to occur. The strong gravitational perturbation of  
919 a gas giant also scatters away most of the mass in the disc, leaving only a narrow annulus  
920 between 0.5 au and 1 au that will be cleared out in due time.

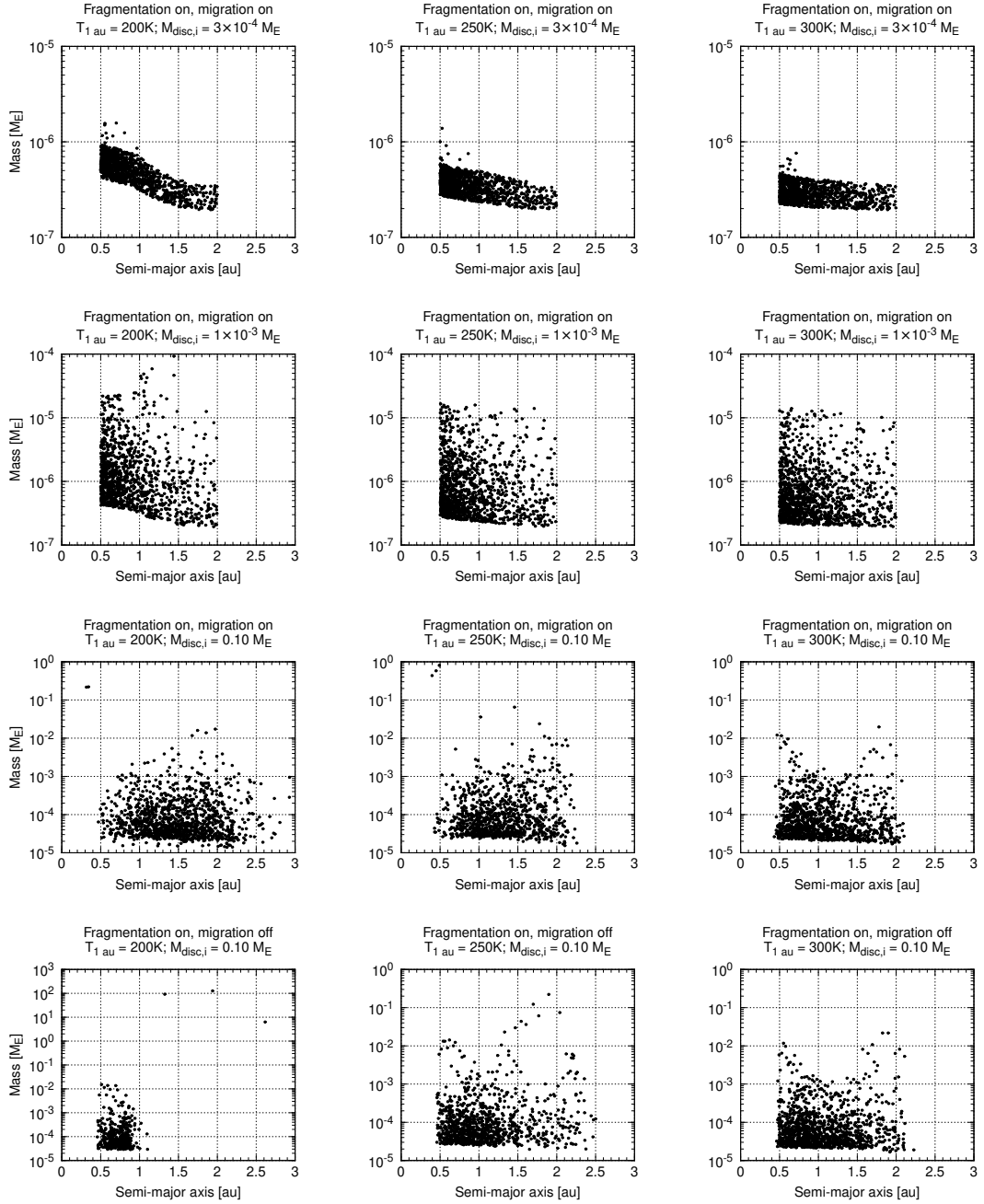


FIGURE 2.4: Distribution of mass in the inner disc at the end of the simulations. Shown here are plots for selected initial conditions representative of all possible outcomes.

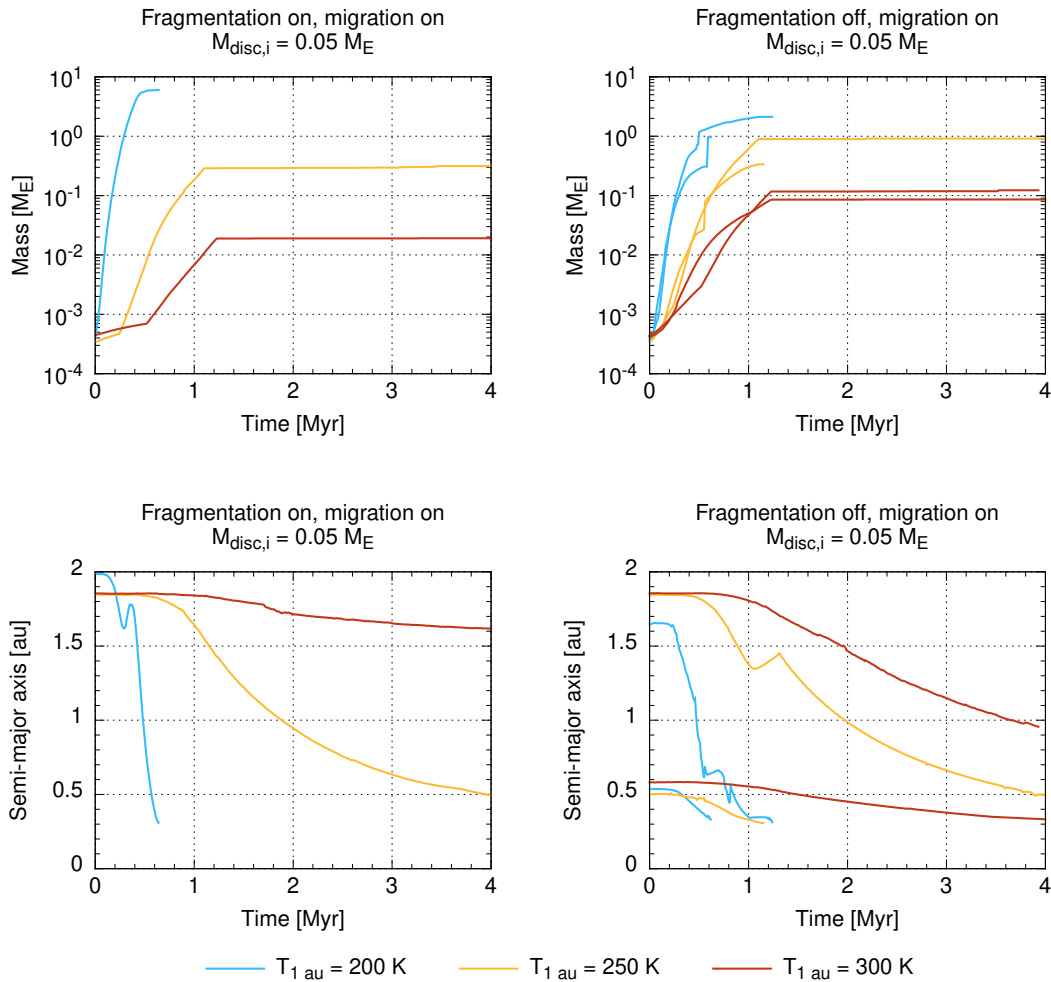


FIGURE 2.5: Selected growth curves of planetesimals in discs of the same mass but with different initial temperature. These planetesimals have diameter over 1000 km so they experience growth more quickly due to their higher pebble accretion efficiency. As migration effects are included in these simulations, these planetesimals will interact with the surrounding gas and migrate inwards to the Sun when they become sufficiently massive. In some cases, these planetesimals do not survive until the end of the simulations (e.g., truncated blue curves in the left and right panels). If we assume that the pebbles do not fragment at the snow line (right panels), then planetesimals near to the inner edge of the solid disc can also grow quickly because of the increased surface density of pebbles in the region closer to the Sun.

### 2.4.2 Establishing a gradient in mass: Lower-mass discs

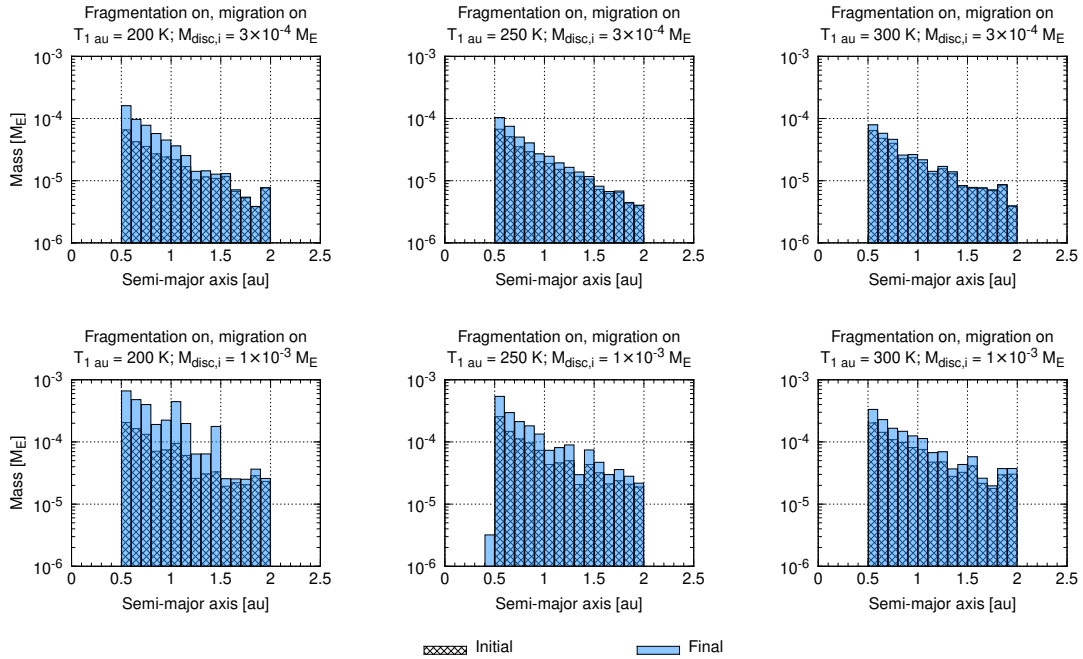


FIGURE 2.6: Initial and final mass distribution in each section of the disc. Shown here are the results for discs containing small planetesimals ( $M_{\text{disc},i} = 3 \times 10^{-4} M_{\text{E}}$  and  $1 \times 10^{-3} M_{\text{E}}$ ) at different initial temperatures, with both fragmentation and migration effects included.

In this and the following subsection we will take an even closer look at the mass distribution in the disc to determine how much mass is accreted in each section of the disc. We divided the inner disc into bins of size 0.1 au each and computed the initial and final mass in each bin. The results for discs containing small planetesimals with  $D \lesssim 300$  km and the inclusion of fragmentation and migration effects (corresponding to the top-left panel of Fig. 2.3) are shown in Fig. 2.6. We observe a trend of inside-out growth: planetesimals closer to the Sun accrete, on average, more mass than those in the region further away (see also the top two rows of Fig. 2.4). The amount of mass accreted also has a dependence on the initial disc mass and the disc temperature, as discussed in the previous subsection. The same inside-out growth trend is also observed for the other simulations using the same initial disc masses with migration effects excluded and thus we opted to not show them. We do not show the results for the simulations with fragmentation effects excluded because the growth is insignificant.

We also computed the value of  $M_{\text{disc},f} - M_{\text{disc},i}$  in each bin with the results shown in Fig. 2.7. In this plot we clearly see the semi-major axis dependence of the amount of mass accreted by the planetesimals. Therefore, if the solid disc is composed of planetesimals with  $D \lesssim 300$  km and the disc is not disturbed by mergers and migration, its isotopic composition will naturally show a gradient.

### 2.4.3 Establishing a gradient in mass: Higher-mass discs

For the case of more massive discs (with  $M_{\text{disc},i} \geq 0.05 M_{\text{E}}$ ), which are composed of larger planetesimals, the inside-out growth trend is not as clear. In Fig. 2.8, we observe a bump each around 1.5 au and inwards of 0.5 au for simulations with fragmentation and migration effects included. The bump around 1.5 au is the result of planetesimal growth caused by the inward migration of the snow line while the bump at  $a < 0.5$  au is due to disc-induced migration

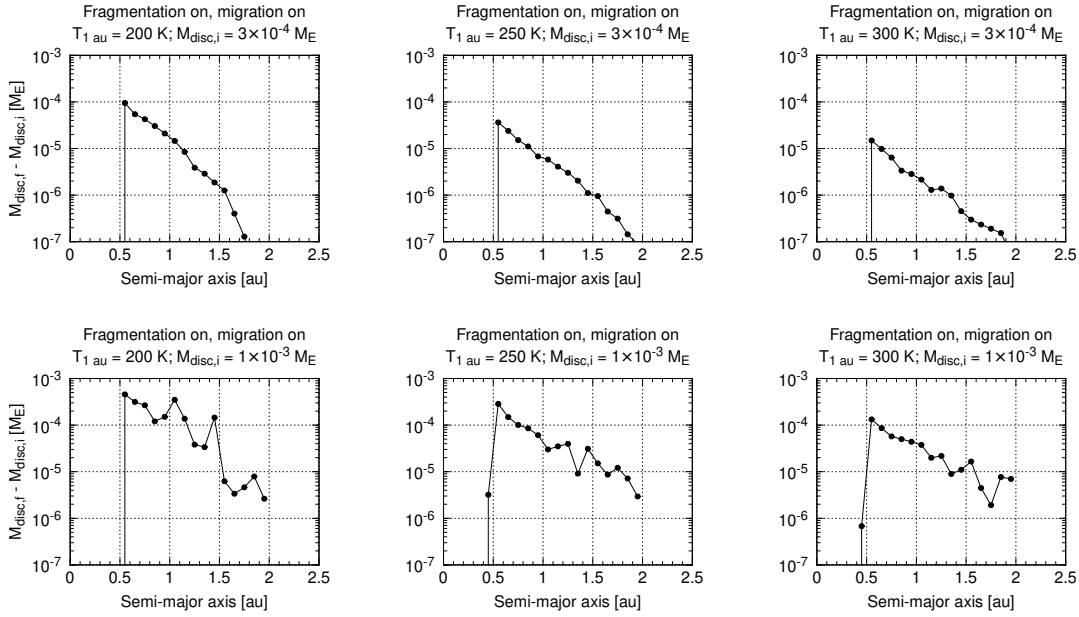


FIGURE 2.7: Mass increase ( $M_{\text{disc},f} - M_{\text{disc},i}$ ) in each section of the disc. Shown here are the results for discs containing small planetesimals ( $M_{\text{disc},i} = 3 \times 10^{-4} M_E$  and  $1 \times 10^{-3} M_E$ ) at different initial temperatures, with both fragmentation and migration effects included.

946 effects causing massive bodies from farther away to migrate inwards and pile up near the  
 947 disc's inner edge. In addition, because the planetesimals in these discs are more massive,  
 948 they will have a higher pebble accretion efficiency which can accelerate their growth and  
 949 thus enable them to perturb nearby smaller planetesimals. In the cold and warm discs where  
 950 the environment is more conducive for planetesimal growth, we observe a wider spread in  
 951 the distribution of mass in the disc due to large planetesimals scattering their nearby smaller  
 952 counterparts away.

953 Unsurprisingly, we also do not observe a strong mass gradient in Fig. 2.9. Only in  
 954 a few cases do we observe the trend but it is confined to the region within 1 au as in the case  
 955 for warm discs or within 1.2 au as in the case of hot discs. This result is in contrast to the  
 956 smoother slopes observed for the simulations using discs composed of smaller planetesimals  
 957 (cf. Fig. 2.7); increasing the number of planetesimals in the more massive discs by including  
 958 smaller bodies will not change the outcome, because the total mass growth is dominated by  
 959 accretion onto the most massive bodies. The combined effect of high accretion efficiency  
 960 and inward migration of large planetesimals in these discs dilute the mass gradient. In the  
 961 case where migration effects are excluded, we observe spikes only in the region around and  
 962 beyond 1.5 au and a mass gradient in the inner region from 0.5 au to about 1.2 au (Fig. 2.10).  
 963 Because the planetesimals remained on their orbits while they grow in the simulations with-  
 964 out migration, several prominent spikes can be seen in the region beyond 1.5 au for cold  
 965 discs due the presence of gas giants. The outcomes for the warm and hot discs in the case  
 966 without migration do not show obvious differences when compared to the outcomes with  
 967 migration included because the higher gas temperature slows down pebble accretion and  
 968 gas giant formation is more difficult.

969 We have seen in Fig. 2.3 that excluding the effects of fragmentation, i.e., allowing  
 970 the pebbles to retain their size and mass when crossing the snow line into the inner regions of  
 971 the disc, results in a general increase in the total mass of the discs. Compared to the case when  
 972 fragmentation effects are implemented, the amount of mass increase is higher regardless of  
 973 the disc temperatures and whether migration effects are included. In Fig. 2.11 we observe a

974 distinct peak in the region within 0.5 au across all disc temperatures because of the inward  
 975 migration of large planetesimals. There is no obvious gradient between 0.5 and 1.2 au, the  
 976 inside-out growth trend is completely masked by the concentration of large bodies in the  
 977 inner region of the disc. When both fragmentation and migration effects are excluded, the  
 978 trend of inside-out growth became apparent once again, in addition to the spikes and peaks  
 979 beyond 1.5 au and the overall larger mass increase in the whole disc (Fig. 2.12).

980 In this and the previous subsection, we show that pebble accretion can generate a  
 981 mass gradient in the terrestrial planet region. This mass gradient does not, however, nec-  
 982 cessarily translate into a corresponding gradient in composition. A composition gradient is  
 983 feasible only if the total mass added by pebbles does not exceed the original mass of the plan-  
 984 etesimal disc, otherwise the composition of the disc becomes almost uniform and dominated  
 985 by the composition of the pebbles.

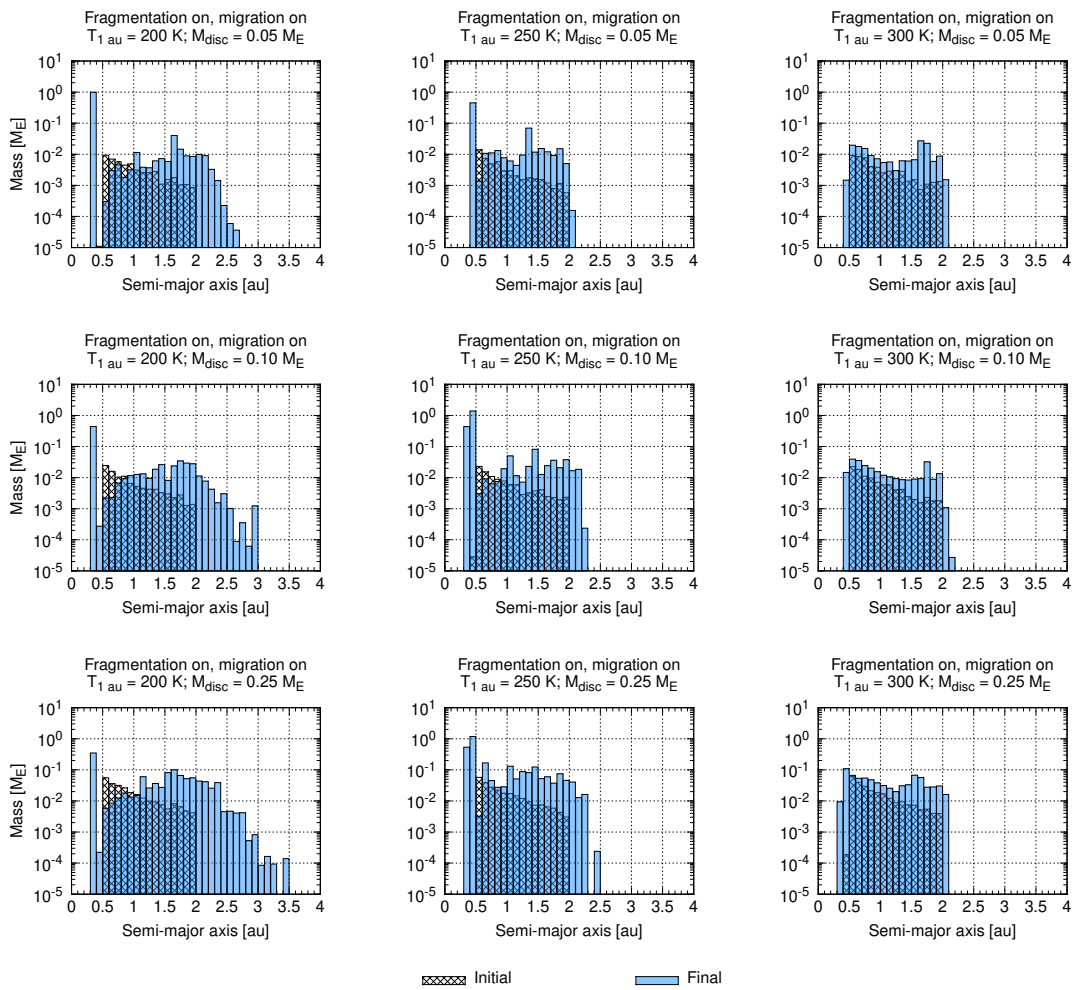


FIGURE 2.8: Initial and final mass distribution in each section of the disc. Shown here are the results for more massive discs containing large planetesimals ( $M_{\text{disc},i} = 0.05 M_E$ ,  $0.10 M_E$ , and  $0.25 M_E$ ) at different initial temperatures, with both fragmentation and migration effects included.

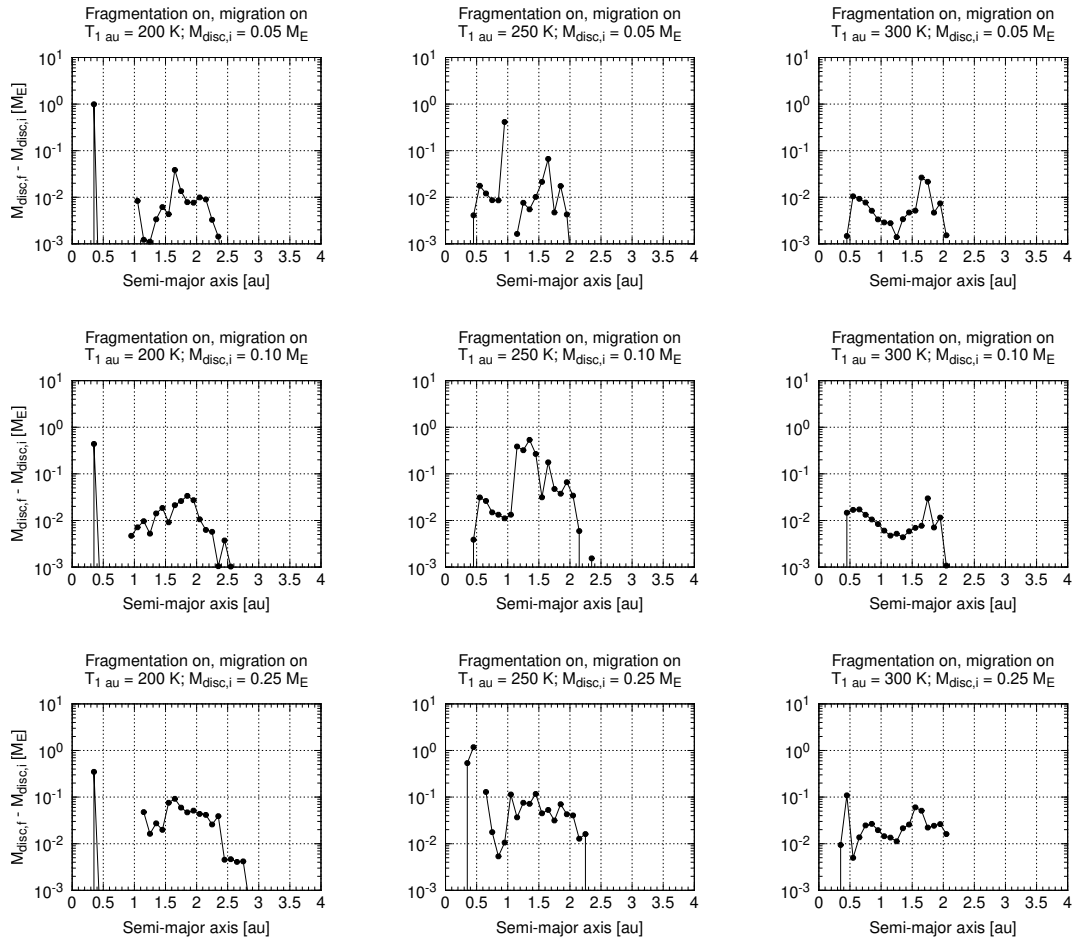


FIGURE 2.9: Mass increase ( $M_{\text{disc},f} - M_{\text{disc},i}$ ) in each section of the disc. Shown here are the results for more massive discs containing large planetesimals ( $M_{\text{disc},i} = 0.05 M_E$ ,  $0.10 M_E$ , and  $0.25 M_E$ ) at different initial temperatures, with both fragmentation and migration effects included.

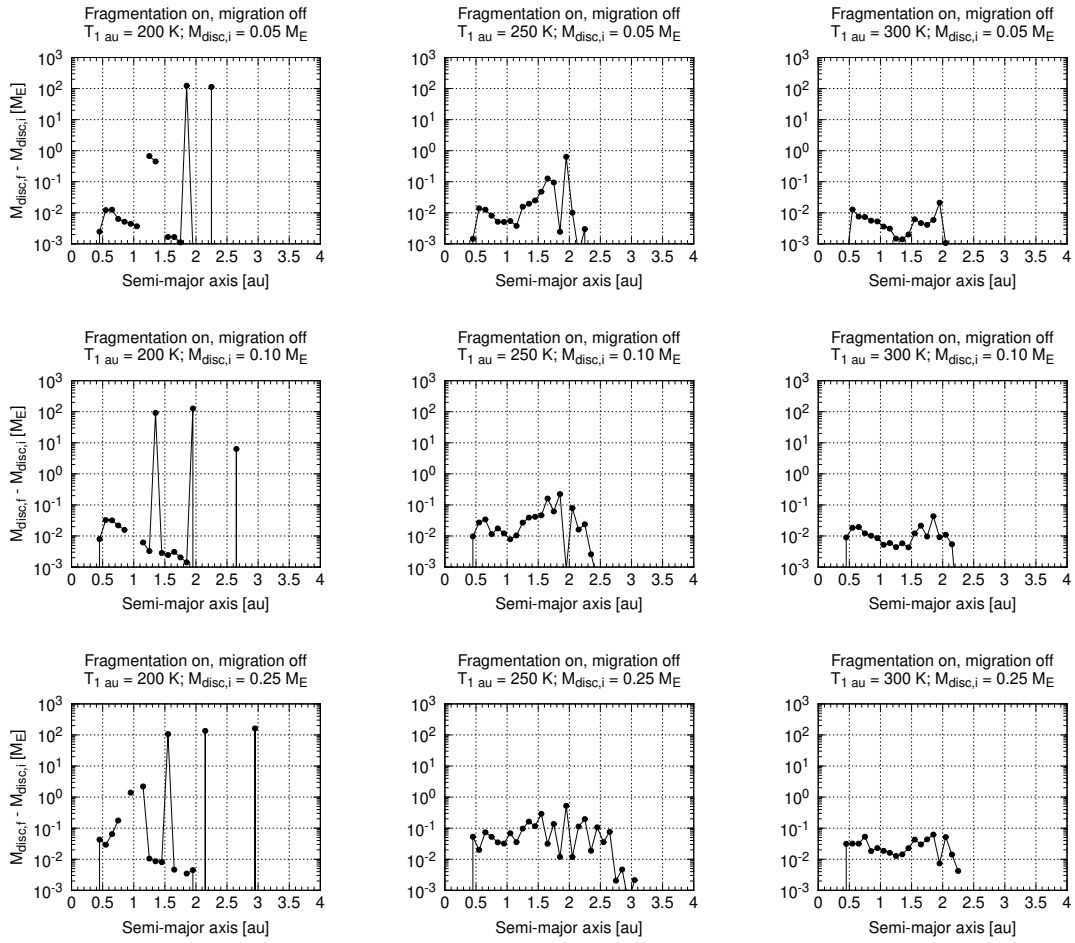


FIGURE 2.10: Mass increase ( $M_{\text{disc},f} - M_{\text{disc},i}$ ) in each section of the disc. Shown here are the results for more massive discs containing large planetesimals ( $M_{\text{disc},i} = 0.05 M_E$ ,  $0.10 M_E$ , and  $0.25 M_E$ ) at different initial temperatures, with fragmentation effects included but migration effects excluded.



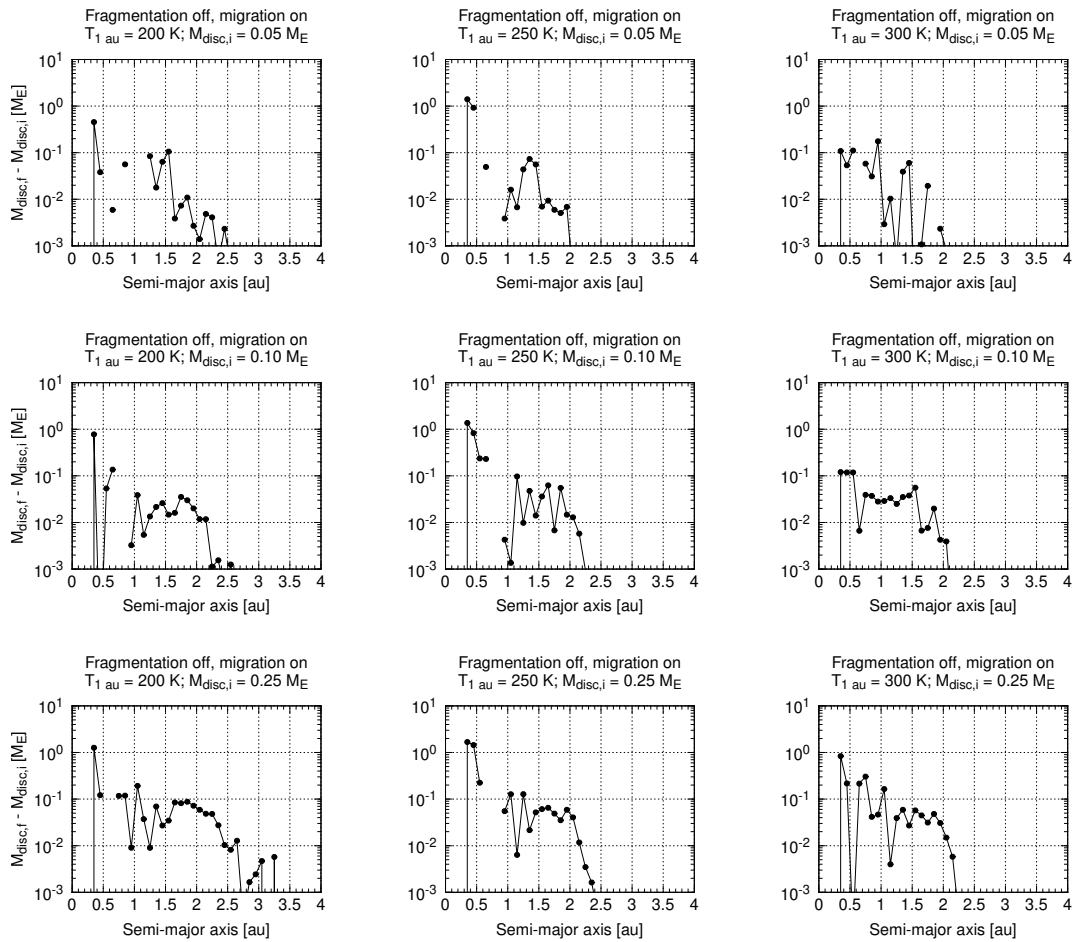


FIGURE 2.11: Mass increase ( $M_{\text{disc},f} - M_{\text{disc},i}$ ) in each section of the disc. Shown here are the results for more massive discs containing large planetesimals ( $M_{\text{disc},i} = 0.05 M_E$ ,  $0.10 M_E$ , and  $0.25 M_E$ ) at different initial temperatures, with fragmentation effects excluded but migration effects included.

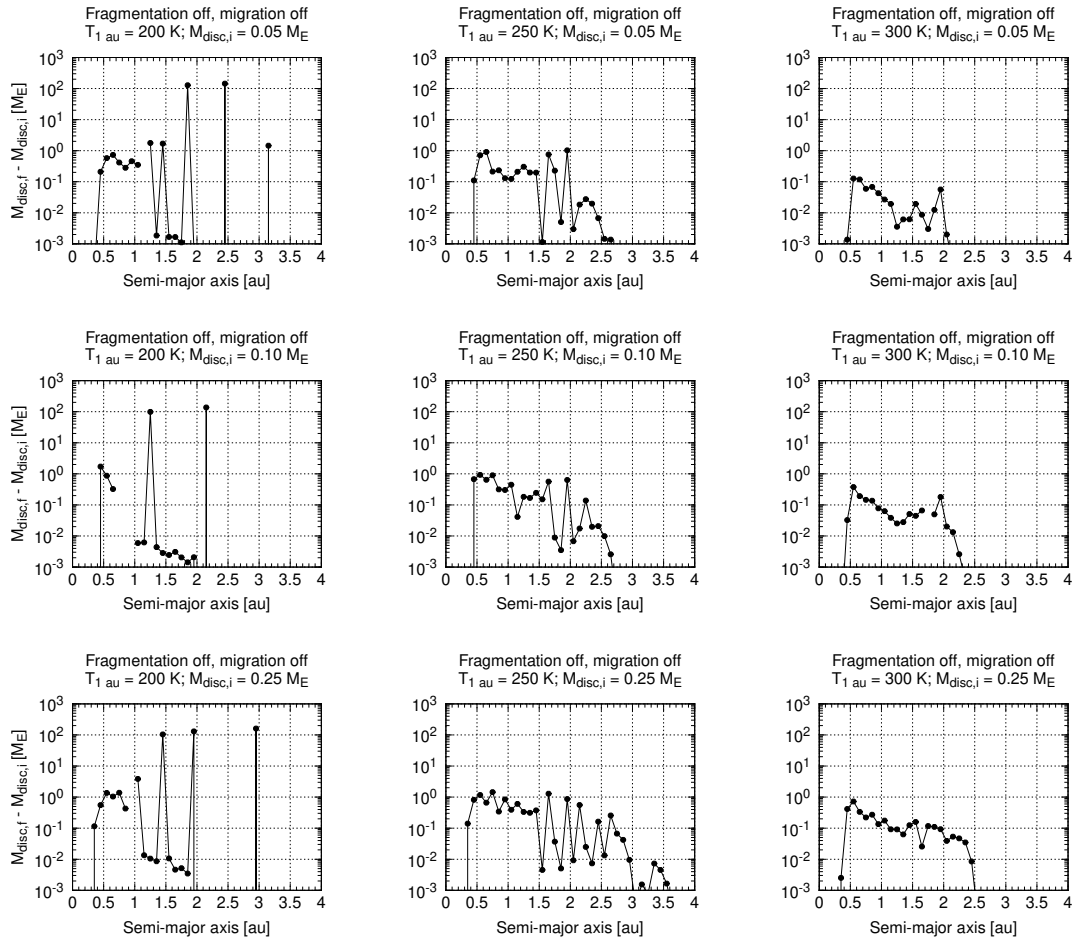


FIGURE 2.12: Mass increase ( $M_{\text{disc},f} - M_{\text{disc},i}$ ) in each section of the disc. Shown here are the results for more massive discs containing large planetesimals ( $M_{\text{disc},i} = 0.05 M_E$ ,  $0.10 M_E$ , and  $0.25 M_E$ ) at different initial temperatures, with both fragmentation and migration effects excluded.

## 2.5 Discussion

### 2.5.1 Jupiter's capacity as a pebble barrier

From the observed isotopic dichotomy among iron meteorites and chondrites that sample the inner and outer Solar System, it is thought that the two reservoirs should have been separated very early and remain separated for at least a few Myr (Kruijer et al., 2017). The means to sustain the separation of the inner and outer Solar System has been suggested to be the growth of Jupiter (e.g., Kruijer et al., 2017). The results of a study by Brassier and Mojzsis (2020) showing large amounts of pebbles could flow past Jupiter while it is still growing and contribute to the growth of planetesimals in the inner Solar System depending on the size of the planetesimal and the temperature of the gas disc raise doubts on the capacity of Jupiter as a pebble barrier.

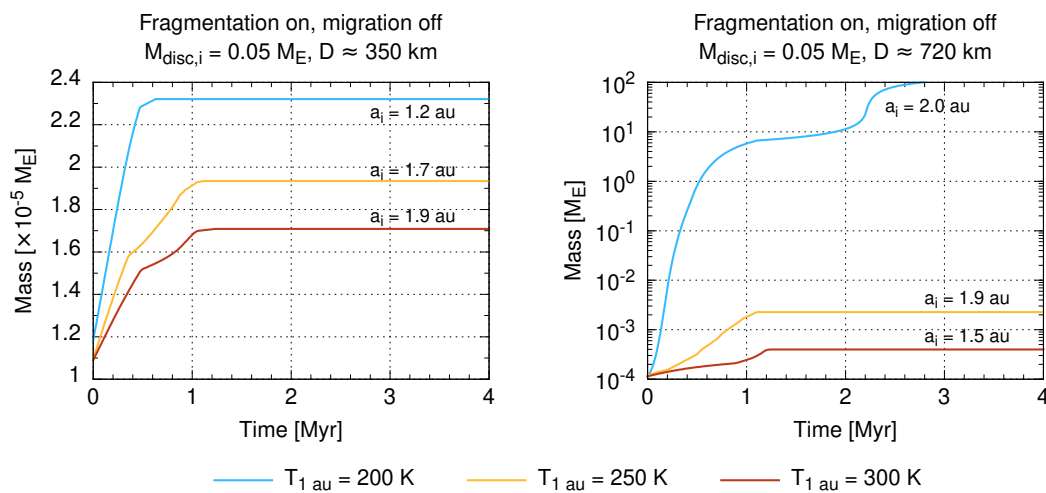


FIGURE 2.13: Growth curves of selected planetesimals of different initial size located beyond 1.2 au over the total simulation time of 4 Myr taken from simulations using the same initial disc mass of  $M_{\text{disc},i} = 0.05 M_{\text{E}}$  but at different disc temperatures. These examples illustrate the substantial mass increase contributed by pebbles (and gas in the case of cold discs) despite Jupiter shutting off the pebble flux when it reaches its isolation mass.

We obtain outcomes similar to those of Brassier and Mojzsis (2020) in that planetesimals with  $D > 300$  km in the region around Mars' orbit can grow substantially after the passage of the snow line under special conditions when Jupiter is growing. Planetesimals in this region can grow to large sizes by mergers and, in some cases, gas accretion, thereby contributing to most of the mass in the disc. In Fig. 2.13 we illustrate this point using growth curves of selected planetesimals of different sizes initially located beyond 1.2 au in discs of different temperature. Our selected 350 km planetesimal in a cold disc increased its mass by 90% while a 720 km planetesimal in the same simulation attained sufficient mass to accrete gas. The swift growth of the larger planetesimal is due to its size and its semi-major axis. Located in the outer edge of the solid disc, it is one of the first few planetesimals to encounter the pebble flux. In a hot disc where the pebble accretion efficiency is lower and the snow line is located farther away, our selected 350 km planetesimal nevertheless managed to increase its mass by 50% from pebbles while its 700 km counterpart increased its mass by about 400%.

Despite Jupiter effectively shutting off the pebble flux once it reaches its pebble isolation mass, we find that planetesimals of 300 km and above have accreted a rather large amount of pebbles during this time which could potentially alter their initial isotopic composition. If the inner Solar System contained a high number of planetesimals with diameter

1014 300 km and above, then the substantial contribution by pebbles can result in the inner Solar  
 1015 System’s final isotopic composition after 4 Myr to be akin to that of the outer Solar System,  
 1016 thus diminishing the isotopic differences between these two reservoirs. In this sense, previ-  
 1017 ous studies suggesting that Jupiter acts as an efficient gatekeeper in preventing pebbles from  
 1018 flowing past its orbit towards the inner disc and maintaining the isotopic dichotomy of the  
 1019 early Solar System (e.g., [Kruijer et al., 2017](#)) may need to be revisited. It is therefore more  
 1020 likely the case that some other factor(s) is/are at play at preserving the isotopic dichotomy,  
 1021 e.g., a structural gap in the protoplanetary disc located just within the orbit of Jupiter, pro-  
 1022 posed by [Brasser and Mojzsis \(2020\)](#).

### 1023 2.5.2 Comparing dynamical outcomes with cosmochemistry data

1024 From chondritic mixing models discussed in Chapter 1, a mass contribution from outer Solar  
 1025 System material by amounts greater than  $\sim 10\%$  poses problems for reconciling the differ-  
 1026 ence in isotopic composition of the terrestrial planets with that of the outer Solar System,  
 1027 and a mass increase beyond 100% will severely dilute the original composition of the inner  
 1028 disc and mostly homogenise it. Discs with initial mass of  $\geq 0.05 M_E$  and containing many  
 1029 planetesimals larger than 300 km in diameter increase their mass by at least a few times the  
 1030 initial value, suggesting that their initial isotopic signatures will be replaced by the isotopic  
 1031 composition of outer Solar System material. If we take 10% as the upper limit for the amount  
 1032 of outer Solar System material present in the Earth and Mars, then the successful cases from  
 1033 our numerical simulations are the cases which fulfil all of the following criteria:

- 1034 •  $M_{\text{disc},i} \leq 1 \times 10^{-3} M_E$ , or if the disc is more massive then all planetesimals have  $D \leq$   
 1035 300 km, and
- 1036 •  $T_{1 \text{ au}} \geq 250 \text{ K}$ , and
- 1037 • pebble fragmentation effects at the snow line are unimportant.

1038 For these cases the overall mass increase in the disc ranges from 0.3% to 5%, consistent with  
 1039 the constraint from mixing models and cosmochemistry data. However, these cases have a  
 1040 critical shortcoming: although the amount of mass increase in the disc appears consistent  
 1041 with cosmochemistry data, the total mass in the disc at the end of 4 Myr is actually too little  
 1042 to build the terrestrial planets in the next stage of planet formation. A 5% mass increase for  
 1043 a disc with  $M_{\text{disc},i} = 1 \times 10^{-3} M_E$  is a mere  $1.05 \times 10^{-3} M_E$ ; at least  $2 M_E$  of solids is required  
 1044 in the disc to form the terrestrial planets. To fulfil both requirements for the amount of mass  
 1045 increase ( $\leq 10\%$ ) and disc mass at the end of the pebble accretion phase ( $\geq 2 M_E$ ), we should  
 1046 ideally start with a solid disc of  $M_{\text{disc},i} = 1.8 M_E$  which will grow to  $2 M_E$  assuming a 10% mass  
 1047 increase and that the disc contained planetesimals of size  $D \leq 300 \text{ km}$ . However, modelling  
 1048 such a massive disc made up entirely of small planetesimals is at the limit of the capabilities  
 1049 of current hardware and  $N$ -body codes ([Woo et al., 2021](#)). We will therefore reserve this study  
 1050 for future work.

1051 It could still be possible for the dynamical outcomes to be reconciled with cos-  
 1052 mochemistry data (e.g., in  $\epsilon^{48}\text{Ca}$ ) by invoking specific assumptions, such as the inner disc  
 1053 planetesimals had a ureilite-like initial composition and the pebbles an isotopic composition  
 1054 akin to CI chondrites ([Schiller et al., 2018](#)). That study argues that the gradual accretion of  
 1055 CI-chondrite-like material from the outer Solar System over the lifetime of the gas disc (about  
 1056 5 Myr) can explain the variation in  $\epsilon^{48}\text{Ca}$  with mass of the major differentiated bodies in the  
 1057 inner Solar System (Vesta, angrite parent body, Mars and Earth). When the gas disc dissipates,  
 1058 the isotopic composition of the planetesimals and planetary embryos stopped changing, with  
 1059 the largest embryos (including proto-Earth) having up to 40% of their mass contributed from

1060 the outer Solar System (Schiller et al., 2020). Indeed, by looking at single isotopes indepen-  
 1061 dently it is always possible to find a combination of end-member meteoritic reservoirs with  
 1062 the correct mixing proportion to explain the isotopic composition of a planetary body. The  
 1063 difficulty is to find a single mixing ratio that matches all isotopes simultaneously.

1064 Schiller et al. (2018) and Schiller et al. (2020) argue for pebble accretion in the inner  
 1065 Solar System based on  $\epsilon^{48}\text{Ca}$  and  $\epsilon^{54}\text{Fe}$  isotopes in the Earth and other meteorites. Their  
 1066 combined results argue for the Earth having 40% CI-chondrite-like material in its mantle. For  
 1067 the ureilite parent body Schiller et al. (2018) list  $\epsilon^{48}\text{Ca} = -1.46 \pm 0.46$  and for the CI chondrite  
 1068 parent body  $\epsilon^{48}\text{Ca} = 2.06 \pm 0.085$ . If we denote by  $x$  the fraction of CI chondrite in Earth's  
 1069 mantle, then according to Schiller et al. (2018)  $x$  is the solution to  $2.06x - 1.46(1 - x) = 0$ ,  
 1070 which yields  $x = 0.41 \pm 0.12$  ( $2\sigma$ ). The uncertainties were computed using a Monte Carlo  
 1071 method. If these results are correct, they should also hold for the isotopes of other elements  
 1072 commonly used as tracers, such as oxygen, chromium and titanium because the Earth can  
 1073 only be made up of a single mixture of sources rather than different mixtures for different  
 1074 elements. For the ureilite parent body  $\Delta^{17}\text{O} = -1.16 \pm 0.55$  (Clayton and Mayeda, 1996) and  
 1075  $\Delta^{17}\text{O} = 0.39 \pm 0.14$  for the CI chondrites (Clayton and Mayeda, 1996). The required mass  
 1076 fraction of CI chondrite based on oxygen isotopes is  $x = 0.75 \pm 0.23$  ( $2\sigma$ ). This fraction is,  
 1077 however, grossly inconsistent with that advocated by Schiller et al. (2018) based on calcium  
 1078 isotopes. In addition, if molybdenum isotopes are considered then there is no acceptable  
 1079 solution for  $x$  as the isotopic anomalies in  $\epsilon^{92}\text{Mo}$  for both ureilites and CI chondrites have  
 1080 the same sign. We arrive at the same conclusion as well if we were to consider the more  
 1081 abundant isotopes of molybdenum ( $\epsilon^{94,95}\text{Mo}$ ).

1082 The above analysis shows that it is difficult to establish whether or not pebble accre-  
 1083 tion occurred in the inner Solar System when using isotopes alone because the end-member  
 1084 case Ureilite + CI chondrite can often be invoked as a mixture to explain the isotopic anoma-  
 1085 lies of the terrestrial planets (albeit not always in the same proportions). It is therefore nec-  
 1086 essary to look beyond nucleosynthetic isotopes alone to establish whether the simple model  
 1087 suggested by Schiller et al. (2018, 2020) and pebble accretion can account for the growth and  
 1088 composition of the terrestrial planets. In the following, we examine the constraints from the  
 1089 major elemental abundances in known meteoritic reservoirs and planetary bodies.

1090 It has been reported (e.g., Drake and Righter, 2002; Dauphas et al., 2015) that the  
 1091 combination of chondritic (and perhaps achondritic) meteorites is unable to reproduce the  
 1092 Mg/Si ratio of the terrestrial planets. Following Drake and Righter (2002) we plot in Fig. 2.14  
 1093 the Mg/Si versus Al/Si elemental ratios for the terrestrial planets and the known meteorite  
 1094 parent body compositions. The CI chondrites are similar in elemental composition to the  
 1095 Sun's photosphere (e.g., Anders and Grevesse, 1989; Lodders, 2003) and there is little variation  
 1096 amongst the carbonaceous chondrites. The non-carbonaceous meteorites, which formed in  
 1097 the same reservoir as the Earth and Mars, all have lower Mg/Si ratios due to nebular and plan-  
 1098 etary processes (e.g., Larimer, 1979; Alexander, 2019); they all have more or less forsterite-  
 1099 or enstatite-rich composition (Dauphas et al., 2015).

1100 The possible compositions of the bulk Silicate Earth (crust and mantle) computed  
 1101 from models based on terrestrial rocks and chondrites (e.g., McDonough and Sun, 1995; Palme  
 1102 and O'Neill, 2014) place it at an end-member location in Fig. 2.14, indicating that the chemical  
 1103 composition of the Earth is unlike any of the known meteorites. An exception is the result of  
 1104 Javoy et al. (2010) (blue square labelled with J10 in the figure) which is obtained by assuming  
 1105 that the Earth is made up entirely of enstatite chondrites. This result should however be  
 1106 interpreted with caution as a more recent study examining the  $\delta^{30}\text{Si}$  and Mg/Si composition

1107 of the Earth showed that it is similar to the enstatite chondrites isotopically but not chemically  
1108 (Dauphas et al., 2015).

1109         There remains uncertainty in the composition of the Earth’s lower mantle, which  
1110 is challenging to determine but important in deriving accurate estimates of the bulk Silicate  
1111 Earth’s composition. Although the different bulk Silicate Earth models make different as-  
1112 sumptions about the composition of the upper and lower mantle, they are all consistent with  
1113 geochemistry (McDonough, 2016). The models of McDonough and Sun (1995) and Palme and  
1114 O’Neill (2014) assume a homogeneous (pyrolitic with Mg/Si  $\sim$  1.3) composition for the whole  
1115 mantle while the model of Javoy et al. (2010) requires that the upper and lower mantle differ  
1116 in their compositions. Results from seismic tomography observations of subducted crustal  
1117 slabs (Fukao and Obayashi, 2013), computations and measurements of mineral elasticities  
1118 (Wang et al., 2015; Kurnosov et al., 2018) support a compositionally homogeneous mantle,  
1119 although there are alternative proposals for a non-pyrolitic and silicon-enriched lower man-  
1120 tle based on its sound-velocity structure (Murakami et al., 2012; Mashino et al., 2020). Be  
1121 that as it may, the Mg/Si ratios of the lower mantle derived from these studies ( $\sim$  1.0 for  
1122 Murakami et al. 2012 and 1.14 for Mashino et al. 2020) still lie above the Mg/Si ratio of the  
1123 known meteorites.

1124         The amount of Si fractionated into the Earth’s core is also uncertain, but it is esti-  
1125 mated to be between 2 wt% to 7 wt% based on geochemical and geophysical constraints (e.g.,  
1126 Badro et al., 2007; Fitoussi et al., 2009; Moynier et al., 2020). We plot in Fig. 2.14 the corre-  
1127 sponding Mg/Si and Al/Si ratios for the Earth assuming different amounts of Si in the core.  
1128 The Earth’s chemical composition is similar within uncertainties to the carbonaceous chon-  
1129 drites if more than 5 wt% of the Si is in the core. Nevertheless, this still does not change the  
1130 fact that the Earth’s chemical composition cannot be reproduced by any mixture of known  
1131 planetary materials, not even the combination of ureilites and CI chondrites as suggested  
1132 by Schiller et al. (2018, 2020) because this mixture would lower the Mg/Si ratio to below the  
1133 7 wt% Si value.

1134         Will the outcome of the N-body simulations change by assuming a changing com-  
1135 position of the pebbles? In our study, we implicitly assume that the pebbles have the same  
1136 composition, which we leave unspecified but one could assume any of the various carbona-  
1137 ceous chondrites as a proxy. In reality, the pebbles that formed at different times and at  
1138 different locations in the disc could potentially have different compositions. The diversity  
1139 in the isotopic compositions of the carbonaceous chondrites possibly reflects their distinct  
1140 formation location and/or their formation time, although this is difficult to prove. For the  
1141 isotopes of O, Cr and Ti the CI and CO chondrites plot in end-member positions of the CC  
1142 group. This could mean that there was also a compositional gradient in the outer Solar Sys-  
1143 tem when these bodies formed. To model the effect of time-dependent pebble compositions,  
1144 we need to understand how the compositional gradient scales with heliocentric distance.  
1145 This information is currently unavailable, although Desch et al. (2018) suggested that the CI  
1146 chondrites form farthest away from the Sun while CO chondrites form closest to the Sun, but  
1147 this suggestion is based mostly on model predictions.

1148         One possible way out of this impasse is to do a similar end-member study by esti-  
1149 mating the contribution of CI or CO chondrites to the composition of the terrestrial planets  
1150 using our isotope mixing models. We show in Fig. 2.15 (which is akin to Fig. 1.2) the com-  
1151 puted best-fit composition of the Earth and Mars as a combination of enstatite chondrites,  
1152 ordinary chondrites and CI or CO chondrites using the Monte Carlo mixing model algo-  
1153 rithm described in Appendix A. With only CI or CO chondrites, the mixing model returns  
1154 the maximum contribution of these chondrite types as  $\leq$  10%, similar to the results obtained

1155 by including various other types of carbonaceous chondrites (Fig. 1.2). For both planets the  
1156 contribution from H-chondrites is most strongly affected by the choice of either CI or CO.  
1157 Thus, even if we were to assume a time-dependent variation in the composition of the peb-  
1158 bles from CO-like at the beginning to CI-like at the end (or vice versa), it still remains difficult  
1159 for our  $N$ -body simulation results to be reconciled with meteorite isotope and elemental ratio  
1160 data of the inner planets: the amount of outer Solar System materials added to the terrestrial  
1161 planets *cannot* be more than 10%!

1162         Based on nucleosynthetic anomalies of several isotopes such as  $^{50}\text{Ti}$  and  $^{54}\text{Cr}$ , the  
1163 contribution of carbonaceous chondrites towards the making of the Earth is limited to 10 –  
1164 25% (e.g., [Warren, 2011](#); [Mezger et al., 2020](#)). We discussed the difficulty for O and Mo iso-  
1165 topes above. Taken together, the isotopic and elemental abundances as well as our modelling  
1166 results argue against the isotopic gradient in the inner Solar System having been established  
1167 through pebble accretion, and against pebble accretion having been a major source of plane-  
1168 tary building blocks if the pebbles were sourced from the outer Solar System. For the gradient  
1169 to have been established early either the injection of nebula material or thermal processing  
1170 of molecular cloud material as suggested by some studies ([Trinquier et al., 2009](#); [Dwarkadas  
1171 et al., 2017](#); [Nanne et al., 2019](#); [Ek et al., 2020](#)) may be the generating mechanism(s), or it  
1172 could be the case that the gradient is primordial and indigenous to the disc at the time of  
1173 Solar System coalescence.

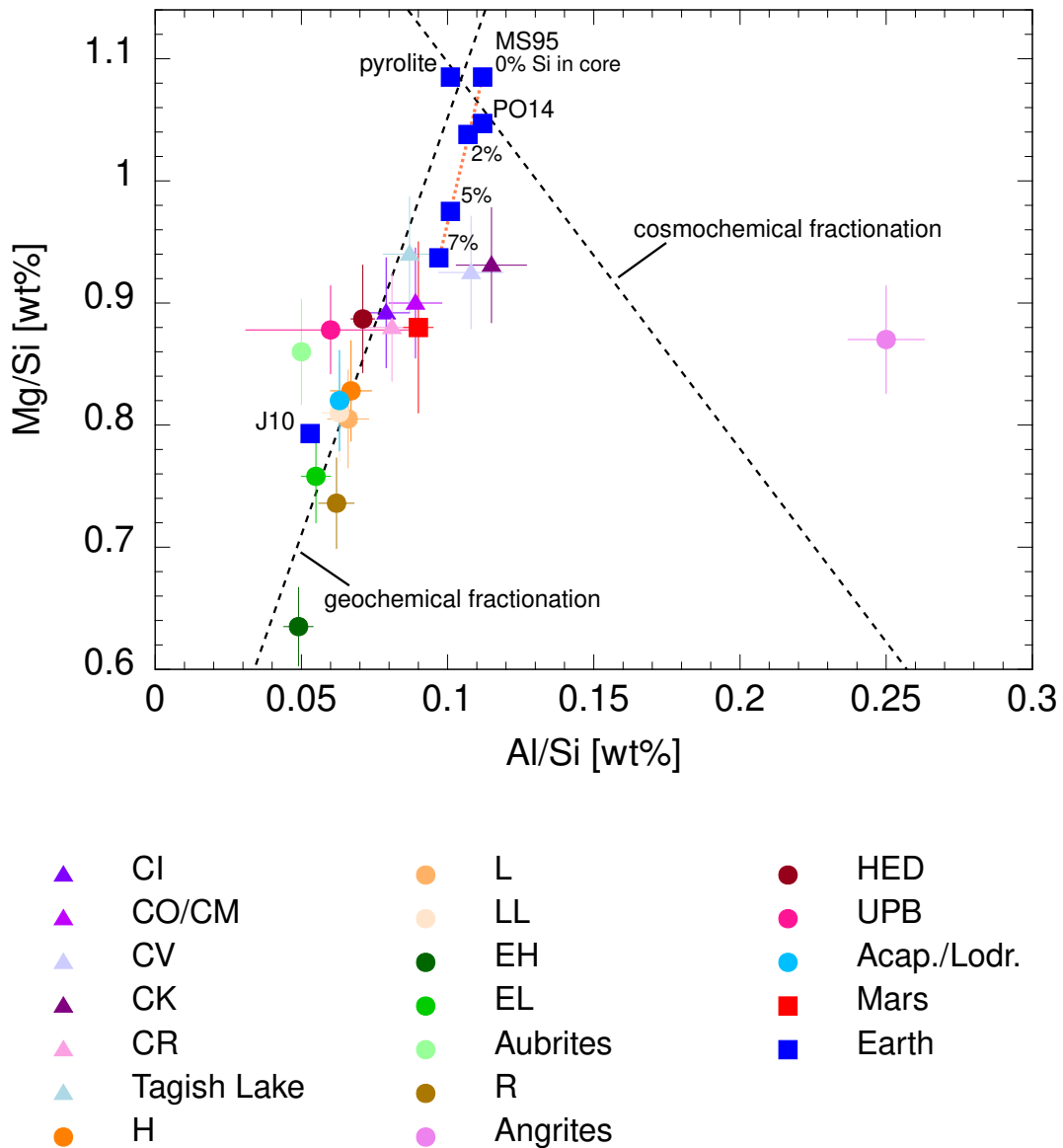


FIGURE 2.14: Mg/Si versus Al/Si for various chondrites, achondrites, Mars and the Earth. For the Earth, we also show the elemental abundance ratios of the Earth for different amount of Si in the core. The fractionation lines and pyrolite composition are from [Jagoutz et al. \(1979\)](#). Error bars are average variations for Mg/Si (5%) and Al/Si (10%) determinations for each parent body. UPB stands for ureilite parent body. Elemental abundance ratio for the Earth sourced from [McDonough and Sun \(1995\)](#), [Javoy et al. \(2010\)](#) and [Palme and O'Neill \(2014\)](#) while the data for meteorites are from [Mason and Wiik \(1962\)](#); [Von Michaelis et al. \(1968\)](#); [Ahrens et al. \(1973\)](#); [Consolmagno and Drake \(1977\)](#); [Dreibus et al. \(1977\)](#); [Hertogen et al. \(1977\)](#); [Morgan et al. \(1978\)](#); [Jagoutz et al. \(1979\)](#); [Watters and Prinz \(1979\)](#); [Jarosewich et al. \(1987\)](#); [Wasson and Kallemeyn \(1988\)](#); [Jarosewich \(1990\)](#); [Kallemeyn et al. \(1991, 1994, 1996\)](#); [Kong et al. \(1997\)](#); [Mittlefehldt et al. \(1998\)](#); [Goodrich \(1999\)](#); [Longhi \(1999\)](#); [Brown et al. \(2000\)](#); [Wolf and Palme \(2001\)](#); [Greenwood et al. \(2010\)](#); [Bischoff et al. \(2011\)](#); [Stracke et al. \(2012\)](#); [Blinova et al. \(2014\)](#); [Hewins et al. \(2014\)](#); [Palme et al. \(2014\)](#); [Collinet and Grove \(2020\)](#); [Yoshizaki and McDonough \(2020\)](#).



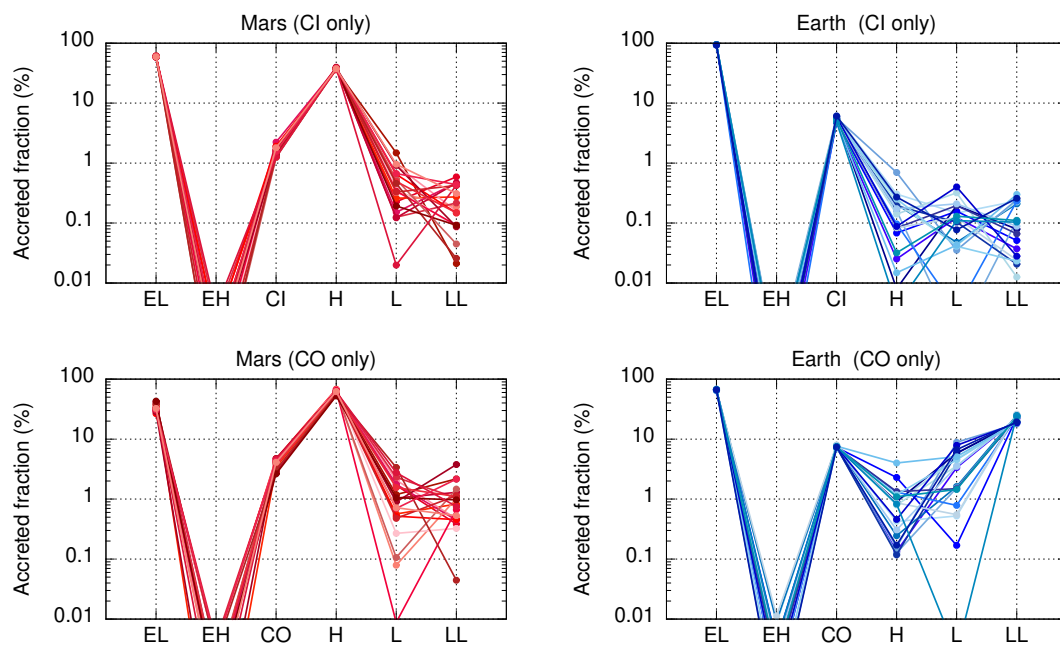


FIGURE 2.15: Best-fit contributions of enstatite chondrites, ordinary chondrites and CI or CO chondrites (end-members of the carbonaceous chondrite group for O, Cr and Ti isotopes) to the building blocks of Earth and Mars computed from 20 Monte Carlo mixing model simulations. The contribution of CI or CO chondrites to the Earth and Mars is limited to  $\leq 10\%$ .

## 1174 2.6 Conclusions

1175 The apparent correlation between semi-major axis and some nucleosynthetic isotope anom-  
 1176 alies ( $\epsilon^{48}\text{Ca}$ ,  $\epsilon^{50}\text{Ti}$ ,  $\epsilon^{54}\text{Cr}$ ) for the Earth, Mars and Vesta can be used to constrain plausible  
 1177 dynamical mechanisms for planet formation in the inner Solar System. This correlation po-  
 1178 tentially points to the existence of isotopic gradients in the inner Solar System, for which the  
 1179 generating mechanism could possibly be the influx of material either from the outer disc or  
 1180 from the Solar nebula.

1181 We investigated the role of the pebble accretion mechanism in the inner Solar Sys-  
 1182 tem by performing  $N$ -body simulations modelling the growth of a disc of planetesimals sub-  
 1183 jected to a flux of pebbles originating from beyond the orbit of Jupiter. We found from simu-  
 1184 lation results that throughout the duration of Jupiter’s growth from a  $0.01 M_{\text{E}}$  planetary body  
 1185 to a  $\sim 300 M_{\text{E}}$  gas giant, depending on disc temperature and whether pebble fragmentation  
 1186 and/or disc-induced migration effects are considered, the final mass in the solid disc can be at  
 1187 least a few times its initial mass if it contained planetesimals of diameter  $D \geq 300$  km; the fi-  
 1188 nal disc mass is at most 3 times the initial mass if the disc is made up of smaller planetesimals  
 1189 of diameter  $D \leq 300$  km.

1190 In particular, the amount of mass increase in warm and hot discs containing plan-  
 1191 etesimals less than 300 km in diameter is consistent with earlier studies (e.g., [Dauphas, 2017](#))  
 1192 reporting that the Earth comprised of at most 10% of (CI) carbonaceous chondrites. However,  
 1193 the major drawback is that the growth of only a few per cent in mass cannot supply the inner  
 1194 disc with sufficient mass for the next stage of planet formation – planetesimal collision and  
 1195 mergers – to form larger bodies, unless the disc was more massive to begin with ( $\geq 1.5 M_{\text{E}}$ )  
 1196 and only consisted of very small planetesimals, which appears to contradict modern models  
 1197 of planetesimal formation. Indeed, the latest models of planetesimal formation show that  
 1198 they form with a fairly shallow size-frequency distribution, with diameters between 100 km  
 1199 to 1000 km (e.g., [Chambers, 2010](#); [Johansen et al., 2014](#); [Klahr and Schreiber, 2020](#)). Instead,  
 1200 if the inner disc had more mass it is expected to have contained many larger planetesimals  
 1201 ( $D \geq 300$  km). In this case the mass increase of the disc due to pebble accretion becomes  
 1202 so large that the final isotopic composition of the planetesimals is akin to those of the (CI)  
 1203 carbonaceous chondrites, even with the assumption that the initial composition of the plan-  
 1204 etesimal disc was ureilite-like ([Schiller et al., 2018](#)).

1205 Based on our results we conclude that pebble accretion played almost no role in the  
 1206 formation of the inner Solar System planetary bodies – the terrestrial planets and asteroid  
 1207 Vesta are more likely to have formed via the merging of planetesimals instead. Furthermore,  
 1208 the isotopic gradients in the inner Solar System were also unlikely to have been established  
 1209 over time by the accretion of outer Solar System material in the form of pebbles. The gradients  
 1210 could instead be (1) the outcome of accreting external material from the Solar nebula very  
 1211 early in the history of the Solar System (e.g., [Dwarkadas et al., 2017](#); [Nanne et al., 2019](#); [Ek  
 1212 et al., 2020](#)), (2) the outcome of thermally processed molecular cloud material ([Trinquier et al.,  
 1213 2009](#)), or (3) innate to the Solar System.



## 3 Formation of the inner Solar System bodies

### 3.1 Introduction

In the previous chapter we showed using cosmochemical trends and  $N$ -body simulations that the isotopic gradients in the inner disc were more likely to have been established via mechanisms like the accretion of nebular material or thermal processing in the disc, rather than the accretion of outer disc material in the form of cm-sized pebbles. Since the contribution of the pebble accretion mechanism to the growth of planetesimals in the inner disc is very minor, it should thus be more likely the case that the terrestrial planets (and possibly the larger asteroids) are products of collisional mergers among the inner disc planetesimals instead. Furthermore, when the planetary bodies in the inner disc were growing, the isotopic gradients should have remained unperturbed as is reflected in their correlated bulk isotopic compositions and semi-major axes (Yamakawa et al., 2010).

What, then, is the preferred formation pathway of the planetary bodies in the inner disc? Previous works that studied the Grand Tack (Walsh et al., 2011) and classical (Chambers, 2001) models to determine the feeding zones of the terrestrial planets found that the terrestrial planet feeding zones are very similar – wide with a large overlapping region – for the Grand Tack model (Brasser et al., 2017; Woo et al., 2018) whereas they are more localised and display a weak but nevertheless existent correlation with semi-major axis for the classical model (e.g., Raymond et al., 2004; O’Brien et al., 2006; Fisher and Ciesla, 2014; Kaib and Cowan, 2015; Woo et al., 2018). These results are verified with new, high-resolution GPU simulations (Woo et al., 2021). Given that the isotopic gradients are present in the inner disc during the formation of the inner Solar System bodies, the distinct isotopic compositions of Earth, Mars and Vesta therefore points to a classical-model-like formation pathway for these planetary bodies.

The major difference between the Grand Tack model and the classical model is that the former features an early gas-driven migration of Jupiter and Saturn while the latter does not. It turns out that this feature exerts a strong influence on the feeding zone outcomes. The migration of the gas giants causes the material in the inner disc to mix and thus homogenising any pre-existing isotopic differences (Carlson et al., 2018). It is therefore not surprising that the terrestrial planets that formed within the framework of the Grand Tack model have very similar feeding zones and isotopic compositions because they all accreted from the same homogenised mixture. If the gas giants did not migrate into the terrestrial region when the terrestrial planets were forming, as in the classical model, then it is more likely for the terrestrial planets to be isotopically distinct. However, the widely-known downside of the classical model is that its Mars analogues are systematically a few times too massive to be consistent with the current Mars unless the surface density slope is much steeper (Izidoro et al., 2015). We therefore need to seek out other dynamical models that can reproduce Mars with the correct mass without invoking the migration of the gas giants.

1252 Here, we investigate the predictions of the depleted disc model (Izidoro et al., 2014)  
 1253 – a less-explored but promising model – for the isotopic compositions of the terrestrial plan-  
 1254 ets. This model was proposed as an alternative to the Grand Tack model to emulate the  
 1255 orbital configuration of the terrestrial planets and the Earth-Mars mass ratio without the mi-  
 1256 gration of Jupiter and Saturn. It features a depletion in the mass of the inner disc around  
 1257 and beyond the orbit of Mars, with the surface density of solids following a steep power law  
 1258 function of distance from the Sun (e.g.,  $\Sigma_s \propto r^{-5.5}$ ; Izidoro et al., 2015). We perform numer-  
 1259 ical simulations to study the formation of the terrestrial planets in this model and compute  
 1260 their corresponding feeding zones. We then determine the formation location of Vesta and  
 1261 compare the outcome with the results from the Grand Tack and classical models. Our aim is  
 1262 to find out whether the isotopic differences measured for the Earth, Mars and Vesta can be a  
 1263 natural consequence of this model.

1264 The results for the feeding zones of the terrestrial planets have been published in  
 1265 Mah and Brasser (2021) while the results for the origin of Vesta is under preparation for  
 1266 submission to a peer-reviewed journal.

## 1267 3.2 Methodology

1268 We begin by simulating the formation of the terrestrial planets in the framework of the de-  
 1269 pleted disc model starting from a disc of planetary embryos (also known as protoplanets) and  
 1270 planetesimals with various reasonable initial conditions and studying the dynamical proper-  
 1271 ties of the resultant planetary systems. Armed with the simulation outputs, we then proceed  
 1272 to identify terrestrial planet analogues – Venus, Earth and Mars – and compute their feeding  
 1273 zones.

1274 Next, we identify the asteroid analogues – Hungaria, Vesta and Hebe – and work  
 1275 out their formation location. We also delve into our  $N$ -body simulation database to select  
 1276 asteroid analogues from the Grand Tack (Walsh et al., 2011) and classical (Chambers, 2001)  
 1277 models and carry out the same analysis as we did for the depleted disc model.

1278 Finally, we compare the results for the terrestrial planets’ feeding zones and the  
 1279 formation location of asteroids across all three dynamical models.

### 1280 3.2.1 Initial conditions of depleted disc model $N$ -body simulations

1281 Our initial setup consists of a sequence of planetary embryos embedded in a disc of planetes-  
 1282 imals (collectively referred to as solids). We set the inner edge of the solid disc to be at 0.5 au  
 1283 and the outer edge at 3.0 au. The free parameters are (1) the semi-major axis beyond where  
 1284 the mass is depleted  $r_{\text{dep}}$ , and (2) the scale or amount of mass depletion. We tested for three  
 1285 values of  $r_{\text{dep}}$ : 1.0 au, 1.25 au and 1.5 au, and three values for the scale of mass depletion: 50%,  
 1286 75% and 95%. This gives us a total of nine sets of initial conditions (Fig. 3.1).

1287 We followed the method of Brasser et al. (2016) to generate the distribution of  
 1288 embryos and planetesimals, assuming that the embryos have undergone oligarchic growth  
 1289 (Kokubo and Ida, 1998). Our method employs the semi-analytical oligarchic approach of  
 1290 Chambers (2006). In the following paragraphs, we provide a brief description of how we  
 1291 generated the initial mass-semi-major axis distribution of the solids in the disc.

1292 As the first step, we computed the total mass in solids between 0.5 au and 3.0 au. We  
 1293 assumed a minimum-mass solar nebula (MMSN) solid surface density of  $\Sigma_s = 7.1 \text{ g cm}^{-2} (r/1 \text{ au})^{-3/2}$   
 1294 (Hayashi, 1981) for the whole disc and scaled the solid surface density down by 50%, 75%, or  
 1295 95% with respect to the MMSN value in the region beyond the depletion radius  $r_{\text{dep}}$ . The

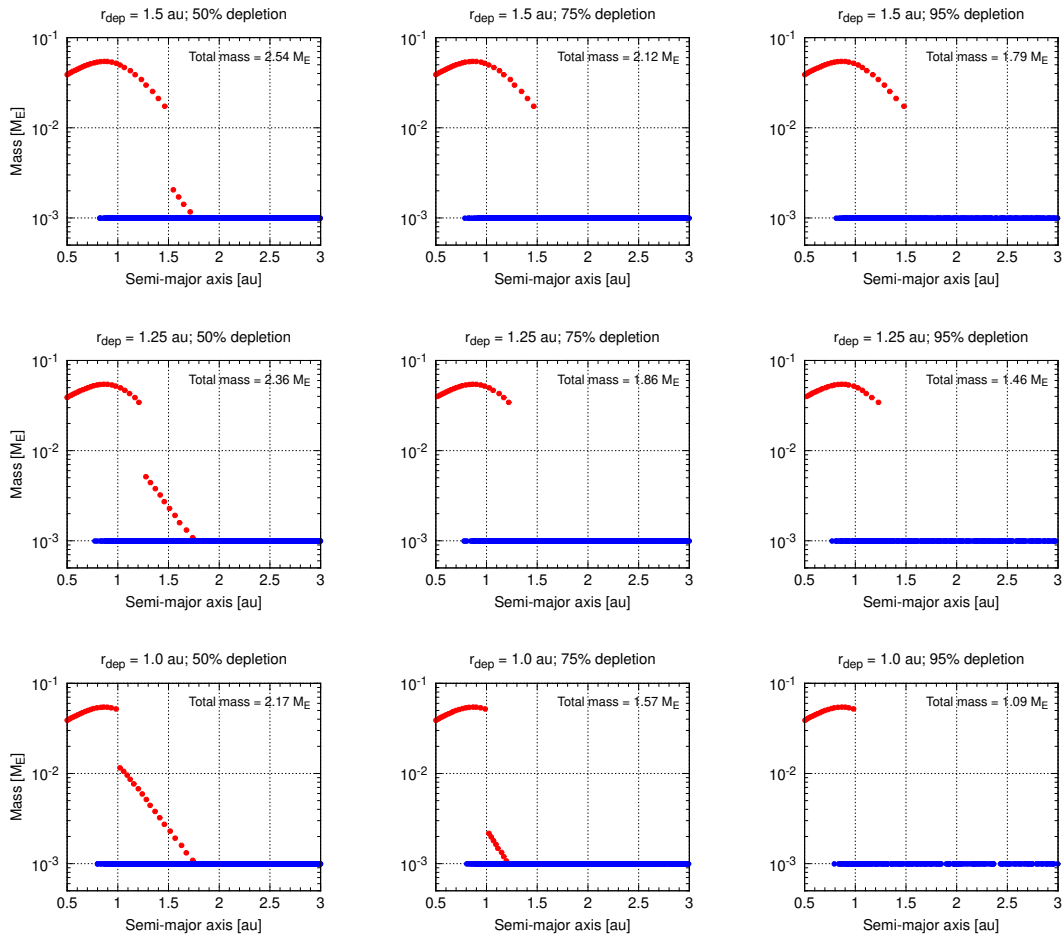


FIGURE 3.1: Initial mass and semi-major axis distribution of planetary embryos (red) and planetesimals (blue) for various values of depletion radius  $r_{\text{dep}}$  and scales of mass depletion.

1296 mass in the solid disc was then distributed into a sequence of feeding annuli for embryos  
 1297 spaced 10 mutual Hill radii apart following the results of [Kokubo and Ida \(1998\)](#). The initial  
 1298 spacing of the embryos is close to a geometric progression  $a_n = a_{n-1} [1 + \beta (2M_{\text{iso}}/3M_{\odot})^{1/3}]$ ,  
 1299 where  $a$  is the semi-major axis,  $n$  is the index of the embryo,  $\beta$  is the mutual spacing between  
 1300 adjacent embryos, and  $M_{\text{iso}} = 2\pi a \Sigma_s \beta$  is the embryo isolation mass. The isolation mass is  
 1301 the maximum mass that the embryos can attain depending on their location in the disc, their  
 1302 distance from adjacent embryos, and the disc's solid surface density.

1303 Next, we computed the masses of the embryos  $M$  in their respective feeding annuli  
 1304 as a function of time according to ([Chambers, 2006](#))

$$M(t) = M_{\text{iso}} \tanh^3 \left( \frac{t}{\tau} \right). \quad (3.1)$$

1305 In the equation above,  $\tau$  is the embryo growth timescale introduced in [Chambers \(2006\)](#). It  
 1306 depends on the radii of the planetesimals  $R$ , in addition to  $a$ ,  $\beta$  and  $\Sigma_s$ . We assumed  $R = 10$  km  
 1307 when computing the embryos' growth timescales. The age of the solid disc when Jupiter has  
 1308 fully formed is denoted by  $t$ . We used  $t = 1$  Myr in this work, based on the results of [Kruijer  
 1309 et al. \(2017\)](#). We chose to conduct this study with only one value of  $t$  to keep the number of  
 1310 simulations reasonable. At  $t = 1$  Myr, the embryos would have attained only a fraction of  
 1311 their isolation masses. Finally, the remaining mass in the feeding annuli was subsequently  
 1312 allocated to planetesimals with masses equal to 0.001 Earth mass ( $M_{\text{E}}$ ) each. The leftover

1313 mass in the disc at this stage is distributed to planetesimals so that the solid disc extends to  
1314 the outer edge at 3.0 au.

1315 The embryos and planetesimals were assigned orbital eccentricities  $e$  and orbital  
1316 inclinations  $I$  from a Rayleigh distribution with scale parameters of the eccentricity distri-  
1317 bution  $\sigma_e = (M/3M_\odot)^{1/3}$ , and the inclination distribution  $\sigma_I = 0.5 \times \sigma_e$ , respectively. The  
1318 remaining orbital angles were chosen at random between  $0^\circ$  and  $360^\circ$  from a uniform distri-  
1319 bution.

1320 The evolution of systems of planetary embryos and planetesimals, including Jupiter  
1321 and Saturn on their current orbits, were simulated using the SyMBA  $N$ -body integrator (Dun-  
1322 can et al., 1998) with a time step of 0.01 yr. In our simulations, the gas giants and the embryos  
1323 were able to gravitationally interact with each other and the planetesimals. The planetesimals  
1324 however, were unable to interact with themselves. Planetary bodies were removed from the  
1325 simulations during collisions in which case they were assumed to have merged into a larger  
1326 body perfectly, or when they ventured too close ( $a < 0.3$  au) to or too far ( $a > 100$  au) from  
1327 the Sun.

1328 The simulations were executed in two phases. In the first 5 Myr, we included the ef-  
1329 fect of a dissipating gas disc adopted from the prescriptions of Ida et al. (2016) which we detail  
1330 in Appendix B.1. The temperature profile  $T(r) \propto r^{-9/10}$  in the inner disc and  $T(r) \propto r^{-3/7}$  in  
1331 the outer disc. The gas disc exerts torques and tidal forces on the planetary bodies which re-  
1332 sult in a combined effect of radial migration and the damping of the orbital eccentricity and  
1333 orbital inclination (Appendix B.2). We excluded the effects of gas-disc-induced migration  
1334 (type-I migration) in all our simulations but retained the effects of eccentricity and inclina-  
1335 tion damping in an attempt to simplify the approach. This is because we want to focus on  
1336 the isotopic composition of the terrestrial planets. We reserve studying the effects of type I  
1337 migration for the future. After 5 Myr, we removed the gas disc artificially assuming that it  
1338 has photoevaporated away completely; we then continued the simulations without the gas  
1339 disc for another 150 Myr.

1340 As the evolution of each system is chaotic, a slight difference in the initial orbital  
1341 configuration of each embryo and planetesimal will give different results. It is therefore  
1342 necessary to perform many simulations to understand the range of possible outcomes. For  
1343 each set of initial condition, we ran 16 simulations for a total of 144. The simulations were  
1344 ran on the computing cluster at the Earth Life Science Institute and on the PC cluster at the  
1345 Center for Computational Astrophysics of the National Astronomical Observatory of Japan.

### 1346 3.2.2 $N$ -body simulation database of Grand Tack and classical models

1347 In addition to the simulations for the depleted disc model, we also tap into our available  
1348 database containing simulation output for the Grand Tack and classical models for a detailed  
1349 comparison between the outcomes of the various models. The results of these simulations  
1350 have already been published in Brasser et al. (2016) and Woo et al. (2018). We briefly sum-  
1351 marise the initial conditions of these simulations below.

1352 The simulations for the Grand Tack model started with Jupiter and Saturn migrat-  
1353 ing inwards through the asteroid belt in the first 0.1 Myr after the beginning of the solar  
1354 system as given by the formation of the calcium-aluminium-rich inclusions (CAI). When  
1355 Jupiter reaches 1.5 au, it reverses its migration direction and ushers Saturn along until they  
1356 reach their proposed semi-major axis at  $\sim 5.4$  au and  $\sim 7.5$  au, respectively (Morbidelli et al.,  
1357 2007) before the late giant planet instability. Within the orbits of Jupiter and Saturn, a solid  
1358 disc composed of embryos and planetesimals having nearly circular and coplanar orbits was

1359 placed between 0.7 and 3 au. The surface density of embryos and planetesimals follows  
 1360  $\Sigma_s \propto r^{-3/2}$ . The initial mass of the embryos are either (a) identical throughout the disc (Ja-  
 1361 cobson and Morbidelli, 2014) with the total mass ratio of embryos to planetesimals being  
 1362 1:1, 4:1 or 8:1, or (b) computed using a semi-analytic oligarchic growth model (Chambers,  
 1363 2006) where the mass and spacing between embryos are dependent on the embryos' isola-  
 1364 tion mass (Kokubo and Ida, 1998). The initial density of the planetesimals are assumed to be  
 1365  $3000 \text{ kg m}^{-3}$ . The simulations were ran for 150 Myr using a time step of 0.02 yr. The gas disc  
 1366 model adopted was based on Bitsch et al. (2015), which features a higher surface gas density  
 1367 than the one employed by Walsh et al. (2011) in their first Grand Tack simulations. The initial  
 1368 gas surface density profile  $\Sigma_g(r) \propto r^{-1/2}$ , and the temperature profile  $T(r) \propto r^{-6/7}$ . Both the  
 1369 gas surface density and temperature profiles decay until  $t = 5 \text{ Myr}$  in the simulation, after  
 1370 which the disc is artificially photoevaporated over the next 100 kyr.

1371 The initial conditions for the classical model simulations are similar to those for the  
 1372 Grand Tack model, except that Jupiter and Saturn stayed on their current orbits throughout  
 1373 the simulations. Woo et al. (2018) only investigated the case where the embryos were assumed  
 1374 to have undergone oligarchic growth (Chambers, 2006).

1375 There are several differences between the initial conditions of the numerical sim-  
 1376 ulations described here and those for the depleted disc model: (1) the inner edge of the solid  
 1377 disc for the Grand Tack and classical model simulations are set at 0.7 au while it is at 0.5 au  
 1378 for the depleted disc model, and (2) the gas disc model adopted for the Grand Tack and clas-  
 1379 sical model simulations is based on Bitsch et al. (2015) with a disc temperature profile of  
 1380  $T(r) \propto r^{-6/7}$  while we employ the gas disc model of Ida et al. (2016) with disc temperature  
 1381 profiles of  $T(r) \propto r^{-9/10}$  in the inner disc and  $T(r) \propto r^{-3/7}$  in the outer disc for the depleted  
 1382 disc model.

### 1383 3.2.3 Selection criteria for terrestrial planet analogues and computation of 1384 feeding zones

1385 At the end of the simulations, we tabulated the number of terrestrial planets produced. We  
 1386 considered all planetary bodies with masses larger than  $0.01 M_E$  to be planets. These planets  
 1387 were further filtered to identify good terrestrial planet analogues. We followed the criteria  
 1388 of Brassier et al. (2016) for the masses  $M$  and final semi-major axes  $a_f$  that the planets must  
 1389 comply with to qualify as good terrestrial planet analogues.

- 1390 • Venus:  $0.4 M_E < M < 1.2 M_E$ ,  $0.55 \text{ au} < a_f < 0.85 \text{ au}$
- 1391 • Earth:  $0.5 M_E < M < 1.5 M_E$ ,  $0.85 \text{ au} < a_f < 1.15 \text{ au}$
- 1392 • Mars:  $0.05 M_E < M < 0.15 M_E$ ,  $1.3 \text{ au} < a_f < 1.7 \text{ au}$

1393 We did not attempt to place constraints for Mercury analogues as there remains many open  
 1394 questions about its formation history.

1395 For each good terrestrial planet analogue, we tracked their accretion histories through-  
 1396 out the simulation to obtain the initial semi-major axis of all the planetary bodies they ac-  
 1397 creted. This information is then used to compute the feeding zones of the terrestrial planet  
 1398 analogues. The feeding zone of a planet provides us with information on the region in the  
 1399 disc where the terrestrial planets sample most of their building blocks from. It is quantified  
 1400 by the mass-weighted mean  $a_{\text{weight}}$  and width  $\sigma_{a_{\text{weight}}}$  of the distribution of the initial semi-  
 1401 major axes of all the solids accreted by the planet throughout its growth history (Kaib and



1402 Cowan, 2015). These quantities are expressed mathematically as (Woo et al., 2018)

$$\begin{aligned}
 a_{\text{weight}} &= \frac{\sum_i^N M_i a_i}{\sum_i^N M_i}, \\
 \sigma_{a_{\text{weight}}} &= \sqrt{\frac{\sum_i^N M_i (a_i - a_{\text{weight}})^2}{\frac{N-1}{N} \sum_i^N M_i}},
 \end{aligned}
 \tag{3.2}$$

1403 where  $M_i$  and  $a_i$  are the mass and semi-major axis of the  $i$ th body accreted by the planet,  
 1404 and  $N$  is the total number of planetary bodies accreted. Together,  $(a_{\text{weight}} \pm \sigma_{a_{\text{weight}}})$  define  
 1405 the feeding zone. The results are then compared with that obtained from the Grand Tack and  
 1406 classical models (Brasser et al., 2016; Woo et al., 2018).

### 1407 3.2.4 Selection criteria for asteroid analogues and computation of forma- 1408 tion location

1409 In total, we analysed 336 simulations from Brasser et al. (2016) for the Grand Tack model and  
 1410 64 simulations from Woo et al. (2018) for the classical model, in addition to the 144 simulations  
 1411 we have for the depleted disc model. We defined all the planetary bodies, regardless of their  
 1412 final mass, in our simulations as Hungaria, Vesta and Hebe analogues if their final semi-major  
 1413 axes  $a_f$  fulfil the following criteria:

- 1414 • Hungaria:  $1.7 \text{ au} < a_f < 2.1 \text{ au}$
- 1415 • Vesta:  $2.1 \text{ au} < a_f < 2.5 \text{ au}$
- 1416 • Hebe:  $2.2 \text{ au} < a_f < 2.6 \text{ au}$

1417 We relax the constraint on the final masses of the asteroid analogues as we are more inter-  
 1418 ested in the range of their initial semi-major axis. This does not affect the outcomes and the  
 1419 conclusions that we will draw for the study because the number of asteroid analogues larger  
 1420 than the mass of planetesimals ( $= 0.001 M_{\oplus}$ ) in our Grand Tack model simulations only con-  
 1421 stitutes  $\sim 21\%$  of the total while the fraction is a mere  $0.6\% - 1\%$  for the classical model and  
 1422  $0.01 - 1.1\%$  for the depleted disc model.

1423 The asteroid analogues had their accretion histories traced back in time to deter-  
 1424 mine the initial semi-major axis of all the bodies that they accreted, or their initial semi-major  
 1425 axis in the case that they did not accrete anything throughout the simulation. We filtered out  
 1426 bodies with initial semi-major axis greater than 3 au because that is defined as the outer edge  
 1427 of the solid disc in our simulations. Finally, from the cumulative distribution of the initial  
 1428 semi-major axis for each asteroid analogue we computed the mass-weighted mean value,  
 1429 and the 5th and 95th percentile values.

## 1430 3.3 Results

### 1431 3.3.1 Depleted disc model: Terrestrial system architecture

1432 In Fig. 3.2, we show the mass and semi-major axis distribution of the terrestrial planets formed  
 1433 at the end of our simulations with varying mass depletion scales at depletion radius 1.5 au,  
 1434 1.25 au and 1.0 au. The peak of the mass distribution is located between 0.75 au and 1 au for  
 1435  $r_{\text{dep}} = 1.5 \text{ au}$  (top panels of Fig. 3.2), although the peak is not clear for the case of 50% mass  
 1436 depletion. The peak shifts inwards when the depletion radius  $r_{\text{dep}}$  is closer in. It is located at  
 1437 the current orbit of Venus for  $r_{\text{dep}} = 1.0 \text{ au}$  (bottom panels of Fig. 3.2).

1438 Most of the terrestrial planets produced in the simulations are generally less mas-  
 1439 sive than the Earth and Venus, albeit with a few exceptions. Planet masses are also smaller

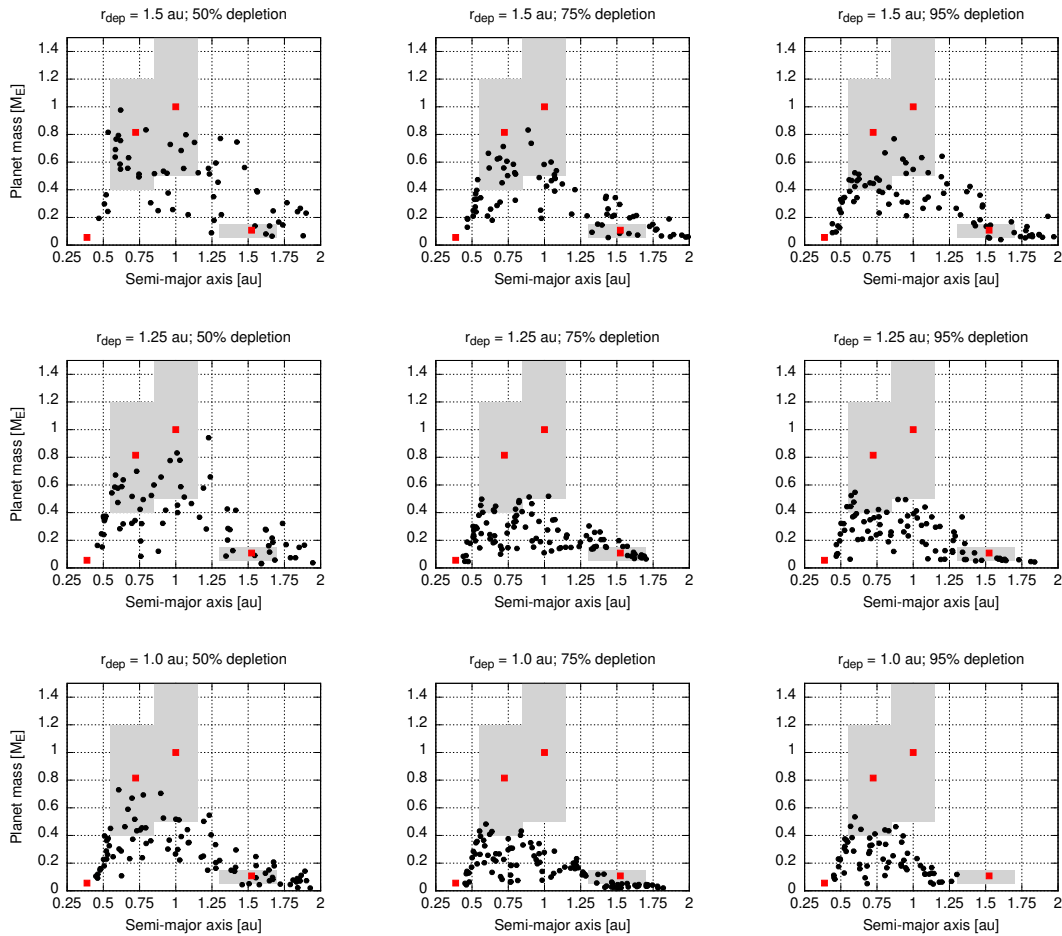


FIGURE 3.2: Mass and semi-major axis distribution of terrestrial planets formed at the end of our simulations for various scales of mass depletion at  $r_{\text{dep}} = 1.5$  au (top row), 1.25 au (middle row) and 1.0 au (bottom row). Red squares are the current terrestrial planets, black circles are planets that formed in our simulations, and grey regions indicate the range within which planets are considered good terrestrial analogues. Plot taken from [Mah and Brasser \(2021\)](#).

1440 when the depletion radius is closer to the Sun because the amount of mass available in the  
 1441 disc to form planets is smaller. This is an artefact of our initial conditions because we chose  
 1442 to keep the solid surface density fixed rather than increasing it in an attempt to reproduce  
 1443 the current masses of the terrestrial planets. Consequently, our simulations tend to produce  
 1444 more Venus analogues than Earth analogues (Table 3.1) because of the low total solid mass  
 1445 in the disc.

1446 We ran additional simulations with increased initial solid surface density and find  
 1447 that increasing the surface density by a factor of 1.5 to 2 times the MMSN value will produce  
 1448 planet analogues with masses closer to those of the current terrestrial planets. The outcomes  
 1449 of these additional simulations are discussed in Appendix C.

1450 Our simulations produce planetary systems with an average of 4 to 6 planets. How-  
 1451 ever, as there usually are planets within Venus' present orbit that could be considered as  
 1452 Mercury analogues, the higher number of planets poses no severe problems for the depleted  
 1453 disc model. From our simulation results, we find 52 planetary systems, out of a total of 144,  
 1454 with Mars analogues. Among these, only 16 have planets with  $a > 1.7$  au (upper limit of our  
 1455 criteria for Mars analogues) that could render them distinct from the Solar System.

TABLE 3.1: Total number of planets  $N$ , average number of planets in a system  $\bar{n}$ , probability of forming Venus, Earth, and Mars analogues for each initial condition, and probability of yielding both Earth and Mars analogues in the same planetary system.

$r_{\text{dep}}$	Mass depletion scale	$N$	$\bar{n}$	Venus analogues	Earth analogues	Mars analogues	Earth & Mars analogues
1.5 au	50%	57	3.6	23%	14%	7%	19%
	75%	78	4.8	15%	8%	8%	13%
	95%	80	5.0	18%	9%	8%	19%
1.25 au	50%	73	4.6	19%	8%	7%	19%
	75%	94	5.9	9%	2%	16%	6%
	95%	85	5.3	8%	0%	18%	0%
1.0 au	50%	86	5.4	12%	5%	9%	6%
	75%	104	6.5	6%	0%	6%	0%
	95%	63	3.9	10%	0%	2%	0%

### 1456 3.3.2 Depleted disc model: Terrestrial system dynamical properties

1457 We also examined the characteristics of final terrestrial systems produced from this model by  
 1458 employing several statistics introduced by [Chambers \(2001\)](#). The first of these is the angular  
 1459 momentum deficit (AMD), defined as

$$\text{AMD} = \frac{\sum_k \mu_k \sqrt{a_k} \left[ 1 - \sqrt{(1 - e_k^2)} \cos I_k \right]}{\sum_k \mu_k \sqrt{a_k}}, \quad (3.3)$$

1460 where  $\mu_k = M_k/M_\odot$ . The second is the mass concentration parameter  $S_c$  which measures  
 1461 the degree of mass concentration in one part of the planetary system, given by

$$S_c = \max \left( \frac{\sum_k \mu_k}{\sum_k \mu_k \log(a/a_k)^2} \right). \quad (3.4)$$

1462 The third is the fraction of total mass in the largest planet of the system  $S_m$ , and the last is  
 1463 the mean orbital spacing statistic  $S_H$ , given by

$$S_H = \frac{2}{N-1} \sum_{k=1}^{N-1} \frac{a_{k+1} - a_k}{a_{k+1} + a_k} \left( \frac{\mu_{k+1} + \mu_k}{3} \right)^{-1/3}. \quad (3.5)$$

1464 We use the mutual Hill sphere as the spacing unit for  $S_H$ , following [Brasser et al. \(2016\)](#).

1465 The values of the aforementioned statistics for all of the planetary systems formed  
 1466 in our simulations are presented in Fig. 3.3. We also plot the current values of the Solar  
 1467 System and its  $2\sigma$  range, obtained using a Monte Carlo method ([Brasser et al., 2016](#)), in grey  
 1468 shaded areas.

1469 In the top panel of Fig. 3.3, we find that the majority of the planetary systems plot  
 1470 away and to the lower left part of the grey region, indicating that their  $S_m$  and  $S_H$  values are  
 1471 lower compared to the Solar System's current value. Their low  $S_m$  and  $S_H$  values mean that  
 1472 the mass difference between planets in the same planetary system are small and the planets  
 1473 are more closely-packed than the current terrestrial planets. Only 20 out of a total of 144  
 1474 planetary systems have  $S_m$  and  $S_H$  values similar to the current terrestrial system and most

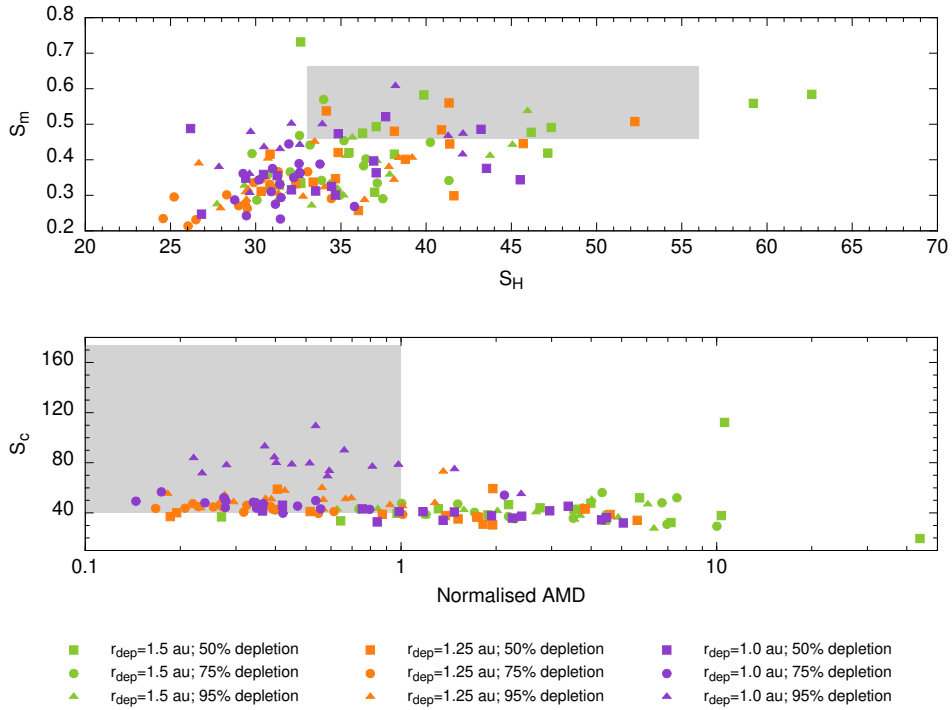


FIGURE 3.3: Top panel: Mass in largest planet as a fraction of the total mass of the planetary system  $S_m$  versus the mean spacing parameter  $S_H$  in units of the mutual Hill sphere. Bottom panel: Mass concentration parameter  $S_c$  versus the angular momentum deficit (AMD) normalised to the current Solar System value. The grey regions encompass the current values of the inner Solar System and the  $2\sigma$  range. Plot taken from Mah and Brasser (2021).

1475 of them correspond to the initial condition of 50% mass depletion (square symbols). Among  
 1476 these systems, 12 possess Earth analogues, 7 possess Mars analogues, and 6 possess both  
 1477 Earth and Mars analogues. There are 6 systems with neither Earth nor Mars analogues.

1478 In terms of the concentration parameter  $S_c$ , the majority of the final planetary sys-  
 1479 tems have low  $S_c$  values but the initial condition of  $r_{\text{dep}} = 1.0$  au and 95% (purple triangles  
 1480 in the bottom panel of Fig. 3.3) is able to produce planetary systems with higher  $S_c$  values  
 1481 that are close to the Solar System's current value. However, these planetary systems failed  
 1482 to form any Earth analogues and barely succeed in forming Mars analogues. In terms of the  
 1483 AMD, the planetary systems have values that range widely from 10 times smaller to 10 times  
 1484 larger than the current value. We chose to define successful cases as planetary systems with  
 1485 AMD less than the current Solar System's value because the AMD is expected to increase in  
 1486 time due to chaotic diffusion (Laskar, 2008). It is thus likely that the AMD at 4.5 Ga ago was  
 1487 lower than what it is today. These results of the dynamical properties of planetary systems  
 1488 formed in the framework of the depleted disc model are expected due to the fixed surface  
 1489 density that we employed.

### 1490 3.3.3 Depleted disc model: Terrestrial planet feeding zones

1491 In Fig. 3.4, we present the feeding zones ( $a_{\text{weight}} \pm \sigma_{a_{\text{weight}}}$ ) of the good terrestrial planet  
 1492 analogues, i.e., those that satisfy the criteria listed in Section 3.2.3. The feeding zones of the  
 1493 terrestrial analogues display a correlation with their final semi-major axis, indicating that  
 1494 the planets tend to accrete material mostly locally.

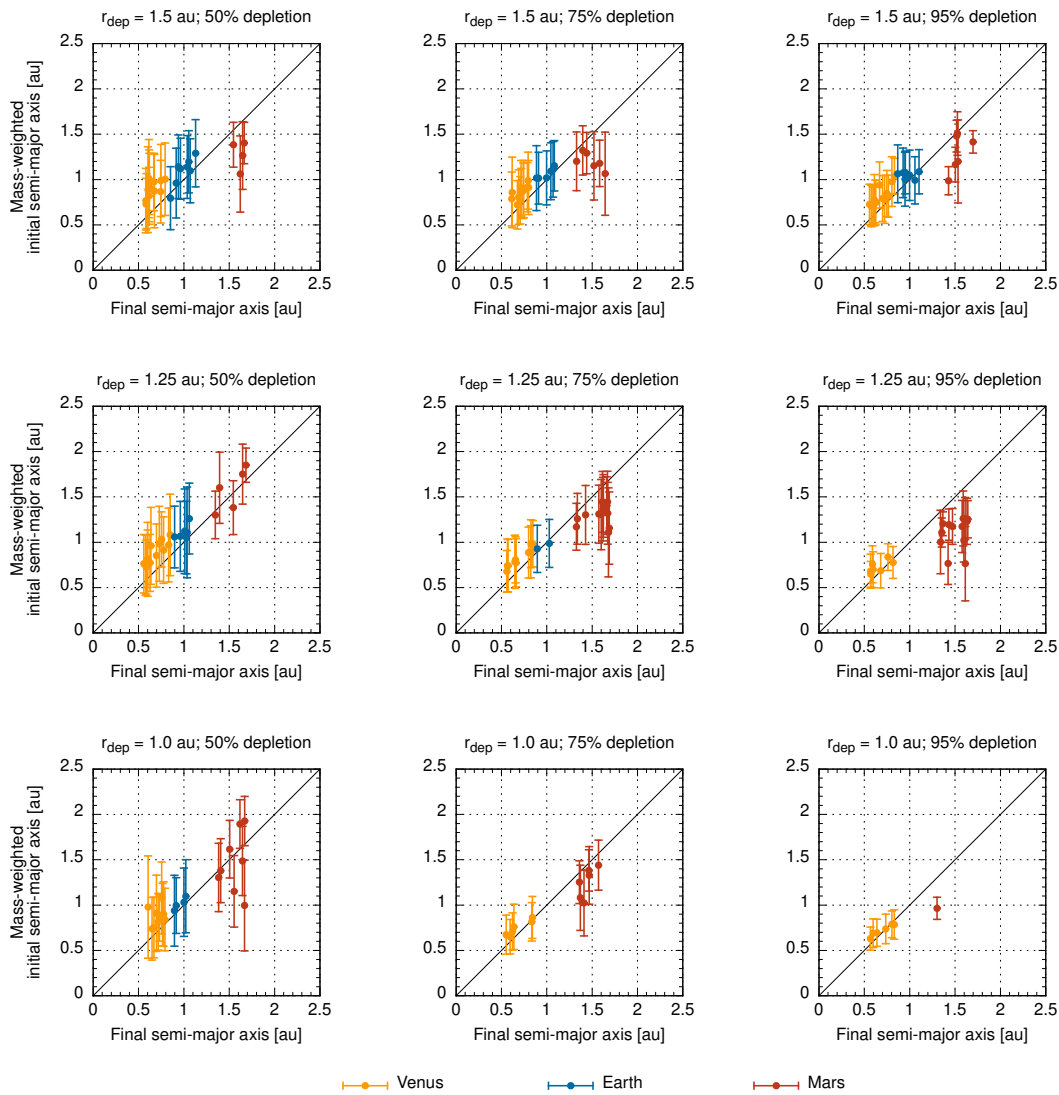


FIGURE 3.4: Feeding zones ( $a_{\text{weight}} \pm \sigma_{a_{\text{weight}}}$ ) of the Venus, Earth and Mars analogues versus their final semi-major axis from simulations of the depleted disc model with different initial conditions. The black line corresponds to the equation  $y = x$ .

1495 The trend of the local feeding zones likely arose from the eccentricity damping  
 1496 effect exerted by the gas on the embryos and planetesimals in the first 5 Myr of the simulation.  
 1497 Planetesimals are kept at low eccentricity (nearly circular) orbits and as a result they tend  
 1498 to get accreted onto nearby embryos. Embryos are typically  $0.1 M_E$  or smaller so the escape  
 1499 velocity at their surfaces is roughly  $5 \text{ km s}^{-1}$  and thus the maximum eccentricity the embryos  
 1500 can obtain from embryo-embryo scattering is about 0.1. Therefore, we expect the feeding  
 1501 zones for the final Earth and Venus analogues obtained from this mode to be narrow and  
 1502 distinct.

1503 For some Mars analogues, however, the same feeding zone trend does not apply.  
 1504 We observe a spread in the feeding zones of our Mars analogues and some of them deviate  
 1505 from the trend. For example, the Mars analogues in the simulations with a 75% mass depletion  
 1506 beyond  $r_{\text{dep}} = 1.5 \text{ au}$  have their feeding zones centered around 1.25 au (top middle panel of  
 1507 Fig. 3.4). We examined the evolution of these Mars analogues that deviate from the trend and  
 1508 found that they were formed closer in initially ( $a < 1.5 \text{ au}$ ) and was subsequently scattered

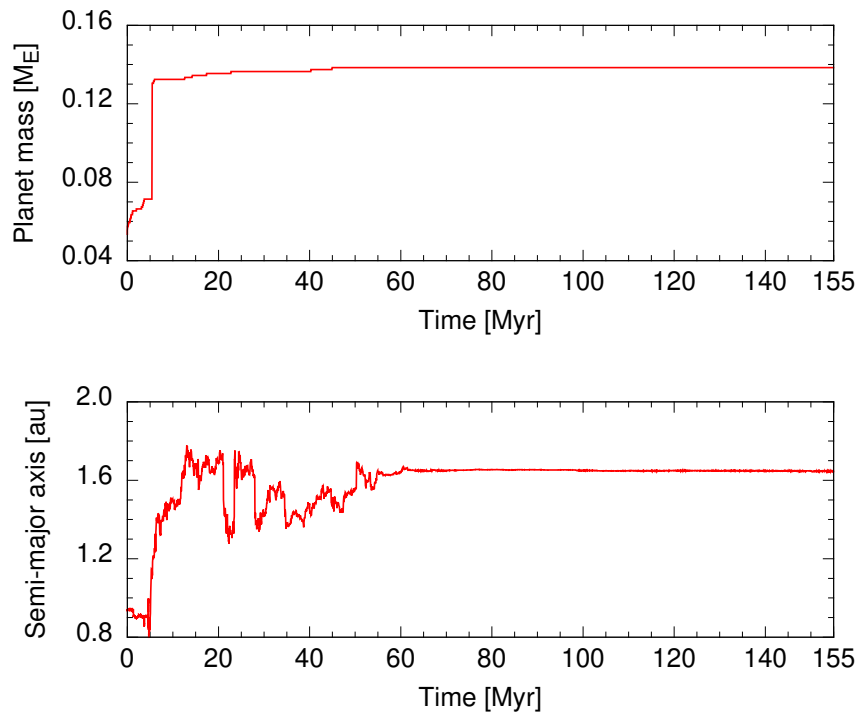


FIGURE 3.5: Time evolution of the mass and semi-major axis of a sample Mars analogue which feeding zone is centered at  $a < 1.5$  au. Plot taken from [Mah and Brassler \(2021\)](#).

1509 outwards to their final orbits (Fig. 3.5). As most of their building blocks comprise material  
 1510 from within 1.5 au, it is reflected in their feeding zones that are centred at  $a \approx 1.25$  au.

### 1511 3.3.4 Formation location of Vesta

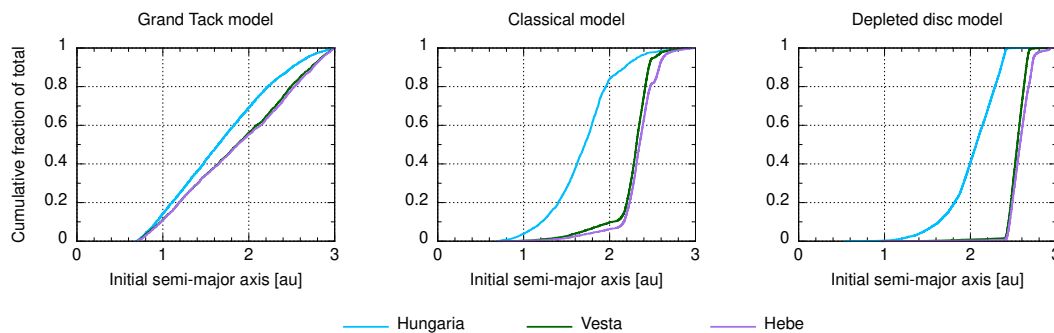


FIGURE 3.6: Cumulative distributions of the initial semi-major axis of Hungaria, Vesta and Hebe analogues in the Grand Tack (left panel), classical (middle panel), and depleted disc (right panel) models. The asteroids have equal probability of originating from anywhere in the disc for the Grand Tack model while their origin locations are more restricted in the classical model and the depleted disc model.

1512 The formation location of asteroid analogues Hungaria, Vesta and Hebe in the  
 1513 Grand Tack, classical, and depleted disc models are shown in Fig. 3.6. In the Grand Tack  
 1514 model, Vesta analogues are equally likely to originate anywhere in the disc between 0.7 au  
 1515 and 3.0 au with a 20% probability of forming within 2.1 au to 2.5 au (left panel of Fig. 3.6). In  
 1516 contrast, in the classical model and the depleted disc model, the initial semi-major axes of the  
 1517 Vesta analogues are severely restricted (middle and right panels of Fig. 3.6). The probability

1518 of Vesta analogues originating from between 2.1 au to 2.5 au is 84% for the classical model  
1519 and 30% for the depleted disc model. The reason for the lower probability in the depleted disc  
1520 model is due to the gas drag exerted on the planetesimals by the gas disc in the first 5 Myr  
1521 of the simulations. The eccentricity damping effect still causes the planetesimals to migrate  
1522 inwards when the gas was present. Consequently, most of the Vesta analogues (68% of the  
1523 total) in the depleted disc model originate from the region between 2.5 au and 2.7 au.

1524 The trend of formation location for Hebe analogues are very similar to that for  
1525 Vesta analogues across the three dynamical models. In particular, for the classical model and  
1526 the depleted disc model, these asteroid analogues ( $a_f > 2$  au) have very restricted formation  
1527 locations because there are no planetary embryos beyond 2 au in the disc to perturb the orbits  
1528 of the planetesimals. The Hungaria analogues on the other hand have a wider distribution for  
1529 their potential formation locations because they are located closer in ( $1.7 \text{ au} < a_f < 2.1 \text{ au}$ )  
1530 and thus are more prone to perturbations by planetary embryos during the formation of the  
1531 terrestrial planets.

1532 It has been suggested in the literature that the asteroid belt was devoid of mass  
1533 when the Solar System formed and was subsequently populated by planetary bodies deriv-  
1534 ing from other regions of the protoplanetary disc, in particular the terrestrial planet region  
1535 (Raymond and Izidoro, 2017b). Vesta's origin in particular has been suggested to be in the  
1536 terrestrial planet region (e.g., Bottke et al., 2006) or even in the outer Solar System (Ray-  
1537 mond and Izidoro, 2017a). However, an origin in the outer disc is inconsistent with isotopic  
1538 data as Vesta would thus be expected to be isotopically akin to (some of) the carbonaceous  
1539 chondrite meteorites (e.g., Warren, 2011). In models where the gas giants remained on their  
1540 current orbits, almost all of the Vesta analogues originated from within the asteroid belt.  
1541 Therefore, Vesta's distinct isotopic composition compared to the terrestrial planets and the  
1542 carbonaceous chondrites, its similarity to several other achondritic meteorite groups such  
1543 as the brachinites and angrites in their oxygen isotopic compositions (Clayton and Mayeda,  
1544 1996), and the narrow range in initial semi-major axis from the dynamical models not involv-  
1545 ing the migration of the gas giants suggest an origin that is most likely in the asteroid belt  
1546 and not in the inner solar system nor the outer solar system.

## 1547 3.4 Discussion

### 1548 3.4.1 Comparison with the Grand Tack and classical models

1549 Comparing the feeding zone trend of the depleted disc model with that of the Grand Tack  
1550 and classical models, we see that the correlation with semi-major axis is strongest for the  
1551 depleted disc model and weakest for the Grand Tack model (Fig. 3.7). The feeding zones of  
1552 the terrestrial planets for the Grand Tack model have a large width and a similar range (from  
1553 0.7 to 2.0 au) with the slope of the best-fit line = 0.06 indicating almost no correlation with  
1554 semi-major axis. The feeding zone trend of the Grand Tack model is due to the gas-driven  
1555 inward-then-outward migration of the gas giants that enhances the mixing of materials in the  
1556 disc. By contrast, in the depleted disc model the feeding zone widths are more restricted and  
1557 the feeding zone range for each planet is different with the slope of the best-fit line having a  
1558 higher value of 0.52. This is because of the limited extent of material mixing in the solid disc  
1559 in the depleted disc model. The mass in the region beyond the orbit of Mars is too low to  
1560 cause sufficient perturbations to the orbits of solid material closer to the Sun. For the case of  
1561 the classical model, the slope of the best-fit line is a combination of two factors: (1) the inner  
1562 edge of the solid disc is set at 0.7 au causing Venus analogues to only accrete material from  
1563 beyond 0.7 au, and (2) there are too few Mars analogues due to the large amount of mass in

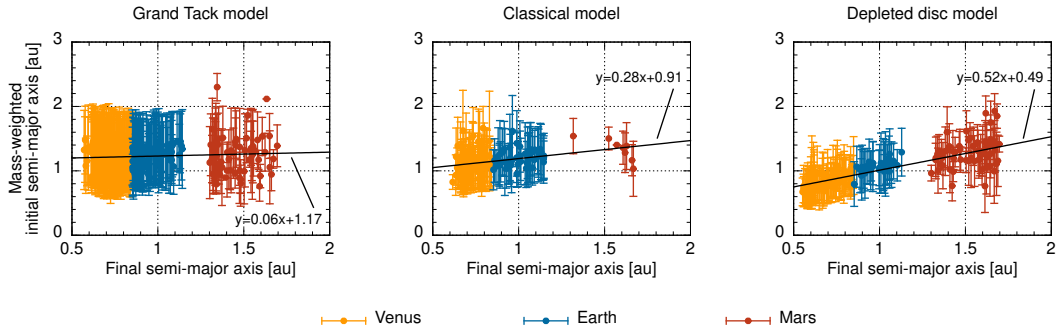


FIGURE 3.7: Comparison of all the Venus, Earth and Mars analogues’ feeding zones for the Grand Tack model (left panel), classical model (middle panel), and depleted disc model (right panel). Feeding zone data for the Grand Tack and classical models are from our simulation database. The Grand Tack simulations used to compute the feeding zones include simulations with different tack locations for Jupiter (1.0 au and 1.5 au), simulations beginning with equal-mass planetary embryos, and simulations with embryos assumed to have undergone oligarchic growth. The results from all the aforementioned Grand Tack simulations are combined because there are no obvious differences between the outcomes from different initial conditions (Brasser et al., 2016).

1564 this region of the disc. It is possible to obtain a steeper value for the slope if the solid disc’s  
 1565 inner edge is extended to 0.5 au and/or if the initial orbital configuration of the gas giants is  
 1566 changed (Woo et al., 2021).

1567 In the ideal case where the planets accrete all their building blocks locally, the  
 1568 feeding zones will display a 1:1 relation with semi-major axis. The slopes of the best-fit line  
 1569 for the three dynamical models examined here deviate from 1 because mixing is inevitably  
 1570 present in the disc in realistic cases due to the gravitational perturbation on the planetesimals  
 1571 by planetary embryos. The feeding zone trend is therefore a reflection of the degree of mixing  
 1572 in the disc. It is strongest for the Grand Tack model and weakest for the depleted disc model.

1573 We next examine how big is the difference between the feeding zones of the Earth  
 1574 and Mars analogues for the depleted disc model and the Grand Tack model. We will not  
 1575 consider the results of the classical model here as it does not form many Mars analogues with  
 1576 the correct size to make good comparisons. From the depleted disc and Grand Tack models,  
 1577 we singled out the planetary systems which possess both Earth and Mars analogues (13 and  
 1578 37 systems, respectively) and computed the difference between  $a_{\text{weight, Mars}}$  and  $a_{\text{weight, Earth}}$ .  
 1579 For systems with multiple Mars analogues, we chose the planet analogue with semi-major  
 1580 axis closest to 1.5 au. The cumulative distribution is presented in Fig. 3.8. We find that the  
 1581 region in the disc where Mars analogues sourced most of their building blocks is generally  
 1582 more distant than the Earth in the depleted disc model, whereas it is closer to the Earth in  
 1583 the case of the Grand Tack model.

1584 To further quantify the difference in the feeding zones of the Earth and Mars ana-  
 1585 logues produced in the depleted disc and Grand Tack models, we computed their overlapping  
 1586 coefficient (OVL). The OVL measures the similarity between the two distributions and is de-  
 1587 fined as the common area under two probability density functions. For planetary systems  
 1588 with both Earth and Mars analogues, we traced their respective accretion histories to obtain  
 1589 the mass-weighted initial semi-major axis of all the planetary embryos and planetesimals  
 1590 accreted onto these two planets. We then combined the mass-weighted initial semi-major  
 1591 axis  $Ma$  data for all the Earth and Mars analogues in each model (Fig. 3.9) to compute the  
 1592 OVL. This is done for better statistics as some of the Mars analogues only accreted a few  
 1593 planetesimals which results in a rather grainy probability function. The OVL is computed as



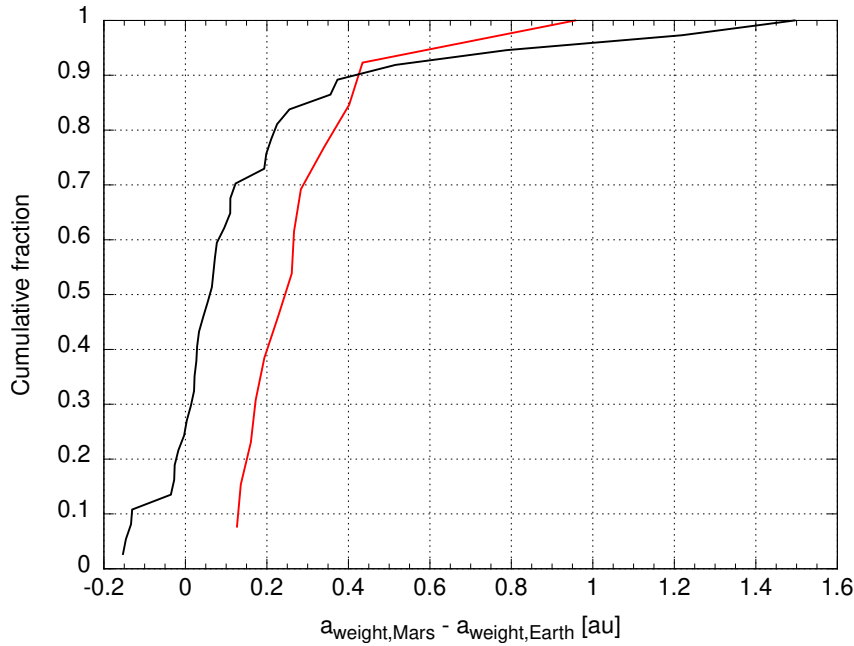


FIGURE 3.8: Cumulative distribution of the difference between the mass-weighted mean initial semi-major axis of all the planetary embryos and planetesimals accreted by both Mars and Earth analogues in the depleted disc model (red) and the Grand Tack model (black). Plot taken from [Mah and Brasser \(2021\)](#).

1594 the sum of the lower value between the probability distribution functions of Earth and Mars  
1595 over the whole range of values for  $Ma$ , expressed as

$$\text{OVL} = \sum_{Ma} \min [f_{\text{Mars}}(Ma), f_{\text{Earth}}(Ma)]. \quad (3.6)$$

1596 We find  $\text{OVL}_{\text{DD}} = 0.79$  for the depleted disc model, and  $\text{OVL}_{\text{GT}} = 0.89$  for the Grand Tack  
1597 model.

1598 The OVL results suggest that the difference in feeding zones between Earth and  
1599 Mars is  $\sim 20\%$  in the depleted disc model, and  $\sim 10\%$  in the Grand Tack model. What does  
1600 this difference actually mean? Naively, one would expect a 10% difference to imply that Mars'  
1601 oxygen isotopes would result in a  $\Delta^{17}\text{O}$  of either 0.10 or  $-0.10\%$  ( $\Delta^{17}\text{O} = 0$  for Earth); instead  
1602 the observed isotopic anomaly of  $0.29\%$  would suggest an OVL difference of  $\sim 30\%$ , which  
1603 is closer to the depleted disc value rather than the Grand Tack value. The question then  
1604 becomes: What did Mars accrete that the Earth did not?

1605 One interpretation of the different OVL values could be in the fraction of ordinary  
1606 chondrites accreted by Mars because it is the only quantity that is potentially significantly  
1607 different when one considers the terrestrial planets to be mixtures of chondrites (e.g., [Lodders  
1608 and Fegley, 1997; Sanloup et al., 1999; Dauphas, 2017; Brasser et al., 2018](#)). We applied the  
1609 same technique to compute the OVL for the distributions from our improved mixing model  
1610 simulation (shown earlier in Fig. 1.2). For the 20 different mixing model iterations, we com-  
1611 puted the OVL by averaging over all possible permutations between the best-fit composition  
1612 of Earth and Mars. We find  $\text{OVL}_{\text{MCMC}} = 0.58 \pm 0.08$ , which is clearly attributed to the in-  
1613 creased H chondrite fraction in Mars versus a higher fraction of carbonaceous material in  
1614 the Earth (Fig. 1.2). Taking the mixing model as our benchmark for the OVL, the depleted  
1615 disc model does a better job than the Grand Tack.

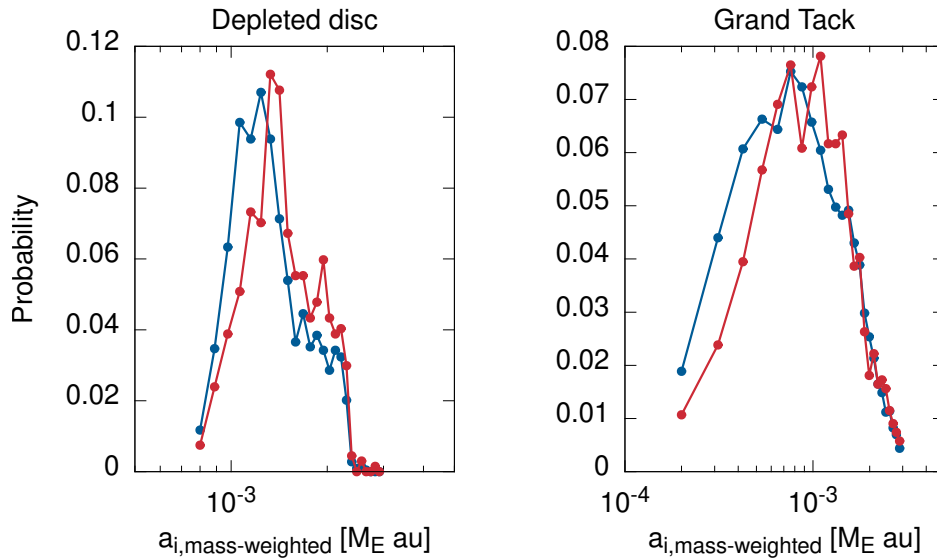


FIGURE 3.9: Probability distribution function of the mass-weighted initial semi-major axis of all the planetary embryos and planetesimals accreted by Earth (blue) and Mars (red) in the depleted disc model and the Grand Tack model. The distribution for Mars is systematically displaced to the right for the depleted disc model. Plot taken from [Mah and Brasser \(2021\)](#).

TABLE 3.2: K-S test results. Maximum difference between each pair of data points  $D$ , and the probability of agreement  $P$  in the cumulative distributions of each planet pair in the Grand Tack, classical and depleted disc models. Also listed is the number of data points  $N$  selected for the test.

	Grand Tack ( $N=1718$ )		Classical ( $N=323$ )		Depleted disc ( $N=2706$ )	
	$D$	$P$ (%)	$D$	$P$ (%)	$D$	$P$ (%)
Venus-Earth	0.014	99.6	0.071	37.7	0.110	0.0
Earth-Mars	0.035	22.5	0.200	0.0	0.086	0.0
Venus-Mars	0.035	24.2	0.258	0.0	0.175	0.0

1616 Finally we conduct a Kolmogorov-Smirnov (K-S) similarity test on the cumulative  
1617 distributions of the initial semi-major axis of all the planetary bodies accreted onto all of  
1618 the Venus, Earth and Mars analogues in the Grand Tack, classical, and depleted disc  
1619 models. We selected  $N = 1718$ ,  $323$  and  $2706$  equally-spaced data points from the cumulative distri-  
1620 butions of the Grand Tack, classical, and depleted disc models for the test. For each planet  
1621 pair (Venus-Earth, Earth-Mars, Venus-Mars) in each model, we computed the maximum dif-  
1622 ference between each pair of data points  $D$  and the corresponding probability of agreement  
1623  $P$ . If the value of  $P$  is greater than 5%, then the two distributions are said to be statistically  
1624 identical. Table 3.2 shows the results of the test for the three dynamical models. The re-  
1625 sults suggest that the accretion regions of the terrestrial planets in the Grand Tack model are  
1626 identical ( $P > 5\%$ ) while the accretion regions are distinct in the depleted disc model. For  
1627 the classical model, the similarity between the accretion regions of Venus and Earth is likely  
1628 due to the inner edge of the solid disc being set to  $0.7$  au in the simulations, which results in  
1629 Venus analogues only sampling material from  $> 0.7$  au in the disc ([Woo et al., 2018](#)).

1630 Given the results of the two statistical tests we conducted (OVL, K-S test), we con-  
1631 clude that the predictions of the depleted disc model comports best with the isotopic compo-  
1632 sitions measured for the Earth and Mars. In this model, the feeding zones of the terrestrial

1633 planets show a clear correlation with semi-major axis. Earth and Mars would accrete mate-  
 1634 rial from different regions in the protoplanetary disc and they can end up with different final  
 1635 mixtures of building material with the presence of isotopic gradients in the disc. This is in  
 1636 stark contrast with the the Grand Tack model which predicts identical isotopic compositions  
 1637 for Earth and Mars.

### 1638 3.4.2 Implications for Venus' isotopic composition

1639 Our simulation results for the depleted disc model show that Venus, Earth and Mars accreted  
 1640 from different, localised regions of the protoplanetary disc. Thus, a direct implication of  
 1641 the model is that Venus should be isotopically distinct from the Earth and Mars. A predic-  
 1642 tion of its isotopic composition for  $\Delta^{17}\text{O}$ - $\varepsilon^{50}\text{Ti}$ - $\varepsilon^{54}\text{Cr}$  can be obtained by making use of the  
 1643 correlation between the feeding zones of the terrestrial planets shown in Fig. 3.7 and the  
 1644 corresponding isotopic anomalies for Earth and Mars. This assumes a linear relationship be-  
 1645 tween the disc's isotopic composition and semi-major axis (Pahlevan and Stevenson, 2007).  
 1646 The predicted isotopic anomalies for Venus  $\varepsilon_V$  can be computed using the relation

$$\varepsilon_V = \frac{a_V - a_E}{a_M - a_E} \times \varepsilon_M, \quad (3.7)$$

1647 where the subscripts V, E and M refer to Venus, Earth and Mars, respectively. We computed  
 1648 the nominal values of the isotopic anomalies of Venus using the current semi-major axes of  
 1649 the terrestrial planets and plotted them as open squares in Fig. 3.10.

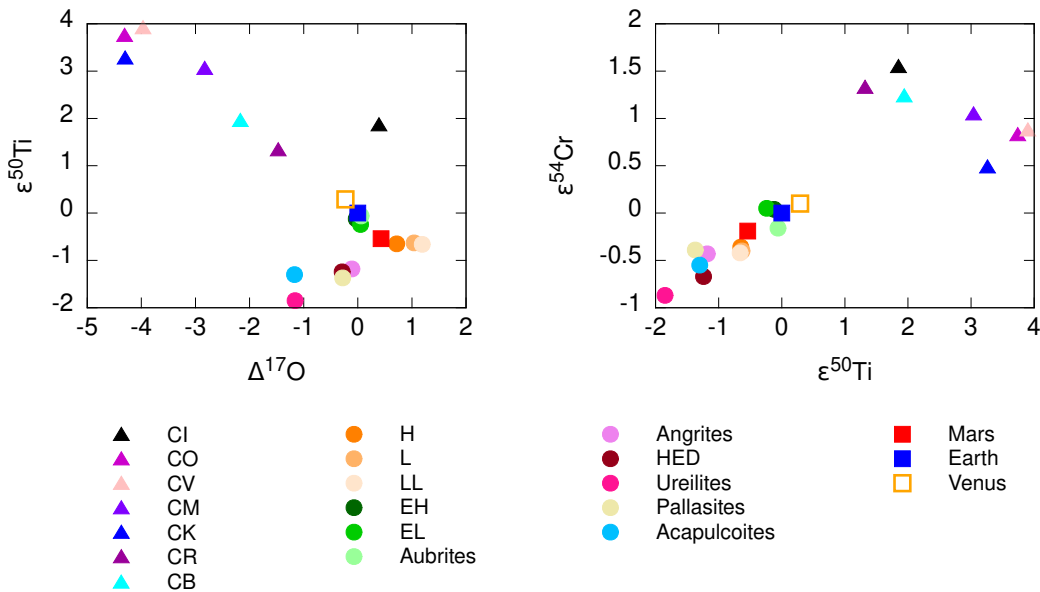


FIGURE 3.10: Predicted isotopic anomalies in chromium, oxygen and titanium for Venus (orange open square) based on terrestrial planet feeding zone trend observed for the depleted disc model. Meteorite isotope anomalies data for  $\Delta^{17}\text{O}$  sourced from Clayton and Mayeda (1983, 1996); Franchi et al. (1999); Rubin et al. (2000); Mittlefehldt et al. (2008); Agee et al. (2013); Wittmann et al. (2015),  $\varepsilon^{50}\text{Ti}$  from Trinquier et al. (2009); Zhang et al. (2011, 2012), and  $\varepsilon^{54}\text{Cr}$  from Shukolyukov and Lugmair (2006); Trinquier et al. (2007, 2008); Qin et al. (2010a,b); Yamashita et al. (2010); Larsen et al. (2011); Petit et al. (2011); Yamakawa and Yin (2014). Martian meteorites used to compute the average value for Mars are ALH 84001, DaG 476, Chassigny, Lafayette, Nakhla, NWA 856, NWA 2737, NWA 7034, Shergotty and Zagami. Plot taken from Mah and Brassier (2021).

1650 In computing the nominal isotopic composition for Venus, we used the Earth-Mars  
 1651 correlation instead of Earth-Mars-Vesta. Although the Earth-Mars-Vesta trend is present for

TABLE 3.3: Predicted values for the isotopic anomalies of Venus computed using a linear extrapolation of the Earth-Mars trend and using a Monte Carlo method, and the fraction of Venus analogues generated by the Monte Carlo method that is more isotopically distinct from the Earth than Mars is.

	Nominal	Monte Carlo	$ \varepsilon_V - \varepsilon_E  >  \varepsilon_E - \varepsilon_M $
$\Delta^{17}\text{O}$	-0.23	$-0.12^{+2.69}_{-2.74}$	50%
$\varepsilon^{50}\text{Ti}$	0.29	$0.26^{+3.37}_{-3.43}$	48%
$\varepsilon^{54}\text{Cr}$	0.10	$0.07^{+1.20}_{-1.19}$	49%

1652  $\varepsilon^{50}\text{Ti}$  and  $\varepsilon^{54}\text{Cr}$ , it is not the case for  $\Delta^{17}\text{O}$  where Vesta has a negative value, in contrast to  
 1653 the positive values of the Earth and Mars. The uncertainties in the isotopic anomalies were  
 1654 computed using a Monte Carlo method. We employed the Box-Mueller transform to generate  
 1655 values for the semi-major axes of Venus, Earth, and Mars, as well as the isotopic anomalies  
 1656 in  $\Delta^{17}\text{O}$ ,  $\varepsilon^{50}\text{Ti}$  and  $\varepsilon^{54}\text{Cr}$  for Mars according to a normal distribution with mean equal to the  
 1657 mean semi-major axes of the feeding zones of the planets, and the standard deviation being  
 1658 a quarter of the feeding zones' width. We then computed the isotopic anomalies of Venus  
 1659 using Eq. 3.7. After  $10^5$  iterations, we obtain the isotopic anomalies and their corresponding  
 1660 uncertainties by computing the mean, 5th percentile and 95th percentile values. We report  
 1661 the values in Table 3.3. There is a huge spread in the predicted isotopic anomalies of Venus,  
 1662 and this is due to the fact that (1) the value of  $(a_V - a_E)/(a_M - a_E)$  can be very small, which  
 1663 results in large variations, and (2) some Mars analogues do not follow the same trend as the  
 1664 Earth and Venus, which skews the values. We also find that about half of the Venus analogues  
 1665 generated by the Monte Carlo method are predicted to have isotopic compositions that are  
 1666 more distinct from the Earth compared to Mars.

1667 Interestingly enough, using the extrapolation from the Earth and Mars trend im-  
 1668 plies that Venus plots in between the Earth and the carbonaceous/jovian material, which  
 1669 could naively be interpreted as Venus having accreted a higher fraction of carbonaceous/jovian  
 1670 material than the Earth, although this interpretation makes little sense dynamically. The  
 1671 Earth-Mars-Vesta trend in  $\varepsilon^{50}\text{Ti}$  and  $\varepsilon^{54}\text{Cr}$  is continued to Venus, but since Vesta is negative  
 1672 in  $\Delta^{17}\text{O}$  there is no such trend for the O isotopes. Our predicted isotopic compositions for  
 1673 Venus also suggest that the angrite meteorites could not have originated from Venus.

1674 Isotope measurements for meteorites or rock samples from Venus will therefore be  
 1675 crucial to know its O isotopic composition (Greenwood and Anand, 2020), and provide evi-  
 1676 dence for or against the presence of a reservoir enriched in *s*-process elements that the Earth  
 1677 is said to have accreted some of its building blocks from (Render et al., 2017). Venus should  
 1678 have accreted a larger fraction of its building blocks from this *s*-process nuclides enriched  
 1679 reservoir given the presence of a potential isotopic gradient in the protoplanetary disc and  
 1680 that it is located closer to the Sun as compared to the Earth.

### 1681 3.5 Conclusions

1682 We examined the masses, orbital configurations, and feeding zones of the terrestrial planets  
 1683 formed in the framework of the depleted disc model by running a large number of *N*-body  
 1684 simulations with different initial conditions and including the effects of a dissipating gas disc  
 1685 during the first few Myr of the simulations. We found that the model outputs planets that  
 1686 are less massive than the current terrestrial planets if we assume a MMSN surface density for  
 1687 the solids in the protoplanetary disc, but the model is successful nevertheless in producing

1688 planets with low mass in the region near Mars' orbit. Increasing the initial surface density of  
1689 the solids in the protoplanetary disc by 1.5 to 2 times the MMSN value will resolve the deficit  
1690 in the terrestrial planets' mass.

1691 Despite the mass depletion in the protoplanetary disc being an ad-hoc assumption,  
1692 the depleted disc model provides a promising initial condition to form Mars with the cor-  
1693 rect mass, a problem that has plagued the classical model and inspired the development of  
1694 subsequent models. The origins of such a concentration of mass in the terrestrial planet re-  
1695 gion of the protoplanetary disc is not yet known. Several suggestions include a difference  
1696 in viscosity in different parts of the disc causing material to preferentially flow towards the  
1697 high-viscosity region (Jin et al., 2008), the growth and inward drift of dust causing the solids  
1698 in the whole disc to redistribute themselves and preferentially pile-up near the inner edge of  
1699 the disc (Drażkowska et al., 2016), and the presence of a potential pressure bump in the disc  
1700 near 5 au causing the outward migration of material originally located in the asteroid belt  
1701 (Brasser and Mojzsis, 2020). However, these scenarios remain speculative as there has not  
1702 yet been any investigation to determine an origin for the depleted disc model to this date.  
1703 We will leave this for future work.

1704 Perhaps more importantly, this model predicts distinct isotopic compositions for  
1705 the Earth, Mars and Vesta, consistent with cosmochemistry data. This is in contrast to the  
1706 Grand Tack model where the most likely outcome for the isotopic compositions of Earth,  
1707 Mars and Vesta is that they are identical. Our results therefore suggest that the early gas-  
1708 driven migration of Jupiter and Saturn into the inner solar system was unlikely to have oc-  
1709 curred but it could have happened at a later time instead (e.g., Clement et al., 2018). Its effect  
1710 on the degree of mixing in the inner disc deserves detailed investigation in the future.

## 1711 4 Summary and future work

### 1712 4.1 The thesis in brief

1713 We presented two studies in this thesis aiming to shed light on the formation pathway of  
 1714 the terrestrial planets, guided by the cosmochemistry observations that the Earth, Mars and  
 1715 Vesta all are distinct in their isotopic compositions and that their isotopic compositions show  
 1716 a correlation with their semi-major axis.

1717 The first study examines the role of pebble accretion in the inner Solar System  
 1718 during the lifetime of the gas disc. This study is motivated by the work of [Levison et al.](#)  
 1719 [\(2015b\)](#) who showed that pebble accretion could help inner disc planetesimals gain enough  
 1720 mass before the gas dissipates, thus preparing them to form the terrestrial planets in the  
 1721 subsequent stages of planetesimal collision and giant impact, and more recently the work  
 1722 of [Johansen et al. \(2021\)](#) who showed that pebble accretion could perhaps contribute a large  
 1723 fraction to the masses of the terrestrial planets. Furthermore, [Schiller et al. \(2018\)](#) proposed  
 1724 that the accretion of outer Solar System material, possibly in the form of pebbles, onto a  
 1725 disc of planetesimals with ureilite-like isotopic compositions could be a possible generating  
 1726 mechanism behind the observed mass-isotopic-composition correlation for Earth, Mars and  
 1727 Vesta.

1728 We simulated the growth of a disc of planetesimals (with a range of diameters) in  
 1729 the terrestrial planet region when they are subjected to a flux of pebbles originating in the  
 1730 outer Solar System. At the end of the simulations ( $t = 4$  Myr), we find that planetesimal discs  
 1731 made up of many planetesimals with diameters  $\geq 300$  km ( $0.05 M_E \leq M_{\text{disc},i} \leq 0.25 M_E$ ) will  
 1732 increase their mass by at least few times their initial mass, depending on the temperature of  
 1733 the gas disc and if gas-induced migration effects are included. This is despite Jupiter almost  
 1734 halting the pebble flux when it reaches its isolation mass. Such a large amount of mass in-  
 1735 crease contributed by outer Solar System pebbles would imply that the isotopic composition  
 1736 of the planetesimals will be replaced by the isotopic signatures of the pebbles. Planetary  
 1737 bodies formed by the subsequent collisions among these planetesimals are expected to have  
 1738 isotopic compositions similar to the outer Solar System bodies, which is inconsistent with  
 1739 the isotopic dichotomy revealed by currently available meteorite samples.

1740 On the other hand, if the planetesimals in the inner Solar System are mostly bodies  
 1741 with diameters  $< 300$  km ( $M_{\text{disc},i} \leq 10^{-3} M_E$ ) then the amount of mass increase in the disc is  
 1742 limited. The mass increase in the disc ranges from 15% to about 300%, depending on the initial  
 1743 mass of the planetesimal disc and assuming that the pebbles sublimate into smaller-sized  
 1744 grains at the snow line. The amount of mass accreted in the form of pebbles is however, still  
 1745 considered to be quite high based on the results of chondritic mixing models (e.g., [Dauphas,](#)  
 1746 [2017](#)) that the maximum contribution of outer Solar System material to the mass of the Earth  
 1747 is about 10%. In the case where we disregard the fragmentation effects, the mass increase in  
 1748 the disc can be less than 10% the initial disc mass. However, the more important problem for  
 1749 these discs with small planetesimals is that the final mass in the disc by the time the gas disc  
 1750 dissipates is insufficient to form the terrestrial planets.

1751 It is more likely that the solid disc in the inner Solar System was more massive  
1752 than  $10^{-3} M_E$  and thus should contain more planetesimals larger than 300 km in diameter.  
1753 Since the growth of these planetesimals proceed at a faster rate (due to their higher accretion  
1754 efficiency), it is expected that the contribution by pebbles to the mass in the terrestrial planet  
1755 region is very large and that such a large contribution can replace the initial isotopic signature  
1756 of the planetesimals. Based on our simulation results, we suggest that it is rather unlikely for  
1757 pebble accretion to play a major role in the formation of the terrestrial planets. Our results  
1758 are in contrast with those of previous studies (Levison et al., 2015b; Johansen et al., 2021)  
1759 mainly because of the different assumptions made. We assumed that the pebbles formed in  
1760 the outer Solar System beyond the orbit of Jupiter whereas the previous studies assume for  
1761 example, that (a) the pebbles form in the inner Solar System (Levison et al., 2015b), or that  
1762 (b) there was a change in the isotopic composition of the pebbles from non-carbonaceous-  
1763 chondrite-like to carbonaceous-chondrite-like within the lifetime of the gas disc (Johansen  
1764 et al., 2021). As the pebble accretion mechanism is widely studied in the community, our  
1765 understanding of it is gradually improving. This leaves room for further examinations of the  
1766 plausibility and validity of the assumptions used by current works.

1767 The second study investigates the predictions of the depleted disc model for the  
1768 isotopic compositions of the terrestrial planets and the formation location of asteroid Vesta.  
1769 In this study, we modelled the growth of a solid disc containing planetesimals and planetary  
1770 embryos when Jupiter has reached its full size and there are no influx of pebbles. We find that  
1771 the terrestrial planet analogues have feeding zones that display a trend with semi-major axis,  
1772 suggesting that the planets accrete mostly local material and there is very little mixing in the  
1773 disc. In addition, the Vesta analogues originate from the asteroid belt in the region close to  
1774 Vesta's current orbit. The distinct feeding zones of the terrestrial planet analogues and the  
1775 formation region of Vesta analogues in the asteroid belt is encouraging because it means that  
1776 the Earth, Mars and Vesta can be distinct in their isotopic compositions – consistent with  
1777 isotopic data – if the solids in the inner Solar System are isotopically heterogeneous. We  
1778 further suggest that (1) isotopic gradients should have been present in the inner Solar System  
1779 before the formation of the planetesimals, and (2) the inner Solar System bodies should have  
1780 formed via local accretion, such that the isotopic heterogeneity is preserved and is reflected  
1781 in the distinct isotopic compositions of Earth, Mars and Vesta.

## 1782 4.2 Future directions

1783 Finally, we list several potential directions that future research could undertake to further our  
1784 understanding of planet formation in our Solar System as well as other exoplanet systems.

- 1785 • Protoplanetary disc models: Since the construction of plausible planet formation mod-  
1786 els is dependent on the current understanding of protoplanetary disc models, it would  
1787 be useful to delve into the study of protoplanetary discs. A good understanding of  
1788 protoplanetary discs could for example aid in understanding how, when and where  
1789 planetesimals form in the disc and the expected size-frequency distribution of the plan-  
1790 etesimals (e.g., Chambers, 2010; Johansen et al., 2014).
- 1791 • High-resolution simulations:  $N$ -body simulations run on graphics processing units  
1792 (GPU) could achieve higher resolution with shorter computing time. Re-examining  
1793 the current terrestrial planet formation models with  $N$ -body codes written for GPUs  
1794 (e.g., GENGA; Grimm and Stadel, 2014) could push the current limits and perhaps re-  
1795 veal new information (e.g., Woo et al., 2021).

- 1796 • Cosmochemistry data: The building blocks of the Earth remain an unresolved puzzle.  
1797 Accurate determination of isotopic anomalies and elemental abundances of a wide va-  
1798 riety of meteorite samples with high-precision equipment coupled with modelling of  
1799 geochemical and geophysical processes could help in cracking the code.
- 1800 • Stellar/Galaxy cluster evolution: On a larger scale, the abundances of short-lived ra-  
1801 dionuclides (SLR) in our Solar System obtained from models of the evolution of the  
1802 Sun's birth cluster (e.g., [Fujimoto et al., 2018](#); [Portegies Zwart et al., 2018](#)) can be com-  
1803 pared to the measured abundances of the daughter isotopes that are radioactive decay  
1804 products of the SLRs. These models could perhaps be employed to study the distribu-  
1805 tion of nucleosynthetic isotopes in different regions of the protoplanetary disc.





# 1806 A Monte Carlo mixing model

1807 Here we describe how we computed the composition of the Earth and Mars as a mixture of  
 1808 chondrites (and angrite meteorites; [Fitoussi et al., 2016](#)) using a Monte Carlo mixing model  
 1809 based on the work of [Dauphas \(2017\)](#). The goal of the mixing model is to derive the best-fit  
 1810 compositions of the Earth and Mars that is consistent with the isotopic anomalies measured  
 1811 for  $\Delta^{17}\text{O}$ ,  $\epsilon^{50}\text{Ti}$ ,  $\epsilon^{54}\text{Cr}$ ,  $\epsilon^{62}\text{Ni}$  and  $\epsilon^{92}\text{Mo}$ . Our model differs from the original model of [Dauphas](#)  
 1812 [\(2017\)](#) in the following ways: (1) we expanded the list of carbonaceous chondrites used in the  
 1813 model to include CM and CR chondrites, (2) we split the enstatite chondrites group into its  
 1814 two components: EL and EH, and (3) we use the  $\epsilon^{62}\text{Ni}$  isotope instead of  $\epsilon^{64}\text{Ni}$ .

## 1815 A.1 Model inputs

TABLE A.1: Measured  $\Delta^{17}\text{O}$ ,  $\epsilon^{50}\text{Ti}$ ,  $\epsilon^{54}\text{Cr}$ ,  $\epsilon^{62}\text{Ni}$  and  $\epsilon^{92}\text{Mo}$  isotopic anomalies of Mars and various meteorite types considered in our Monte Carlo mixing model. The isotopic anomalies for the Earth is 0. All values taken from the compilation of [Dauphas \(2017\)](#) except for  $\epsilon^{62}\text{Ni}$  which we source from the compilation of [Burkhardt et al. \(2017\)](#).

	$\Delta^{17}\text{O}$	$\epsilon^{50}\text{Ti}$	$\epsilon^{54}\text{Cr}$	$\epsilon^{62}\text{Ni}$	$\epsilon^{92}\text{Mo}$
Mars	$0.27 \pm 0.03$	$-0.54 \pm 0.17$	$-0.19 \pm 0.04$	$0.040 \pm 0.022$	$0.20 \pm 0.53$
EL	$-0.01 \pm 0.07$	$-0.28 \pm 0.06$	$0.06 \pm 0.04$	$-0.025 \pm 0.044$	$0.30 \pm 0.74$
EH	$-0.03 \pm 0.10$	$-0.10 \pm 0.02$	$0.04 \pm 0.08$	$0.026 \pm 0.021$	$0.36 \pm 0.43$
H	$0.72 \pm 0.05$	$-0.61 \pm 0.17$	$-0.38 \pm 0.03$	$-0.065 \pm 0.044$	$0.78 \pm 0.26$
L	$1.03 \pm 0.04$	$-0.63 \pm 0.02$	$-0.39 \pm 0.07$	$-0.051 \pm 0.020$	$0.61 \pm 0.62$
LL	$1.19 \pm 0.06$	$-0.65 \pm 0.04$	$-0.43 \pm 0.04$	$-0.076 \pm 0.013$	$0.87 \pm 1.13$
CI	$0.39 \pm 0.10$	$1.83 \pm 0.09$	$1.57 \pm 0.03$	$0.198 \pm 0.057$	$0.82 \pm 0.41$
CO	$-4.32 \pm 0.26$	$3.76 \pm 0.66$	$0.75 \pm 0.21$	$0.113 \pm 0.018$	$2.00 \pm 1.40$
CV	$-3.62 \pm 0.48$	$3.64 \pm 0.29$	$0.87 \pm 0.04$	$0.103 \pm 0.038$	$2.59 \pm 0.67$
CM	$-2.92 \pm 0.04$	$3.01 \pm 0.09$	$1.10 \pm 0.18$	$0.095 \pm 0.030$	$5.71 \pm 0.94$
CR	$-1.48 \pm 0.55$	$2.35 \pm 0.04$	$1.32 \pm 0.08$	$0.095 \pm 0.035$	$3.00 \pm 1.80$
Angrites	$-0.11 \pm 0.11$	$-1.15 \pm 0.02$	$-0.41 \pm 0.09$	$0.028 \pm 0.082$	$-0.14 \pm 0.75$

1816 The reservoirs we include in our model are the EL, EH, CI, CO, CV, CM, CR, H, L  
 1817 and LL chondrites, and the angrite meteorite (a type of achondrite). Other than the  $\Delta^{17}\text{O}$ ,  
 1818  $\epsilon^{50}\text{Ti}$ ,  $\epsilon^{54}\text{Cr}$ ,  $\epsilon^{62}\text{Ni}$  and  $\epsilon^{92}\text{Mo}$  values for these meteorites, the model also requires the respec-  
 1819 tive uncertainties of these isotopic anomalies and the concentration of these elements in the  
 1820 meteorites. In addition, the model also takes in the mass fraction of the five elements O, Ti,  
 1821 Cr, Ni and Mo in the mantle of the Earth and Mars that was delivered at each stage of the ac-  
 1822 cretion process. We follow [Dauphas \(2017\)](#) and assume that the accretion process comprises

TABLE A.2: Measured O, Ti, Cr, Ni and Mo elemental concentrations of the meteorites considered in our Monte Carlo mixing model. The values for chondritic meteorites are from [Wasson and Kallemeyn \(1988\)](#) while the values for angrites are from [Fitoussi et al. \(2016\)](#).

	O (mg/g)	Ti ( $\mu\text{g/g}$ )	Cr (mg/g)	Ni (mg/g)	Mo (ng/g)
EL	310	580	3.05	13.0	1131
EH	280	450	3.15	17.5	1131
CI	460	420	2.65	10.7	920
CO	370	780	3.55	14.0	1900
CV	370	980	3.60	13.4	2100
CM	432	580	3.05	12.0	1500
CR	420	647	3.75	13.6	1210
H	357	600	3.66	16.0	1700
L	377	630	3.88	12.0	1300
LL	400	620	3.74	10.2	1100
Angrites	359	867	3.78	14.9	1523

TABLE A.3: Mass fractions of elements O, Ti, Cr, Ni and Mo present in the mantle of the Earth and Mars at various accretion stages. The values are from [Dauphas \(2017\)](#).

	O		Ti		Cr		Ni		Mo	
	Earth	Mars	Earth	Mars	Earth	Mars	Earth	Mars	Earth	Mars
Stage 1	0.6	0.6	0.6	0.6	0.447	0.365	0.046	0	0	0
Stage 2	0.395	0.392	0.395	0.392	0.546	0.632	0.916	0.849	0.873	0.985
Stage 3	0.005	0.008	0.005	0.008	0.007	0.003	0.038	0.151	0.127	0.015

1823 three distinct stages. The inputs for our mixing model are summarised in Tables [A.1](#), [A.2](#)  
1824 and [A.3](#).

## 1825 A.2 Governing equations

1826 The isotopic composition ( $\Delta^{17}\text{O}$ ,  $\epsilon^{50}\text{Ti}$ ,  $\epsilon^{54}\text{Cr}$ ,  $\epsilon^{62}\text{Ni}$  and  $\epsilon^{92}\text{Mo}$ ) of the Earth and Mars, a quan-  
1827 tity to be computed in our model, is given by ([Dauphas, 2017](#))

$$\epsilon_{\text{mantle,comp}} = \sum_j X_j \frac{\sum_i f_{i,j} C_i \epsilon_i}{\sum_i f_{i,j} C_i}, \quad (\text{A.1})$$

1828 where  $X_j$  is the mass fraction of the element that was accreted onto the planet in stage  $j$   
1829 ( $\sum_j X_j = 1$ ),  $f_{i,j}$  is the mass fraction of meteorite reservoir  $i$  that was accreted onto the  
1830 planet in stage  $j$  ( $\sum_i f_{i,j} = 1$ ),  $C_i$  is the concentration of the element in reservoir  $i$ , and  $\epsilon_i$   
1831 is the measured isotopic composition of reservoir  $i$ . All quantities are fixed and given in  
1832 Tables [A.1](#), [A.2](#) and [A.3](#) except for  $f_{i,j}$  which we leave as a free parameter.

1833 In our model, Eq. [A.2](#) is decomposed into two parts, representing the contribution  
1834 by EL chondrites, and all reservoirs other than EL chondrites. The corresponding equations

1835 are

$$\begin{aligned}\varepsilon_{\text{EL}} &= \sum_j X_j \frac{f_{j,\text{EL}} C_{\text{EL}} \varepsilon_{\text{EL}}}{f_{j,\text{EL}} C_{\text{EL}} + (1 - f_{j,\text{EL}}) \sum_i f_{i,j,\text{nEL}} C_{i,\text{nEL}}}, \\ \varepsilon_{\text{nEL}} &= \sum_j X_j \frac{(1 - f_{j,\text{EL}}) \sum_i f_{i,j,\text{nEL}} C_{i,\text{nEL}} \varepsilon_{i,\text{nEL}}}{f_{j,\text{EL}} C_{\text{EL}} + (1 - f_{j,\text{EL}}) \sum_i f_{i,j,\text{nEL}} C_{i,\text{nEL}}},\end{aligned}\tag{A.2}$$

1836 where  $\varepsilon_{\text{EL}} + \varepsilon_{\text{nEL}} = \varepsilon_{\text{mantle,comp}}$ . The uncertainties for  $\varepsilon_{\text{EL}}$  and  $\varepsilon_{\text{nEL}}$  are computed as

$$\begin{aligned}\sigma_{\varepsilon_{\text{EL}}} &= \sum_j X_j \frac{f_{j,\text{EL}} C_{\text{EL}}}{f_{j,\text{EL}} C_{\text{EL}} + (1 - f_{j,\text{EL}}) \sum_i f_{i,j,\text{nEL}} C_{i,\text{nEL}}}, \\ \sigma_{\varepsilon_{\text{nEL}}} &= \sum_j X_j \frac{(1 - f_{j,\text{EL}}) \sum_i f_{i,j,\text{nEL}} C_{\text{EL}}}{f_{j,\text{EL}} C_{\text{EL}} + (1 - f_{j,\text{EL}}) \sum_i f_{i,j,\text{nEL}} C_{i,\text{nEL}}},\end{aligned}\tag{A.3}$$

1837 Combining the uncertainties for the EL and non-EL reservoirs gives the total uncertainty in  
1838  $\varepsilon_{\text{mantle,comp}}$ :

$$\sigma_{\varepsilon_{\text{mantle,comp}}} = \sqrt{\left( \frac{\sqrt{\sum_i f_{i,j,\text{nEL}} C_{i,\text{nEL}} \sigma_{i,\text{nEL}}^2}}{\sum_i f_{i,j,\text{nEL}} C_{i,\text{nEL}}} \right)^2 \sigma_{\varepsilon_{\text{nEL}}}^2 + \sigma_{\text{EL}}^2 \sigma_{\varepsilon_{\text{EL}}}^2}.\tag{A.4}$$

1839 Here,  $\sigma_{i,\text{nEL}}$  and  $\sigma_{\text{EL}}$  are the uncertainties in the isotopic compositions of the meteoritic reser-  
1840 voirs listed in Table A.1.

1841 Finally, the chi-square statistic  $\chi^2$  is computed as

$$\chi^2 = \frac{(\varepsilon_{\text{mantle,comp}} - \varepsilon_{\text{mantle,meas}})^2}{\left(\frac{1}{2}\sigma_{\varepsilon_{\text{mantle,comp}}}\right)^2 + \left(\frac{1}{2}\sigma_{\varepsilon_{\text{mantle,meas}}}\right)^2},\tag{A.5}$$

1842 where  $\varepsilon_{\text{mantle,meas}}$  are the measured isotopic compositions of the Earth (or Mars) and  $\sigma_{\varepsilon_{\text{mantle,meas}}}$   
1843 are the corresponding uncertainties (Table A.1).

### 1844 A.3 Model algorithm

1845 The first step of the computation concerns the initialisation of the isotopic compositions  
1846 (Eq. A.2), their corresponding uncertainties (Eq. A.3 and A.4) and the chi-square values (Eq. A.5).  
1847 For the free parameter  $f_{i,j}$ , we chose at random  $f_{1,\text{EL}} = 1$ ,  $f_{2,\text{EL}} = 0.2$ ,  $f_{3,\text{EL}} = 1$ , and  
1848  $f_{i,j,\text{nEL}} = 0$ . With these initial values we compute  $\varepsilon_{\text{mantle,comp}}$ ,  $\sigma_{\varepsilon_{\text{mantle,comp}}}$  and  $\chi_{\text{old}}^2$ .

1849 We next proceed to compute new values of  $f_{i,j}$  using a Box-Muller transform. We  
1850 made the assumption that  $f_{i,j}$  are distributed normally with a standard deviation of 0.005.  
1851 As the Box-Muller transform generates two variables at once, we compute the new values of  
1852  $f_{i,j}$  in pairs, according to

$$\begin{aligned}f_{i,j,\text{new}} &= f_{i,j,\text{old}} + 0.005z_1, \\ f_{i,j,\text{new}} &= f_{i,j,\text{old}} + 0.005z_2,\end{aligned}\tag{A.6}$$

1853 where  $z_1$  and  $z_2$  are given by

$$\begin{aligned}z_1 &= \sqrt{-2 \log u} \sin(2\pi v), \\ z_2 &= \sqrt{-2 \log u} \cos(2\pi v).\end{aligned}\tag{A.7}$$

1854 Here,  $u$  and  $v$  are selected at random from a uniform distribution with interval  $[0,1)$ . We  
 1855 also imposed the following constraints for the values of  $f_{i,j}$  generated by the Box-Muller  
 1856 transform:

$$\begin{aligned} 0 &\leq f_{j,\text{EL}} \leq 1, \\ 0 &\leq f_{i,j,\text{nEL}} \leq 1, \\ \sum_i f_{i,j,\text{nEL}} &\leq 1. \end{aligned} \quad (\text{A.8})$$

1857 With the new values of  $f_{i,j}$  we compute  $\varepsilon_{\text{mantle,comp}}$ ,  $\sigma_{\varepsilon_{\text{mantle,comp}}}$  and the corresponding value  
 1858 of  $\chi_{\text{new}}^2$ . This is then followed by an acceptance test according to the Metropolis-Hastings  
 1859 algorithm (Metropolis et al., 1953) with the acceptance ratio computed as

$$\alpha' = \exp(-0.5\chi_{\text{new}}^2 + 0.5\chi_{\text{old}}^2). \quad (\text{A.9})$$

1860 We accept the new  $f_{i,j}$  values and update  $\chi_{\text{old}}^2$  with  $\chi_{\text{new}}^2$  if the value of  $y$  selected at random  
 1861 from a uniform distribution ranging from  $[0,1)$  fulfils the condition  $y < \alpha'$ .

1862 Finally, we repeat the algorithm described in the previous paragraph over  $10^6$  it-  
 1863 erations for Earth and  $2 \times 10^6$  iterations for Mars. We excluded the output from the first  
 1864  $2 \times 10^4$  iterations for the Earth and  $2 \times 10^5$  iterations for Mars when the system has yet to  
 1865 reach equilibrium before searching for the best-fit combination of  $f_{i,j}$  which gives the low-  
 1866 est value of  $\chi^2$ . We also repeated the same Monte Carlo simulation 20 times to obtain other  
 1867 best-fit combinations of  $f_{i,j}$ .

## 1868 A.4 Model output

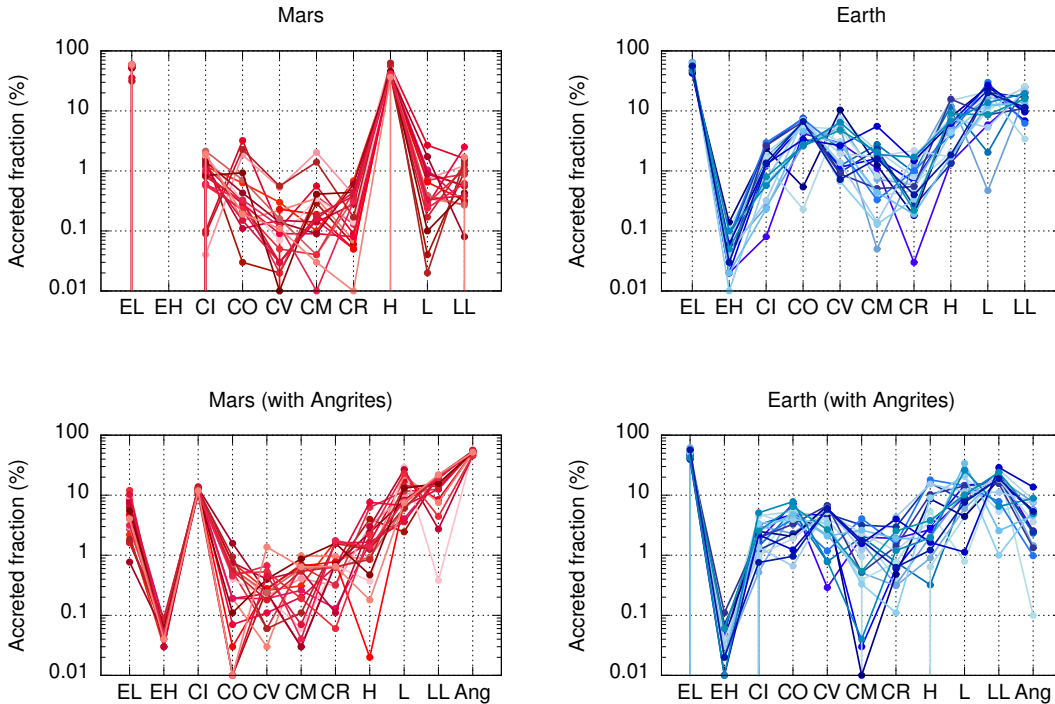


FIGURE A.1: Contribution of various meteorite types to the composition of Earth and Mars computed from our mixing model. Shown here are the best-fit compositions obtained from 20 simulations. The top panels shows the results for the simulations where only chondrites are considered while the bottom panels shows the results when we include angrites into the list of potential building blocks.

1869 Fig. A.1 shows the best-fit compositions of the Earth and Mars obtained from our  
 1870 mixing model. If we only consider chondritic reservoirs, the mixing model outputs the fol-  
 1871 lowing combination for the Earth and Mars:

- 1872 • Earth =  $(52 \pm 6)\%$  EC +  $(36 \pm 4)\%$  OC +  $(12 \pm 2)\%$  CC
- 1873 • Mars =  $(53 \pm 9)\%$  EC +  $(45 \pm 8)\%$  OC +  $(2 \pm 1)\%$  CC

1874 The major contributors to the composition of Earth are EL (52%), CO (5%), CV (3%), H (7%),  
 1875 L (15%) and LL (15%) chondrites. For Mars, the major contributors are EL (53%) and H (43%)  
 1876 chondrites. In computing these numbers, we have taken the average and the standard devi-  
 1877 ation from the outputs of 20 Monte Carlo simulations. Our results are consistent with those  
 1878 from previous studies (e.g., [Sanloup et al., 1999](#); [Tang and Dauphas, 2014](#); [Dauphas, 2017](#);  
 1879 [Brasser et al., 2018](#)).

1880 If we include angrites to the mix, the model gives the following results instead:

- 1881 • Earth =  $(48 \pm 7)\%$  EC +  $(34 \pm 4)\%$  OC +  $(13 \pm 2)\%$  CC +  $(5 \pm 3)\%$  angrites
- 1882 • Mars =  $(5 \pm 3)\%$  EC +  $(29 \pm 2)\%$  OC +  $(14 \pm 1)\%$  CC +  $(52 \pm 3)\%$  angrites

1883 In this case the major contributors are EL (48%), CO (4%), CV (4%), H (6%), L (12%), LL (16%)  
 1884 and angrites (5%) for the Earth, and EL (5%), CI (12%), L (12%), LL (15%) and angrites (52%)  
 1885 for Mars. The model gives a very different composition for Mars when angrites are consid-  
 1886 ered: Angrites are now the favoured major contributor, the contribution of EC is drastically  
 1887 reduced and the contribution of CC is increased. This outcome is also consistent with the  
 1888 results of [Fitoussi et al. \(2016\)](#). However, this result should not be overinterpreted mainly  
 1889 because the bulk chemical composition of the angrite parent body is not well constrained  
 1890 (as is also the case with other achondrites) and thus it is unclear if the measured isotopic  
 1891 anomalies of the angrites that we use in our mixing model is truly representative of that of  
 1892 its parent body.

1893 From our mixing model study, we show that it is always possible to find a com-  
 1894 bination of chondrites (and achondrites) which, when mixed in the correct proportion, can  
 1895 reproduce the isotopic compositions of the Earth and Mars. The large uncertainties in the  
 1896 measurement of some isotopic anomalies (e.g.,  $\epsilon^{92}\text{Mo}$ ) can affect the mixing model output  
 1897 for the contribution of each chondritic (and achondritic) reservoir. It is therefore imperative  
 1898 to identify new constraints (e.g., major element abundance ratio) to be incorporated into the  
 1899 model in order to obtain more conclusive results.



## 1900 B Numerical methods

### 1901 B.1 Gas disc model

1902 The gas disc model employed in our simulations is based on the model of [Ida et al. \(2016\)](#).  
 1903 The accretion rate of the gas onto the central star (the Sun in our case) is assumed to occur  
 1904 at a steady rate given by

$$\dot{M}_* = 3\pi\alpha\Sigma_g H_g^2 \Omega_K, \quad (\text{B.1})$$

1905 where  $\Sigma_g$  is the gas surface density,  $H_g$  is the disc scale height and  $\Omega_K$  is the Keplerian  
 1906 frequency. The disc  $\alpha$ -viscosity  $\alpha$  was set to  $10^{-3}$  and assumed to be constant throughout  
 1907 ([Shakura and Sunyaev, 1973](#)). It is given by

$$\alpha = \nu / (c_s^2 \Omega_K), \quad (\text{B.2})$$

1908 where  $\nu$  is the gas viscosity and  $c_s$  is the sound speed. As a result, the gas surface density  
 1909 is comparable to that of the MMSN. The scale height of the disc  $H_g$  is a function of the  
 1910 temperature  $T$  and the sound speed  $c_s$  via  $H_g = c_s / \Omega_K$ , where  $c_s = (\gamma k_B T / \mu m_p)$ . The heat  
 1911 capacity ratio  $\gamma$  is set to 7/5,  $k_B$  is the Boltzmann constant,  $\mu = 2.3$  is the mean atomic mass  
 1912 of the gas and  $m_p$  is the mass of the proton. In the simulations, the gas accretion rate varies  
 1913 with time according to [Hartmann et al. \(1998\)](#)

$$\log\left(\frac{\dot{M}_*}{M_\odot \text{ yr}^{-1}}\right) = -8 - \frac{7}{5} \log\left(\frac{t}{1 \text{ Myr}} + 0.1\right) \quad (\text{B.3})$$

1914 where the extra 0.1 Myr was added to avoid the logarithmic singularity ([Bitsch et al., 2015](#)).

1915 The temperature in different regions of the disc is predominantly dictated by the  
 1916 heating source. In general, viscous heating dominates the inner region close to the star while  
 1917 stellar irradiation has a stronger influence in the far away regions. At the midplane, the  
 1918 disc temperature is given by  $T = \max(T_{\text{vis}}, T_{\text{irr}})$ , where  $T_{\text{vis}}$  and  $T_{\text{irr}}$  are temperatures in the  
 1919 viscous region and irradiative region, respectively. The empirically fitted expressions for  $T_{\text{vis}}$   
 1920 and  $T_{\text{irr}}$  based on the constant-opacity disc model of [Garaud and Lin \(2007\)](#) are

$$\begin{aligned} T_{\text{vis}} &= T_{0v} \alpha_3^{-1/5} \dot{M}_{*8}^{2/5} \left(\frac{r}{1 \text{ au}}\right)^{-9/10} \text{ K}, \\ T_{\text{irr}} &= 150 \left(\frac{r}{1 \text{ au}}\right)^{-3/7} \text{ K}, \end{aligned} \quad (\text{B.4})$$

where  $T_{0v}$  is the initial temperature at 1 au and  $r$  is the distance to the Sun. The power exponents in the equation are derived analytically. We additionally defined the following normalised parameters

$$\alpha_3 \equiv \frac{\alpha}{10^{-3}}, \quad (\text{B.5})$$

$$\dot{M}_{*8} \equiv \frac{\dot{M}_*}{10^{-8} M_\odot \text{ yr}^{-1}}. \quad (\text{B.6})$$



1921 With the disc temperature profiles defined, the reduced disc scale height  $h_g = H_g/r$  can thus  
1922 be computed as

$$\begin{aligned} h_{g,\text{vis}} &= 0.034 \left( \frac{T_{0v}}{200 \text{ K}} \right)^{1/2} \alpha_3^{-1/10} \dot{M}_{*8}^{1/5} \left( \frac{r}{1 \text{ au}} \right)^{1/20}, \\ h_{g,\text{irr}} &= 0.029 \left( \frac{r}{1 \text{ au}} \right)^{2/7}. \end{aligned} \quad (\text{B.7})$$

1923 The actual reduced scale height of the disc is  $h_g = \max(h_{g,\text{vis}}, h_{g,\text{irr}})$ . This gives the disc  
1924 a flaring shape in the irradiative region and a constant scale height in the viscous region.  
1925 Equations (B.1), (B.4) and (B.7) are then combined to compute the gas surface density in the  
1926 viscous and irradiative regions

$$\begin{aligned} \Sigma_{g,\text{vis}} &= 1320 \left( \frac{T_{0v}}{200 \text{ K}} \right)^{-1} \alpha_3^{-4/5} \dot{M}_{*8}^{3/5} \left( \frac{r}{1 \text{ au}} \right)^{-3/5} \text{ g cm}^{-2}, \\ \Sigma_{g,\text{irr}} &= 1785 \alpha_3^{-1} \dot{M}_{*8} \left( \frac{r}{1 \text{ au}} \right)^{-15/14} \text{ g cm}^{-2}. \end{aligned} \quad (\text{B.8})$$

1927 The corresponding pressure gradient  $d \ln P / d \ln r$  in the viscous and irradiative regimes are

$$\begin{aligned} \left( \frac{d \ln P}{d \ln r} \right)_{\text{vis}} &= \frac{51}{20}, \\ \left( \frac{d \ln P}{d \ln r} \right)_{\text{irr}} &= \frac{39}{14}. \end{aligned} \quad (\text{B.9})$$

1928 Finally, the boundary between the viscous and irradiative region, determined by  $T_{\text{vis}} = T_{\text{irr}}$ ,  
1929 occurs at

$$\begin{aligned} r_{\text{vis/irr}} &= \left( \frac{T_{0v}}{150 \text{ K}} \right)^{70/33} \alpha_3^{-14/33} \dot{M}_{*8}^{28/33} \\ &\approx 1.84 \alpha_3^{-14/33} \dot{M}_{*8}^{28/33} \text{ au}. \end{aligned} \quad (\text{B.10})$$

## 1930 B.2 Disc-induced orbital evolution

1931 The gas disc exerts torques and tidal forces on all the planetary bodies (with mass  $M$  and  
1932 radius  $R$ ) embedded in the disc which result in a combined effect of radial migration and the  
1933 damping of the orbital eccentricity  $e$  and orbital inclination  $I$ . Low-mass planetary bodies,  
1934 i.e., those that are unable to clear the surrounding gas, experience type I migration (Tanaka  
1935 et al., 2002) while massive bodies experience type II migration (Lin and Papaloizou, 1986).  
1936 The computation of the torques and the direction of migration is based on the prescriptions  
1937 of Coleman and Nelson (2014). The normalised torque is given by

$$\frac{\gamma \Gamma}{\Gamma_0} = \frac{\Gamma_C}{\Gamma_0} F_C + \frac{\Gamma_L}{\Gamma_0} F_L \quad (\text{B.11})$$

1938 where  $\Gamma_C$  and  $\Gamma_L$  are the corotation and Lindblad torques respectively (Paardekooper et al.,  
1939 2011) and

$$\Gamma_0 = \left( \frac{M}{M_*} \right)^2 h_g^{-2} \Sigma_g \Omega_K^2 \quad (\text{B.12})$$

1940 is a normalisation constant. The factors  $F_L$  and  $F_C$  are defined as (Cresswell and Nelson,  
1941 2008; Fendyke and Nelson, 2014)

$$\begin{aligned} \ln F_C &= -\frac{e}{e_f}, \\ \frac{1}{F_L} &= P_e + \text{sign}(P_e)(0.07\hat{I} + 0.085\hat{I}^4 - 0.08\hat{e}^2\hat{I}^2), \end{aligned} \quad (\text{B.13})$$

where  $e_f = 0.01 + \frac{1}{2}h_g$ ,  $\hat{e} = e/h_g$ ,  $\hat{I} = \sin(I)/h_g$  and

$$P_e = \frac{1 + (0.444\hat{e})^{1/2} + (0.352\hat{e})^6}{1 - (0.495\hat{e})^4}.$$

1942 The eccentricity damping timescale  $\tau_e = -e/\dot{e}$  is

$$\tau_e = 1.282t_{\text{wav}} \left( 1 - 0.14\hat{e}^2 + 0.06\hat{e}^3 + 0.18\hat{e}^2\hat{I}^2 \right), \quad (\text{B.14})$$

1943 where the wave timescale is (Tanaka and Ward, 2004)

$$t_{\text{wav}} = \left( \frac{M_*}{M} \right) \left( \frac{M_*}{\Sigma_g R^2} \right) h_g^4 \Omega_K^{-1}. \quad (\text{B.15})$$

1944 The inclination damping time scale  $\tau_I = -I/(dI/dt)$  is

$$\tau_I = 1.838t_{\text{wav}} (1 - 0.30\hat{I}^2 + 0.24\hat{I}^3 + 0.14\hat{e}^2\hat{I}^2). \quad (\text{B.16})$$

1945 For planetary bodies in the type I migration regime, the migration timescale is defined as  
1946  $\tau_m = -L/\Gamma$  where  $L$  and  $\Gamma$  are the angular momentum and the torque. We compute the  
1947 migration timescale as

$$\tau_{\text{mig},1} = -\frac{t_{\text{wav}}\Gamma_0}{h_g^2\Gamma}, \quad (\text{B.17})$$

1948 in the simulations. For bodies in the type II regime, the migration timescale is computed as

$$\tau_{\text{mig},2} = \frac{2R^2}{3\nu} \max \left( 1, \frac{M}{2\pi\Sigma_g R^2} \right). \quad (\text{B.18})$$

1949 The first term in the parentheses corresponds to the case when the planet is less massive than  
1950 the disc interior to its orbit and the migration occurs on the disc's viscous evolution timescale  
1951 of  $\tau_{\text{mig},2} \simeq (2/3)(R^2/\nu)$  (Lin and Papaloizou, 1986), whereas the second term corresponds to  
1952 the opposite case where the planet is more massive and thus the migration occurs on a longer  
1953 timescale  $\tau_{\text{mig},2} \simeq M/\dot{M}_*$  (Hasegawa and Ida, 2013).

### 1954 B.3 Gas envelope accretion for massive planets

1955 Gas accretion commences for planetary bodies that fulfil two criteria: (1) they have reached  
1956 a critical core mass, and (2) the accretion rate of solids onto said planetary core is sufficiently  
1957 low that it does not affect the cooling and contraction of the gas envelope. The critical core  
1958 mass of a planetary body is given by (Ikoma et al., 2000)

$$M_{\text{crit}} = 10 \left( \frac{\dot{M}_{\text{core}}}{10^{-6}M_E \text{ yr}^{-1}} \right)^{1/4} M_E, \quad (\text{B.19})$$

1959 where the core accretion rate is equal to the pebble accretion rate of the planetary body  
1960  $\dot{M}_{\text{core}} = \dot{M}$  (see Eq. 2.1). The collapse and accretion of the gas envelope then proceeds on the  
1961 Kelvin-Helmholtz timescale (Ikoma et al., 2000) according to

$$\tau_{\text{KH}} = 10^9 \left( \frac{M}{M_E} \right)^{-3} \text{ yr}. \quad (\text{B.20})$$

1962 This process of runaway gas accretion is bounded by the gas accretion rate throughout the  
1963 disc  $\dot{M}_*$ . Gas accretion ceases when the Hill radius of the planet is approximately equal to

1964 that of the disc scale height. Taking all these effects into account, the gas accretion rate onto  
 1965 the planetary core is written as

$$\dot{M}_g = \min \left[ \frac{M}{\tau_{\text{KH}}}, \dot{M}_* \exp \left( -\frac{M}{M_{\text{H}}} \right) \right], \quad (\text{B.21})$$

1966 where  $M_{\text{H}} = 3(h_g/R)^3 M_*$  is the required planetary mass for its Hill radius to be comparable  
 1967 to the disc scale height. The gas accretion rate is limited to the Bondi accretion rate of

$$\dot{M}_{\text{g,B}} = \frac{4\pi\rho_g G^2 M^2}{c_s^3}, \quad (\text{B.22})$$

1968 where  $\rho_g \sim \Sigma_g/(\sqrt{2\pi}h_g)$  is the gas disc's density and  $G$  is the gravitational constant. We  
 1969 keep track of the amount of mass in solids and in gas accreted by the planet.

## 1970 **C Depleted disc model simulations** 1971 **with higher solid surface density**

1972 In our depleted disc model simulations adopting a fixed value (MMSN) for the solid surface  
1973 density (Chapter 3) we find that the planets that formed in the terrestrial region have masses  
1974 that are lower than the current terrestrial planets. This issue could be resolved by increasing  
1975 the surface density of the disc so that there is more mass in the disc to form more massive  
1976 planets. We carried out additional simulations with a higher solid surface density (1.5 and/or  
1977 2 times the MMSN value) for the cases where the initial mass in the solid disc is less than  
1978  $\sim 2 M_E$ . Fig. C.1 shows the initial conditions of our additional simulations. In most cases,  
1979 the initial mass of solids in the disc is now well over  $\sim 2 M_E$ , sufficient to form the terrestrial  
1980 planets.

1981 With the disc's solid surface density increased, the final mass of planets in the  
1982 terrestrial region are now closer to the current mass of the terrestrial planets (Fig. C.2). In  
1983 particular, planets at around 1 au now have masses comparable to that of the Earth. However,  
1984 planets that formed in the region around 1.5 au tend to be more massive than Mars. From the  
1985 initial conditions that we investigated here, we find that increasing the solid surface density  
1986 produces more Venus and Earth analogues but less Mars analogues. A larger degree of mass  
1987 depletion is thus required to form planets around 1.5 au with masses equivalent to that of  
1988 Mars. For example, a mass depletion of  $> 95\%$  is needed for the case of  $r_{\text{dep}} = 1.5$  au and a  
1989 mass depletion of  $> 75\%$  up to about  $95\%$  is needed for the case of  $r_{\text{dep}} = 1.0$  au.

1990 As the planets are now more massive on average, we observe an increase in the  
1991 values of  $S_m$  and  $S_H$  (top panel of Fig. C.3). The results for the concentration parameter  $S_c$  and  
1992 AMD of the terrestrial planet systems are, however, similar to the outcomes for simulations  
1993 with MMSN surface density (bottom panel of Fig. C.3).

1994 We also find the same trend of correlated feeding zones with semi-major axis for  
1995 the Venus and Earth analogues and a large variation in the feeding zones of Mars analogues  
1996 (Fig. C.4).

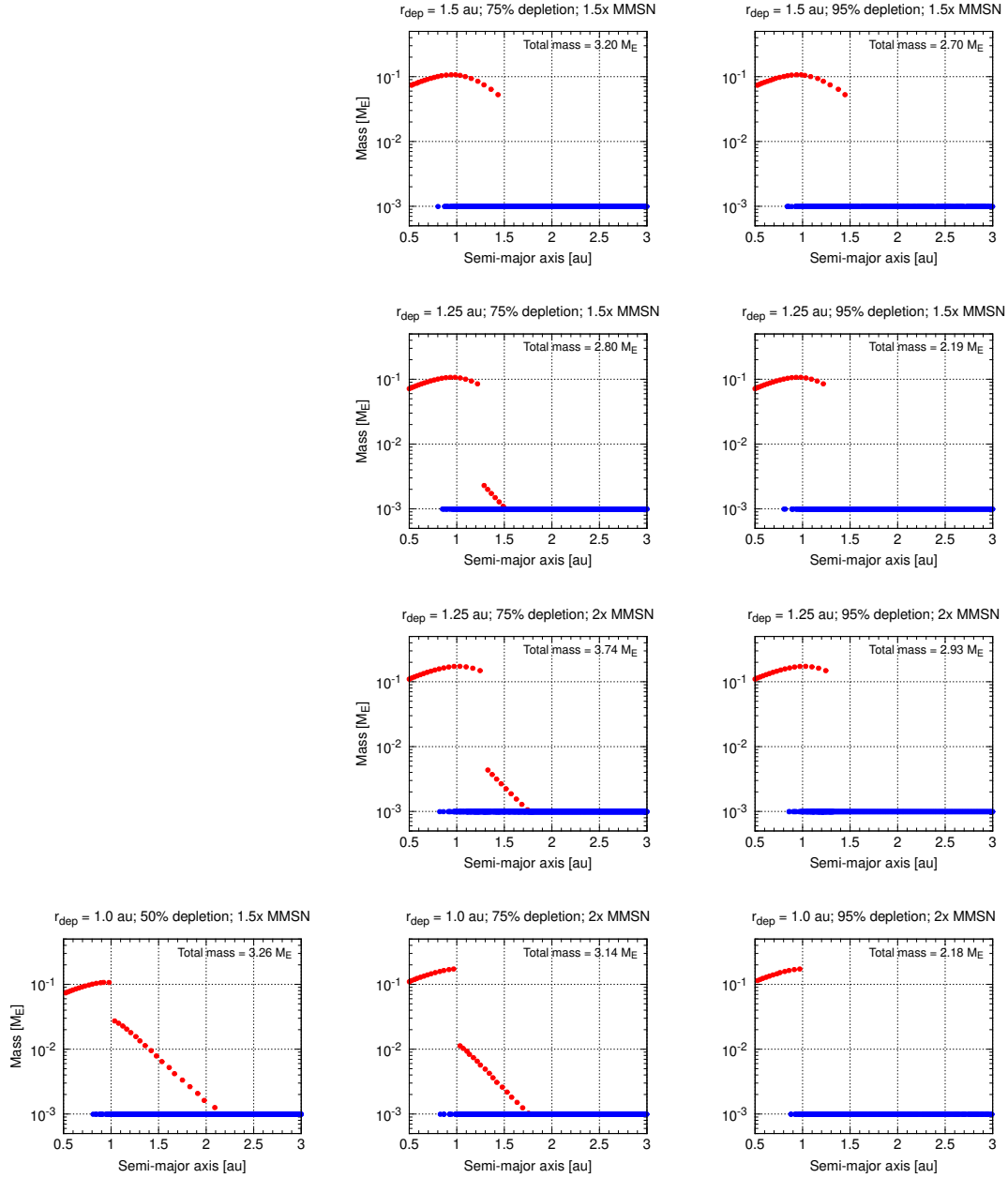


FIGURE C.1: Initial mass and semi-major axis distribution of planetary embryos (red) and planetesimals (blue) for additional depleted disc model simulations starting with higher solid surface density.

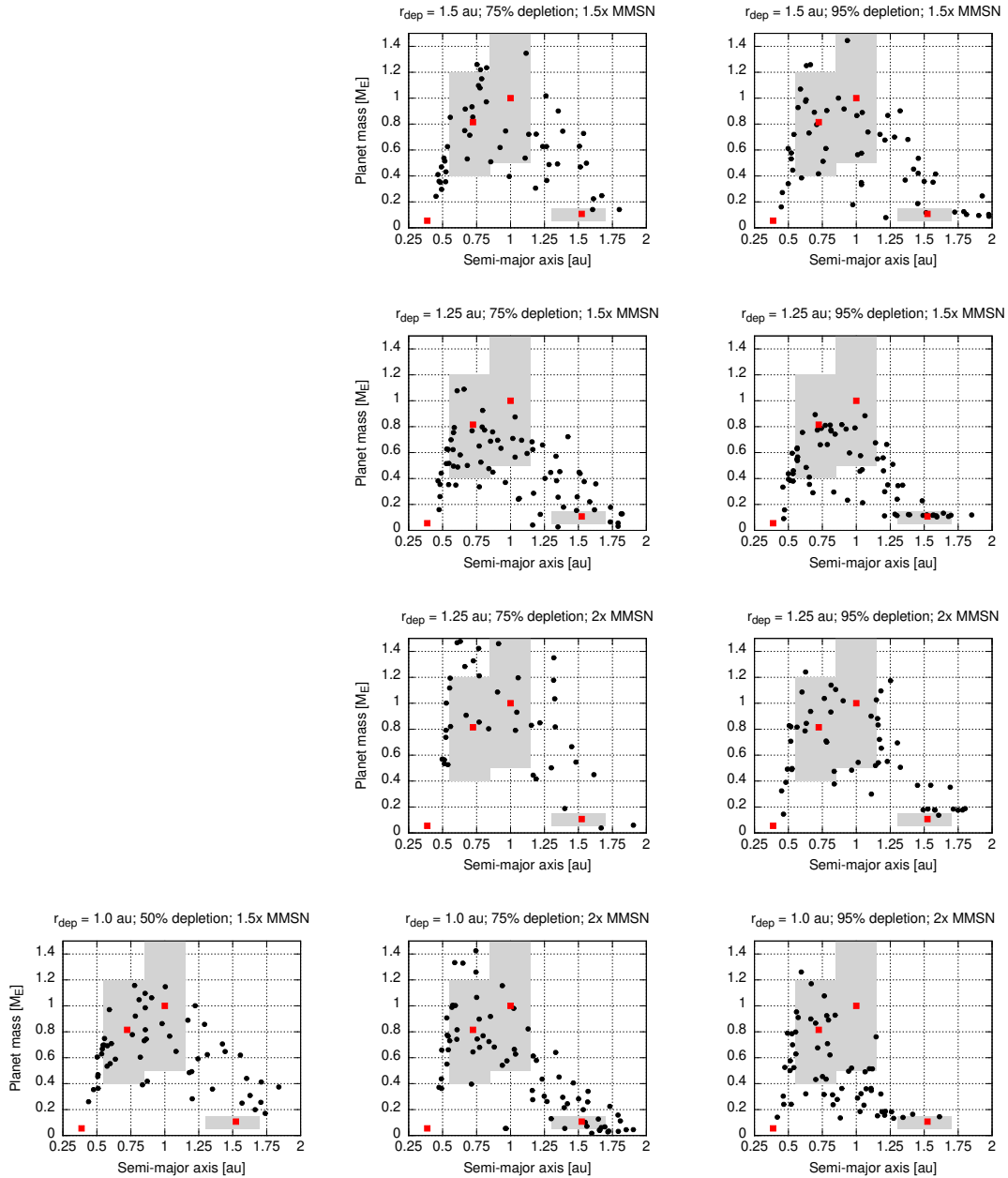


FIGURE C.2: Distribution of final planet mass versus semi-major axis for simulations starting with higher solid surface density. Red squares are the current terrestrial planets, black circles are planets that formed in the simulations, and grey regions indicate the range within which planets are considered good terrestrial planet analogues.

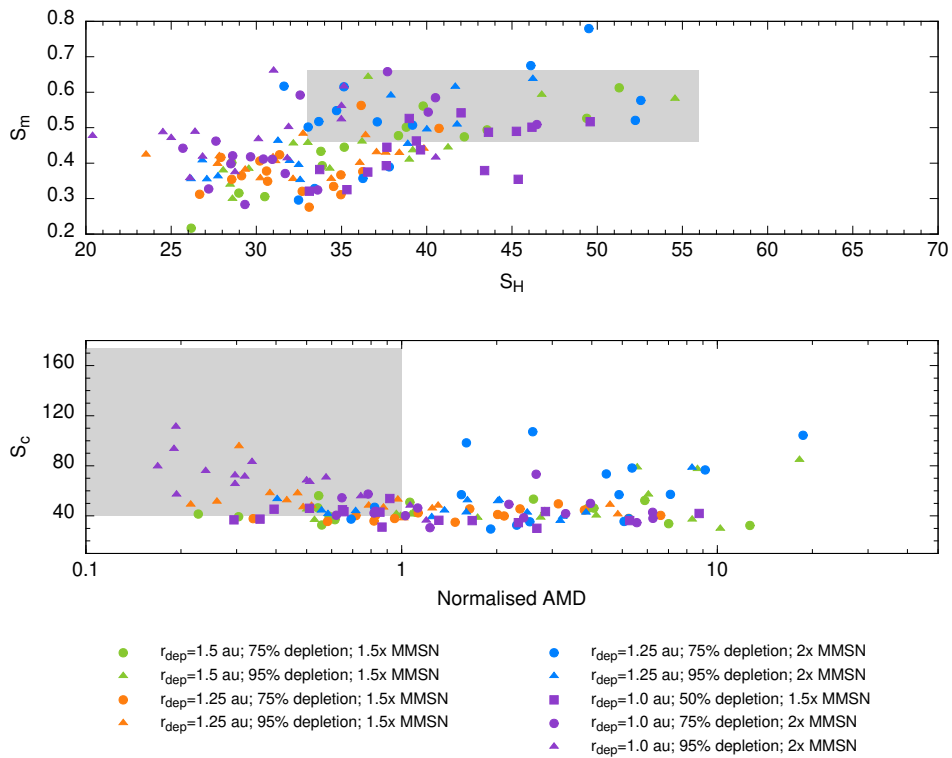


FIGURE C.3: Top panel: Mass in largest planet as a fraction of the total mass of the planetary system  $S_m$  versus the mean spacing parameter  $S_H$  in units of the mutual Hill sphere. Bottom panel: Mass concentration parameter  $S_c$  versus the angular momentum deficit (AMD) normalised to the current Solar System value. Grey regions encompass the current values of the inner Solar System and the  $2\sigma$  range.

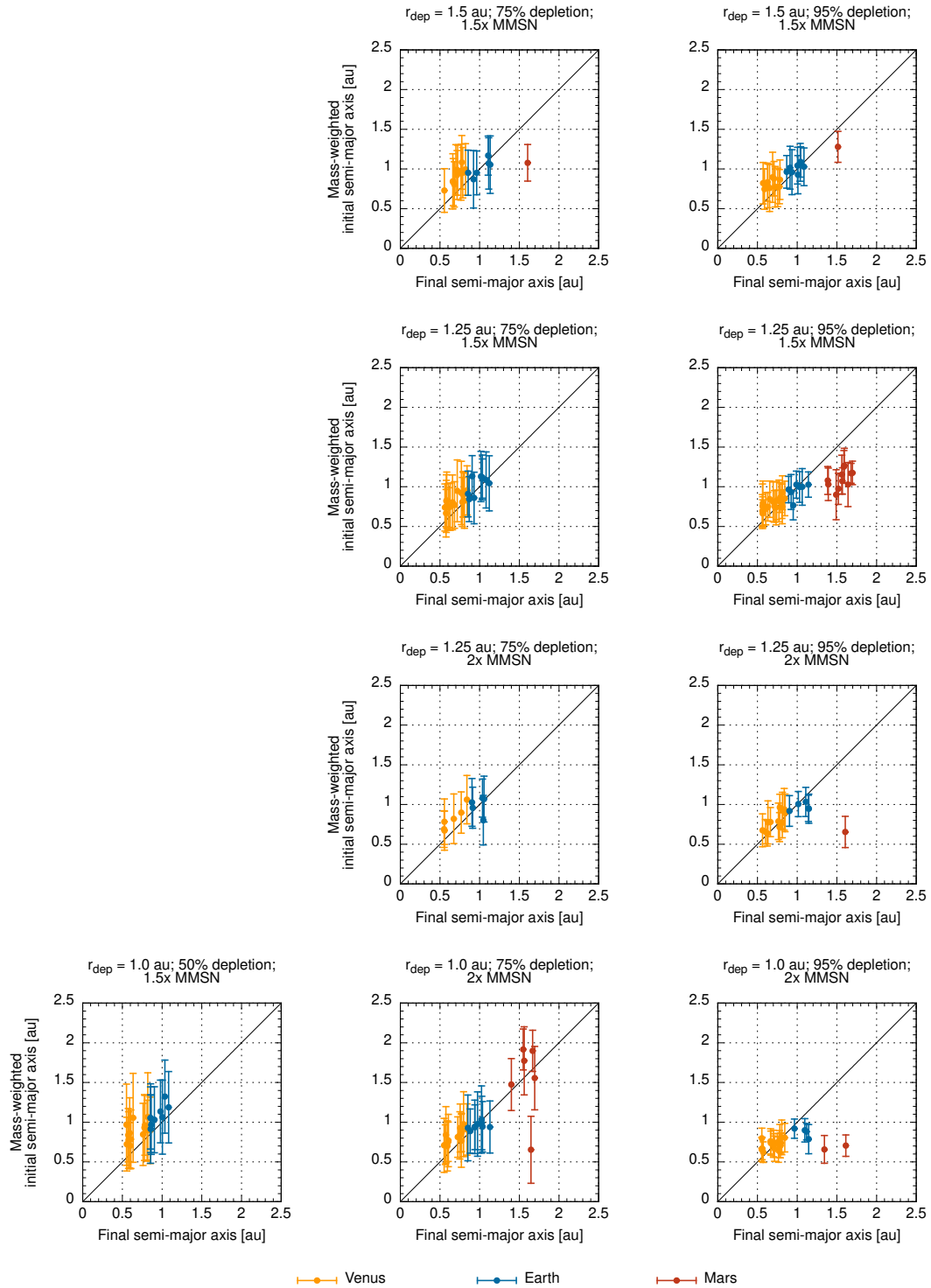


FIGURE C.4: Feeding zones of the Venus, Earth and Mars analogues versus their final semi-major axis from additional depleted disc model simulations starting with higher solid surface density. Black lines correspond to the equation  $y = x$ .





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