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### NEW INSIGHTS ON THE FORMATION OF THE TERRESTRIAL PLANETS

by Jingyi Ман

A thesis submitted to the Department of Earth and Planetary Sciences of the Tokyo Institute of Technology in partial fulfilment of the requirements for the degree of Doctor of Science

### 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 2 endeavour motivated in part by humanity's curiosity of our own origins. How did the Earth 3 form? What made the Earth? Where can we find clues? These seemingly basic questions turn 4 out to be complex puzzles that require contributions from multiple fields such as astronomy, 5 cosmochemistry and planetary science, to name a few. In recent years, researchers from these 6 apparently disparate but complementary fields have taken notice of the developments in each 7 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, 9 challenge long-held perceptions and lead to even more questions, but our understanding of 10 planet formation nevertheless increases because of the debate that these results ignited. 11

In this thesis, we synthesise state-of-the-art knowledge from theories of planet for-12 mation and cosmochemistry data and use this information to answer the question of whether 13 the terrestrial planets grew by the accumulation of small (cm-sized) solids or were they the 14 products of mergers between large (km-sized) planetary bodies. We will put forward a pro-15 posal to explain cosmochemistry data trends based on the outcomes of our numerical inves-16 tigations. The thesis consists of two studies, each examining the formation of the terrestrial 17 planets from one of the two aforementioned pathways. We aim to convey the message that 18 utilising a variety of relevant cosmochemistry data can help to distinguish between differ-19 ent planet formation models and point to the direction(s) that future studies could follow 20 in the quest of gaining full understanding of how the terrestrial planets take shape. In the 21 following sections we will review several dynamical models of planet formation, introduce 22 relevant cosmochemistry data used in our work, and outline the motivation and approach of 23 the studies presented in this thesis. 24

### **1.1** Developments in planet formation theories

Studies to unravel the mysteries surrounding the formation pathways of the terrestrial plan-26 ets have made considerable advances since the initial proposal by Safronov (1969) on the 27 genesis of planetesimals via the agglomeration of dust particles in the protoplanetary disc. It 28 is commonly accepted in the community that the terrestrial planets formed from collisions 29 among protoplanets (also known as planetary embryos) of increasing size, although, as we 30 will later discuss, this paradigm is starting to be challenged. The Classical model of terres-31 trial planet formation (Chambers, 2001) was built upon the results of early analytical deriva-32 tions (e.g., Wetherill, 1980; Wetherill and Stewart, 1989) and numerical simulations (Kokubo 33 and Ida, 1995, 1996, 1998) of the evolution of a self-gravitating solid disc of planetesimals. 34 Several planetesimals in the solid disc will grow much faster than the rest and produce a 35 bimodal population in the disc comprising larger-sized planetary embryos and smaller-sized 36 planetesimals (Kokubo and Ida, 1998). The embryos continue growing by accreting nearby 37 planetesimals until they exhaust all the planetesimals in their feeding zones, by which time 38

the embryos will collide and merge among themselves to finally form the terrestrial planets. Chambers (2001) shows that the growth timescales of the terrestrial planets are around several tens of millions of years.

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

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

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

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

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

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

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

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

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

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

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

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

### **1.3** Cosmochemistry data and trends

#### 175 **1.3.1** Isotopic dichotomy in the Solar System

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

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



FIGURE 1.1: Measured  $\varepsilon^{50}$ Ti and  $\varepsilon^{54}$ 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); Petitat et al. (2011); Zhang et al. (2011, 2012); Yamakawa and Yin (2014).

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

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

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

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

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

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

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



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).

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

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

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



FIGURE 1.3: Measured  $\varepsilon^{92}$ Mo and  $\varepsilon^{100}$ 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  $\varepsilon^{92}$ 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);  $\varepsilon^{100}$ Ru data are from Chen et al. (2010); Fischer-Gödde et al. (2015); Bermingham et al. (2018); Worsham et al. (2017); Fischer-Gödde and Kleine (2017); Bermingham et al. (2018); Worsham et al. (2019).

It has been shown (e.g., by Drake and Righter, 2002 and more recently, a review 297 by Mezger et al., 2020) that the current repository of known meteorites does not constitute 298 the whole picture of the Earth's building blocks. Earth's location as an end-member in plots 299 of Ti versus Cr (Fig. 1.1; Trinquier et al., 2009; Warren, 2011) and Ru versus Mo (Fig. 1.3; 300 Dauphas et al., 2014a; Fischer-Gödde et al., 2015) could also hint at an additional reservoir 301 in the region closer to the Sun than where the ECs are thought to have formed. Fig 1.3302 illustrates the fact that one cannot get the isotopic composition of the Earth by mixing EC, 303 OC and CC. This therefore prompted the suggestion of the existence of an additional reservoir 304 characterised by an enrichment in s-process isotopes. The Earth should have accreted some 305 material from this reservoir to offset the s-process deficit signature of the other meteorites 306 (Fischer-Gödde and Kleine, 2017; Render et al., 2017). However, meteorite samples from this 307 s-process-enriched reservoir have not been found to date and it has been suggested that 308 all the material from this reservoir have been accreted into the terrestrial planets (Drake 309 and Righter, 2002; Burkhardt et al., 2011, 2016). Indeed, Fischer-Gödde et al. (2020) may 310 have found evidence of this reservoir in ancient terrestrial rocks that show positive  $\varepsilon^{100}$ Ru 311 anomalies, but more measurements are needed to confirm this hypothesis. 312

### 1.3.3 Potential isotopic gradients in the inner Solar System and the origins 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  $\varepsilon^{92}$ 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.

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

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

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

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

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

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

### <sup>380</sup> 1.4 Key questions and structure of thesis

High-precision isotope data of meteorites made available in the past decade have been grad-381 ually adopted by studies seeking to understand how the terrestrial planets formed. The dis-382 tinct isotopic compositions of the Earth and Mars have been employed to constrain dynamical 383 models of planet formation. Previous studies examining the classical model (Chambers, 2001) 38/ found that the feeding zones (region of the protoplanetary disc where a planet sourced most 385 of its building material) of the terrestrial planets show a correlation with their semi-major 386 axis (e.g., Raymond et al., 2004; O'Brien et al., 2006; Fisher and Ciesla, 2014; Kaib and Cowan, 387 2015; Woo et al., 2018). This is because the planets are thought to grow by the accretion of 388 solid material within their respective feeding zones in the classical model. Consequently, 389 Earth and Mars' isotopic differences can be reproduced if the material that these two planets 390 accreted have different isotopic compositions. However, forming Mars analogues at 1.5 au 391 with the correct mass is a fundamental shortcoming of this model. 392

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

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

In this thesis, we will study the formation of planetary bodies in the inner Solar System as a whole. We will use the correlation between isotopic compositions of Earth, Mars and Vesta and their respective semi-major axis, as well as the distinct compositions of these planetary bodies as additional constraints to help us understand their formation pathway and formation location. To this end, we will employ a two-pronged approach. We will examine two different models of planet formation — the pebble accretion model (Ormel and Klahr, <sup>424</sup> 2010; Lambrechts and Johansen, 2012), and the depleted disc model (Izidoro et al., 2014, 2015)
<sup>425</sup> - with the aim of answering the following questions:

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

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

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

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

# <sup>457</sup> 2 Role of pebble accretion the inner <sup>458</sup> Solar System

### 459 2.1 Introduction

In this chapter we study the effects of pebble accretion in the inner Solar System when Jupiter 460 is still growing. We will use N-body simulations to model the growth of planetesimals in 461 the inner Solar System that are subjected to a flux of pebbles over the course of Jupiter's 462 growth, with the aim of quantifying the amount of mass delivered to the inner disc by pebble 463 accretion. Our motivation stems from the promising results of several previous works, both 464 from the aspects of planetary dynamics and cosmochemistry, that reported the potential of 465 the pebble accretion mechanism (e.g., Lambrechts and Johansen, 2012) to lay the groundwork 466 for the formation of the terrestrial planets (e.g., Levison et al., 2015b; Johansen et al., 2021) 467 and its capability of explaining the correlation between the  $\varepsilon^{48}$ Ca isotopic composition and 468 the mass (or size) of the Earth, Mars and Vesta (Schiller et al., 2018). However, there have 469 also been reports (Brasser and Mojzsis, 2020; Kleine et al., 2020) challenging the efficiency of 470 Jupiter as a competent barrier in preventing excessive pebbles from entering the inner Solar 471 System and maintaining the isotopic dichotomy. In the following we briefly describe the 472 method and outcome of several previous works that investigated the feasibility of the pebble 473 accretion mechanism in forming the terrestrial planets. 474

The work of Levison et al. (2015b) employed numerical simulations to study the 475 effect of pebble accretion in the inner Solar System. They subjected a population of plan-476 etesimals distributed between 0.7 au and 2.7 au to a flux of inward drifting pebbles that are 477 continuously generated in the same region over a period of 2 Myr. The planetesimals are 478 embedded in a gas disc with an  $r^{-1}$  (r is the distance to the star) surface density function. 479 Since the pebbles are formed continuously in the inner Solar System, the surface density of 480 the gas was chosen to be about 5 times the minimum mass solar nebula (MMSN; Hayashi, 481 1981), a value deemed sufficient to sustain continuous pebble formation in the disc in their 482 simulations. Simulations with sufficient mass to form the terrestrial planets are continued for 483 another 120 Myr. Levison et al. (2015b) found that the small mass of Mars is a natural outcome 484 of their model because the efficiency of planetesimals to grow via pebble accretion decreases 485 with distance from the star. The key assumption of this work is the local formation of pebbles 486 that contributed to the mass of planetesimals that went on to form the terrestrial planets via 487 planetesimal mergers. It is based on observations that show the composition of outer Solar 488 System material to be too distinct to have contributed much to the terrestrial planets as well 489 as the fact that the flux of pebbles necessary to form the giant planets (Levison et al., 2015a) 490 is too great to form the terrestrial planets. The assumption of local pebble formation over 491 time is, however, rather peculiar and deviates from the more common assumption used in 492 many studies (including ours) that the pebbles originate in the outer Solar System. 493

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

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

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

In the next subsection we will describe how pebble accretion works for planetesimals of different sizes and a minor but important modification to our numerical code that we inherited from Matsumura et al. (2017). This is followed by a description of the initial conditions of our simulations and the simulation outcomes. The content that we will henceforth present is currently in preparation for submission to a peer-reviewed journal.

### <sup>537</sup> 2.2 Pebble accretion onto planetesimals

#### 538 2.2.1 Basic formulation

<sup>539</sup> Based on the formulation of Ormel and Klahr (2010) and Ormel and Kobayashi (2012) and <sup>540</sup> modified by Ida et al. (2016), the accretion rate of cm-sized pebbles onto a planetesimal of mass M and located at distance r from the central star is derived to be

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

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

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

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

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

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

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

<sup>561</sup> The Stokes number itself is given by

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

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

$$\rho_{\rm g} = \frac{\Sigma_{\rm g}}{\sqrt{2\pi}H_{\rm g}},\tag{2.6}$$

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

$$\lambda = \frac{\mu m_{\rm H}}{\sigma_{\rm H_2} \rho_{\rm g}},\tag{2.7}$$

where  $\mu$  is the mean molecular weight of the gas (mostly hydrogen),  $m_{\rm H}$  is the mass of a hy-

 $_{569}$  drogen atom (mostly that of the proton), and  $\sigma_{
m H_2}$  is the collisional cross section of a hydrogen

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

571 Kobayashi, 2012)

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

<sup>572</sup> where the quantity  $\mathcal{S}^*$  is defined as

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

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

$$\eta = \frac{1}{2} h_{\rm g}^2 \left| \frac{\mathrm{d} \ln P}{\mathrm{d} \ln r} \right|. \tag{2.10}$$

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

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

578 and

$$h_{\rm peb} = \left(1 + \frac{S}{\alpha_{\rm t}}\right)^{-1/2} h_{\rm g},\tag{2.12}$$

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

#### 583 2.2.2 Application to small planetesimals

According to Ormel and Klahr (2010) pebble accretion causes rapid growth onto planetesimals with diameters of ~ 200 km or greater. To understand how pebble accretion works on small(er) bodies the question becomes which of the paths in the min() statements in Equations 2.1, 2.3, 2.9 and 2.11 dominate.

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

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

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

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

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

#### <sup>632</sup> 2.2.3 The role of the snow line and fragmentation

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

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

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

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

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

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

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

<sup>686</sup> Without fragmentation (right column of Fig. 2.1) only planetesimals with  $M \gtrsim$ <sup>687</sup>  $3 \times 10^{-5} M_{\rm E}$  ( $D \gtrsim 500$  km) will efficiently accrete pebbles, with a slight dependence on <sup>688</sup> their initial location in the disc; everything smaller will barely accrete anything (large purple <sup>689</sup> region in the left part of the panels in the right column of Fig. 2.1). Fragmentation, on the <sup>691</sup> other hand, allows for the creation of a narrow annulus of large bodies between 0.8 au to at <sup>691</sup> most 1.5 au whose exact extent depends on the time of the formation of the planetesimals <sup>692</sup> 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  $M_{\rm f}$  of planetesimals after a phase of pebble accretion as a function of their initial mass  $M_{\rm i}$  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  $\log(D/1 \text{ km}) = \frac{1}{6} \log(M/1 M_{\rm E}) + 3.597$ , so that  $M/M_{\rm E} = 10^{-5}$  corresponds to D = 580 km.

reach inside 0.75 au so accretion inside of this distance can be inefficient if planetesimals are 693 predominantly small ( $D \leq 300$  km) and formed late ( $t_{\text{off}} \gtrsim 1$  Myr). In our fiducial model the 694 snow line is at 1.2 au when  $t+t_{off} = 1$  Myr, and it passes 2 au by the time  $t+t_{off} = 0.44$  Myr, thus 695 substantial pebble accretion in the terrestrial planet region can only occur if planetesimals 696 form very early and/or form large. In the asteroid belt region accretion generally stops really 697 early on, at a time comparable to the formation age of the iron meteorites, and possibly before 698 most chondrule formation ages - typically about 1.5 Myr (Luu et al., 2015) - because of the 699 rapid inward migration of the snow line. Beyond 2 au accretion is generally insubstantial for 700 small planetesimals. 701

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

<sup>709</sup> In essence, we investigate the growth of a disc of planetesimals that is subjected to a flux of <sup>710</sup> inward drifting pebbles ( $\rho_{peb} = 1000 \text{ kg m}^{-3}$ ,  $R_{peb} = 10 \text{ cm}$ ) originating from a pebble front <sup>711</sup> located in the outer Solar System beyond the orbit of Jupiter (e.g., Lambrechts and Johansen, <sup>712</sup> 2014; Ida et al., 2016) over the lifetime of the gas disc.

#### 713 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 714 detailed prescriptions given in Appendix B.1. The gas disc is a steady accretion disc with a 715 constant value for  $\alpha$  (viscosity parameter; Shakura and Sunyaev, 1973). The temperature of 716 the disc depends on two heating sources, i.e., viscous dissipation or stellar irradiation, which 717 dominate at different regions of the disc. Equations describing the disc temperature profiles 718 Eq. B.4 due to the aforementioned heating sources are obtained from empirical fits to the 719 disc model of Garaud and Lin (2007). The thermal structure of the disc in turn determines 720 the scale height and surface density. 721

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  $\dot{M}_F(t = t_0)$  in the simulation. It also plays a role in computing the subsequent values of  $\dot{M}_*(t)$  and  $\dot{M}_F(t)$  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  $\dot{M}_F =$  $10^{-4} M_E \text{ yr}^{-1}$ .

#### 734 2.3.2 Pebble accretion

The pebble accretion formulation we use in this work is based on previous studies that have 735 developed and refined the formulation (e.g., Ormel and Klahr, 2010; Ormel and Kobayashi, 736 2012; Ida et al., 2016), and studies which applied it to the formation of the giant planets in 737 our Solar System and found success in building the cores of giant planets quick enough to 738 allow gas envelope accretion before the dissipation of the gas (e.g., Lambrechts and Johansen, 739 2012, 2014). We apply the equations derived by Ida et al. (2016) for the pebble accretion rate at 740 different locations in a steady state accretion disc while taking into account the various prop-741 erties of the gas disc (e.g., temperature, surface density, scale height). We chose to use this 742 particular pebble accretion formulation for its simplicity and elegance, and because it does 743 not invoke any additional assumptions (such as was done by Levison et al., 2015b; Johansen 744 et al., 2021). 745

The pebbles are assumed to have originated in the outer regions of the protoplane-746 tary disc where most of the solids (dust) are located (e.g., Youdin and Shu, 2002; Garaud, 2007; 747 Birnstiel et al., 2012). In this region, sub-micron-sized dust grains can grow into pebbles be-748 cause their growth timescale is much shorter than their migration timescale and the collision 749 rate is low (Birnstiel et al., 2012). Upon reaching a critical size (or a critical Stokes number), 750 the migration timescale becomes comparable to the growth timescale and the pebbles com-751 mence their inward migration towards the Sun by virtue of gas drag (Ida et al., 2016). Due 752 to the strong radial dependence of the growth timescale, there will be a location in the disc 753 where dust clumps have just reached pebble size and start to migrate inwards. This is known 754 as the pebble formation front and it moves outwards with time until it reaches the outer edge 755 of the protoplanetary disc (Lambrechts and Johansen, 2014; Ida et al., 2016), after which the 756 pebble flux is severely reduced because all the solids in the disc have been consumed (e.g., 757 Chambers, 2016; Sato et al., 2016). 758

We implemented the pebble accretion prescriptions of Ida et al. (2016) into the N-759 body code based on that presented in Matsumura et al. (2017). We do not directly compute 760 the growth of planetesimals by accretion of physical pebbles, but instead compute their mass 761 increase based on the pebble flux at their respective locations in the disc. Pebble accretion 762 onto planetesimals occurs outside in, that is, planetesimals at the outer edge of our solid disc 763 are the first to encounter the pebbles. They will accrete a fraction of the pebbles, reducing the 764 pebble flux by a factor of  $1 - \dot{M}_{\rm p} / \dot{M}_{\rm F}$ . The planetesimals that are next in line will see a reduced 765 pebble flux and the amount of pebbles they can accrete is computed from the reduced pebble 766 flux. Furthermore, when a planetesimal (or more accurately, planetary embryo) reaches its 767 pebble isolation mass  $M_{\rm p,iso} \sim 1/2 (h_{\rm g}/r)^3 M_*$  we assume that its accretion stops and pebbles 768 are prevented from flowing past its orbit to other planetary bodies residing closer to the Sun. 769 We assume that pebbles were fragmented (or sublimated) into grains of 1 mm when they 770 cross the snow line on their path towards the Sun (Morbidelli et al., 2016). We also study the 771 outcome of excluding this effect. 772

#### 773 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°,1°), respectively. The remaining orbital angles (longitude of ascending node  $\Omega$ , argument of periapsis  $\omega$  and mean anomaly *M*) are assigned values between 0° and 360°, also randomly chosen from a uniform distribution. The semi-major axis of the planetesimals ranges from 0.5 au < *a* < 2.0 au and they are
distributed according to an  $r^{-1}$  surface density profile. Our choice to limit the outer edge of the solid disc to 2 au is guided by the analytical results in Fig. 2.1 and our intent to save computation time (our simulations contain a fairly large number of planetesimals and they are all self-gravitating). Furthermore, planetesimals smaller than  $D \leq 500$  km located beyond 2 au are not expected to grow by much (Fig. 2.1), whereas for bodies with diameter larger 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  $T_{1 \text{ au}} = 200 \text{ K}$ , 250 K, and 300 K.

$M_{\rm disc,i}~(M_{\rm E})$	D (km)	$N_{ m plt}$	
$3  imes 10^{-4}$	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	$\sim 2000$	

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

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

1000 km (e.g., Chambers, 2010; Johansen et al., 2014; Klahr and Schreiber, 2020), with a size-797 frequency distribution that follows a shallow power law  $N(>D) \propto D^{-1.8}$  for diameter, 798 corresponding to  $N(> M) \propto M^{-0.6}$  for mass (e.g., Johansen et al., 2015; Simon et al., 2016; 799 Schäfer et al., 2017; Abod et al., 2019). Models of the collisional evolution of the asteroid belt 800 also suggest that the primordial asteroids were typically 100 km in diameter (Morbidelli et al., 801 2009). The combined results of these studies suggest that the initial planetesimal population 802 likely consisted of many small planetesimals and a few massive bodies. Vesta could be one 803 of the early-formed massive bodies at the tail end of the distribution. 804

In addition to the planetesimal disc, following the work of Brasser and Mojzsis 805 (2020) our initial set-up also includes a 0.01  $M_{\rm E}$  planetary embryo placed at 5.2 au that would 806 eventually become Jupiter. When Jupiter reaches its pebble isolation mass (20  $M_{\rm E}$ ; Lam-807 brechts et al., 2014) in about 1 Myr (Kruijer et al., 2017), it starts to open a partial gap in 808 the disc around its orbit that prevents pebbles from beyond its orbit to spiral in towards 809 the Sun, effectively shutting off the pebble flux to the inner Solar System (Lambrechts et al., 810 2014), although particles with sizes  $\lesssim 100 \ \mu m$  are still able to pass through unobstructed 811 (Paardekooper and Mellema, 2006). 812

<sup>813</sup> We employ the SyMBA *N*-body code (Duncan et al., 1998) modified to include a <sup>814</sup> pebble accretion subroutine (described in Section 2.2; Matsumura et al., 2017) and all the <sup>815</sup> additional effects described in this paragraph to carry out our simulations. For each value <sup>816</sup> of  $M_{\text{disc},i}$  we ran one simulation for each permutation of initial conditions (disc temperature <sup>817</sup>  $T_{1 \text{ au}}$ , fragmentation on/off, migration on/off). In total we ran 60 simulations. The simulations <sup>818</sup> 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 819 the accretion of pebbles by computing the ratio of the final mass of the planetesimal disc ver-820 sus its initial mass  $M_{\rm disc,f}/M_{\rm disc,i}$ . For the more massive discs ( $M_{\rm disc,i} \ge 0.05 M_{\rm E}$ ), the larger 821 planetesimals will accrete pebbles efficiently and they can grow to large masses quickly, as we 822 will show in the following section. Therefore, the final disc mass for these cases do not only 823 reflect growth via pebble accretion, but also additional growth due to mergers and gas en-824 velope accretion. However, the additional growth processes from mergers and gas envelope 825 accretion should not affect the cosmochemical outcome and the conclusion of this study. 826

#### 827 2.4 Results

#### 828 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  $(M_{\text{disc. f}}/M_{\text{disc. i}})$ 829 in the region between 0.5 au and 2.0 au plotted with respect to the initial disc mass and the 830 disc temperature in Fig. 2.3. We find that the final mass of the solid disc depends mostly on its 831 initial mass. A higher initial disc mass results in a higher final disc mass because these discs 832 have, on average, a higher number of large planetesimals which are more efficient at accret-833 ing pebbles. This result is similar to the outcome of the single-planetesimal computations 834 shown earlier in Fig. 2.1, which illustrates that a planetesimal's accretion regime abruptly 835 transitions from the less efficient geometric regime to the more efficient settling regime when 836 their masses are above a critical threshold given a specific set of gas disc parameters. We also 837 observe a general inverse correlation between the amount of mass increase and the initial 838 temperature of the gas disc because (1) for hotter discs the scale height is higher and this 839 lowers the pebble accretion efficiency (Ida et al., 2016), and (2) the snow line is on average 840 farther away in hotter discs than in cooler discs. 841



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.

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

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

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

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

We show the results of  $M_{\text{disc},i} = 0.1 M_{\text{E}}$  with fragmentation effects included (rows 3 and 4 of Fig. 2.4) as they are representative of the outcomes for the higher-mass disc ( $M_{\text{disc},i} \ge$ 0.05  $M_{\text{E}}$ ) simulations. Other than the difference in the amount of growth in the disc, there are no obvious differences in the mass versus semi-major axis distribution of solids in discs 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 inside-out growth trend for the higher-mass discs. This could be due to the discs containing

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



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.



#### 921 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 922 distribution in the disc to determine how much mass is accreted in each section of the disc. 923 We divided the inner disc into bins of size 0.1 au each and computed the initial and final 924 mass in each bin. The results for discs containing small planetesimals with  $D \leq 300$  km and 925 the inclusion of fragmentation and migration effects (corresponding to the top-left panel of 926 Fig. 2.3) are shown in Fig. 2.6. We observe a trend of inside-out growth: planetesimals closer 927 to the Sun accrete, on average, more mass than those in the region further away (see also 928 the top two rows of Fig. 2.4). The amount of mass accreted also has a dependence on the 929 initial disc mass and the disc temperature, as discussed in the previous subsection. The same 930 inside-out growth trend is also observed for the other simulations using the same initial disc 931 masses with migration effects excluded and thus we opted to not show them. We do not 932 show the results for the simulations with fragmentation effects excluded because the growth 933 is insignificant. 934

<sup>935</sup> We also computed the value of  $M_{\rm disc,f} - M_{\rm disc,i}$  in each bin with the results shown <sup>936</sup> in Fig. 2.7. In this plot we clearly see the semi-major axis dependence of the amount of mass <sup>937</sup> accreted by the planetesimals. Therefore, if the solid disc is composed of planetesimals with <sup>938</sup>  $D \leq 300$  km and the disc is not disturbed by mergers and migration, its isotopic composition <sup>939</sup> will naturally show a gradient.

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

For the case of more massive discs (with  $M_{\text{disc},i} \ge 0.05 M_{\text{E}}$ ), 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  $(M_{\text{disc},\text{f}} - M_{\text{disc},\text{i}})$  in each section of the disc. Shown here are the results for discs containing small planetesimals  $(M_{\text{disc},\text{i}} = 3 \times 10^{-4} M_{\text{E}} \text{ and } 1 \times 10^{-3} M_{\text{E}})$  at different initial temperatures, with both fragmentation and migration effects included.

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

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

We have seen in Fig. 2.3 that excluding the effects of fragmentation, i.e., allowing the pebbles to retain their size and mass when crossing the snow line into the inner regions of the disc, results in a general increase in the total mass of the discs. Compared to the case when fragmentation effects are implemented, the amount of mass increase is higher regardless of the disc temperatures and whether migration effects are included. In Fig. 2.11 we observe a distinct peak in the region within 0.5 au across all disc temperatures because of the inward migration of large planetesimals. There is no obvious gradient between 0.5 and 1.2 au, the inside-out growth trend is completely masked by the concentration of large bodies in the inner region of the disc. When both fragmentation and migration effects are excluded, the trend of inside-out growth became apparent once again, in addition to the spikes and peaks beyond 1.5 au and the overall larger mass increase in the whole disc (Fig. 2.12).

In this and the previous subsection, we show that pebble accretion can generate a mass gradient in the terrestrial planet region. This mass gradient does not, however, necessarily translate into a corresponding gradient in composition. A composition gradient is feasible only if the total mass added by pebbles does not exceed the original mass of the planetesimal disc, otherwise the composition of the disc becomes almost uniform and dominated 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 ( $M_{\text{disc,i}} = 0.05 M_{\text{E}}$ , 0.10  $M_{\text{E}}$ , and 0.05  $M_{\text{E}}$ ) at different initial temperatures, with both fragmentation and migration effects included.



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



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

# 986 2.5 Discussion

#### 987 2.5.1 Jupiter's capacity as a pebble barrier

From the observed isotopic dichotomy among iron meteorites and chondrites that sample 988 the inner and outer Solar System, it is thought that the two reservoirs should have been 989 separated very early and remain separated for at least a few Myr (Kruijer et al., 2017). The 990 means to sustain the separation of the inner and outer Solar System has been suggested to be 991 the growth of Jupiter (e.g., Kruijer et al., 2017). The results of a study by Brasser and Mojzsis 992 (2020) showing large amounts of pebbles could flow past Jupiter while it is still growing and 993 contribute to the growth of planetesimals in the inner Solar System depending on the size of 994 the planetesimal and the temperature of the gas disc raise doubts on the capacity of Jupiter 995 as a pebble barrier. 996



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 Brasser and Mojzsis (2020) in that that 997 planetesimals with D > 300 km in the region around Mars' orbit can grow substantially after 998 the passage of the snow line under special conditions when Jupiter is growing. Planetesimals 999 in this region can grow to large sizes by mergers and, in some cases, gas accretion, thereby 1000 contributing to most of the mass in the disc. In Fig. 2.13 we illustrate this point using growth 1001 curves of selected planetesimals of different sizes initially located beyond 1.2 au in discs of 1002 different temperature. Our selected 350 km planetesimal in a cold disc increased its mass by 1003 90% while a 720 km planetesimal in the same simulation attained sufficient mass to accrete 1004 gas. The swift growth of the larger planetesimal is due to its size and its semi-major axis. 1005 Located in the outer edge of the solid disc, it is one of the first few planetesimals to encounter 1006 the pebble flux. In a hot disc where the pebble accretion efficiency is lower and the snow line 1007 is located farther away, our selected 350 km planetesimal nevertheless managed to increase 1008 its mass by 50% from pebbles while its 700 km counterpart increased its mass by about 400%. 1009

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

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

## 1023 2.5.2 Comparing dynamical outcomes with cosmochemistry data

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

•  $M_{\text{disc},i} \le 1 \times 10^{-3} M_{\text{E}}$ , or if the disc is more massive then all planetesimals have  $D \le 300 \text{ km}$ , and

•  $T_{1 \text{ au}} \ge 250 \text{ K}$ , and

• pebble fragmentation effects at the snow line are unimportant.

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

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

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

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

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

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

The possible compositions of the bulk Silicate Earth (crust and mantle) computed from models based on terrestrial rocks and chondrites (e.g., McDonough and Sun, 1995; Palme and O'Neill, 2014) place it at an end-member location in Fig. 2.14, indicating that the chemical composition of the Earth is unlike any of the known meteorites. An exception is the result of Javoy et al. (2010) (blue square labelled with J10 in the figure) which is obtained by assuming that the Earth is made up entirely of enstatite chondrites. This result should however be interpreted with caution as a more recent study examining the  $\delta^{30}$ Si and Mg/Si composition of the Earth showed that it is similar to the enstatite chondrites isotopically but not chemically
 (Dauphas et al., 2015).

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

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

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

One possible way out of this impasse is to do a similar end-member study by estimating the contribution of CI or CO chondrites to the composition of the terrestrial planets using our isotope mixing models. We show in Fig. 2.15 (which is akin to Fig. 1.2) the computed best-fit composition of the Earth and Mars as a combination of enstatite chondrites, ordinary chondrites and CI or CO chondrites using the Monte Carlo mixing model algorithm described in Appendix A. With only CI or CO chondrites, the mixing model returns the maximum contribution of these chondrite types as  $\leq 10\%$ , similar to the results obtained by including various other types of carbonaceous chondrites (Fig. 1.2). For both planets the contribution from H-chondrites is most strongly affected by the choice of either CI or CO. Thus, even if we were to assume a time-dependent variation in the composition of the pebbles from CO-like at the beginning to CI-like at the end (or vice versa), it still remains difficult for our *N*-body simulation results to be reconciled with meteorite isotope and elemental ratio data of the inner planets: the amount of outer Solar System materials added to the terrestrial planets *cannot* be more than 10%!

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



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

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

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

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

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

# 3 Formation of the inner Solar System bodies

# 1216 3.1 Introduction

In the previous chapter we showed using cosmochemical trends and N-body simulations that 1217 the isotopic gradients in the inner disc were more likely to have been established via mech-1218 anisms like the accretion of nebular material or thermal processing in the disc, rather than 1219 the accretion of outer disc material in the form of cm-sized pebbles. Since the contribution 1220 of the pebble accretion mechanism to the growth of planetesimals in the inner disc is very 1221 minor, it should thus be more likely the case that the terrestrial planets (and possibly the 1222 larger asteroids) are products of collisional mergers among the inner disc planetesimals in-1223 stead. Furthermore, when the planetary bodies in the inner disc were growing, the isotopic 1224 gradients should have remained unperturbed as is reflected in their correlated bulk isotopic 1225 compositions and semi-major axes (Yamakawa et al., 2010). 1226

What, then, is the preferred formation pathway of the planetary bodies in the inner 1227 disc? Previous works that studied the Grand Tack (Walsh et al., 2011) and classical (Chambers, 1228 2001) models to determine the feeding zones of the terrestrial planets found that the terrestrial 1229 planet feeding zones are very similar – wide with a large overlapping region – for the Grand 1230 Tack model (Brasser et al., 2017; Woo et al., 2018) whereas they are more localised and display 1231 a weak but nevertheless existent correlation with semi-major axis for the classical model (e.g., 1232 Raymond et al., 2004; O'Brien et al., 2006; Fisher and Ciesla, 2014; Kaib and Cowan, 2015; Woo 1233 et al., 2018). These results are verified with new high-resolution GPU simulations (Woo et al., 1234 2021). Given that the isotopic gradients are present in the inner disc during the formation 1235 of the inner Solar System bodies, the distinct isotopic compositions of Earth, Mars and Vesta 1236 therefore points to a classical-model-like formation pathway for these planetary bodies. 1237

The major difference between the Grand Tack model and the classical model is that 1238 the former features an early gas-driven migration of Jupiter and Saturn while the latter does 1239 not. It turns out that this feature exerts a strong influence on the feeding zone outcomes. The 1240 migration of the gas giants causes the material in the inner disc to mix and thus homogenising 1241 any pre-existing isotopic differences (Carlson et al., 2018). It is therefore not surprising that 1242 the terrestrial planets that formed within the framework of the Grand Tack model have very 1243 similar feeding zones and isotopic compositions because they all accreted from the same 1244 homogenised mixture. If the gas giants did not migrate into the terrestrial region when 1245 the terrestrial planets were forming, as in the classical model, then it is more likely for the 1246 terrestrial planets to be isotopically distinct. However, the widely-known downside of the 1247 classical model is that its Mars analogues are systematically a few times too massive to be 1248 consistent with the current Mars unless the surface density slope is much steeper (Izidoro 1249 et al., 2015). We therefore need to seek out other dynamical models that can reproduce Mars 1250 with the correct mass without invoking the migration of the gas giants. 1251

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

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

# 1267 **3.2 Methodology**

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• Venus: 0.4  $M_{\rm E} < M <$  1.2  $M_{\rm E}$ , 0.55 au <  $a_{\rm f} <$  0.85 au 1390 - Earth: 0.5  $M_{\rm E} < M <$  1.5  $M_{\rm E},$  0.85 au  $< a_{\rm f} <$  1.15 au 1391 • Mars: 0.05  $M_{\rm E} < M < 0.15 M_{\rm E}$ , 1.3 au  $< a_{\rm f} < 1.7$  au 1392

1394

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

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

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

$$a_{\text{weight}} = \frac{\sum_{i}^{N} M_{i} a_{i}}{\sum_{i}^{N} M_{i}},$$

$$\sigma_{a_{\text{weight}}} = \sqrt{\frac{\sum_{i}^{N} M_{i} \left(a_{i} - a_{\text{weight}}\right)^{2}}{\frac{N-1}{N} \sum_{i}^{N} M_{i}}},$$
(3.2)

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

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

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

• Hungaria: 1.7 au  $< a_{\rm f} < 2.1$  au

• Vesta: 2.1 au <  $a_{\rm f}$  < 2.5 au

• Hebe: 2.2 au  $< a_{\rm f} < 2.6$  au

We relax the constraint on the final masses of the asteroid analogues as we are more interested in the range of their initial semi-major axis. This does not affect the outcomes and the conclusions that we will draw for the study because the number of asteroid analogues larger than the mass of planetesimals (=  $0.001 M_E$ ) in our Grand Tack model simulations only constitutes ~ 21% of the total while the fraction is a mere 0.6% - 1% for the classical model and 0.01 - 1.1% for the depleted disc model.

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

## 1430 3.3 Results

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

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

Most of the terrestrial planets produced in the simulations are generally less massive 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  $r_{dep} = 1.5$  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).

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

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

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

r <sub>dep</sub>	Mass depletion scale	Ν	ñ	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%

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.

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

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

$$AMD = \frac{\sum_{k} \mu_{k} \sqrt{a_{k}} \left[ 1 - \sqrt{\left(1 - e_{k}^{2}\right)} \cos I_{k} \right]}{\sum_{k} \mu_{k} \sqrt{a_{k}}},$$
(3.3)

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

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

The third is the fraction of total mass in the largest planet of the system  $S_{\rm m}$ , and the last is the mean orbital spacing statistic  $S_{\rm H}$ , given by

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

We use the mutual Hill sphere as the spacing unit for  $S_{\rm H}$ , following Brasser et al. (2016).

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

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

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

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

#### <sup>1490</sup> 3.3.3 Depleted disc model: Terrestrial planet feeding zones

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

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

For some Mars analogues, however, the same feeding zone trend does not apply. We observe a spread in the feeding zones of our Mars analogues and some of them deviate from the trend. For example, the Mars analogues in the simulations with a 75% mass depletion beyond  $r_{dep} = 1.5$  au have their feeding zones centered around 1.25 au (top middle panel of Fig. 3.4). We examined the evolution of these Mars analogues that deviate from the trend and found that they were formed closer in initially (a < 1.5 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 Brasser (2021).

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

#### **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.

The formation location of asteroid analogues Hungaria, Vesta and Hebe in the Grand Tack, classical, and depleted disc models are shown in Fig. 3.6. In the Grand Tack model, Vesta analogues are equally likely to originate anywhere in the disc between 0.7 au 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 contrast, in the classical model and the depleted disc model, the initial semi-major axes of the Vesta analogues are severely restricted (middle and right panels of Fig. 3.6). The probability of Vesta analogues originating from between 2.1 au to 2.5 au is 84% for the classical model and 30% for the depleted disc model. The reason for the lower probability in the depleted disc model is due to the gas drag exerted on the planetesimals by the gas disc in the first 5 Myr of the simulations. The eccentricity damping effect still causes the planetesimals to migrate inwards when the gas was present. Consequently, most of the Vesta analogues (68% of the total) in the depleted disc model originate from the region between 2.5 au and 2.7 au.

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

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

# 1547 **3.4 Discussion**

### <sup>1548</sup> 3.4.1 Comparison with the Grand Tack and classical models

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



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 underwent 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).

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

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

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

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


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).

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

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

We find  $OVL_{DD} = 0.79$  for the depleted disc model, and  $OVL_{GT} = 0.89$  for the Grand Tack model.

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

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



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	l (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	

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

Given the results of the two statistical tests we conducted (OVL, K-S test), we conclude that the predictions of the depleted disc model comports best with the isotopic compositions measured for the Earth and Mars. In this model, the feeding zones of the terrestrial planets show a clear correlation with semi-major axis. Earth and Mars would accrete material from different regions in the protoplanetary disc and they can end up with different final mixtures of building material with the presence of isotopic gradients in the disc. This is in stark contrast with the the Grand Tack model which predicts identical isotopic compositions for Earth and Mars.

#### 1638 3.4.2 Implications for Venus' isotopic composition

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

$$\varepsilon_{\rm V} = \frac{a_{\rm V} - a_{\rm E}}{a_{\rm M} - a_{\rm E}} \times \varepsilon_{\rm M},\tag{3.7}$$

where the subscripts V, E and M refer to Venus, Earth and Mars, respectively. We computed the nominal values of the isotopic anomalies of Venus using the current semi-major axes of 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  $\Delta^{17}$ 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),  $\varepsilon^{50}$ Ti from Trinquier et al. (2009); Zhang et al. (2011, 2012), and  $\varepsilon^{54}$ Cr from Shukolyukov and Lugmair (2006); Trinquier et al. (2007, 2008); Qin et al. (2010a,b); Yamashita et al. (2010); Larsen et al. (2011); Petitat 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 Brasser (2021).

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

	Nominal	Monte Carlo	$ \epsilon_V - \epsilon_E  >  \epsilon_E - \epsilon_M $
$\Delta^{17}O$	-0.23	$-0.12^{+2.69}_{-2.74}$	50%
$\epsilon^{50} Ti$	0.29	$0.26^{+3.37}_{-3.43}$	48%
$\epsilon^{54}Cr$	0.10	$0.07^{+1.20}_{-1.19}$	49%

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.

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

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

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

#### 1681 3.5 Conclusions

We examined the masses, orbital configurations, and feeding zones of the terrestrial planets formed in the framework of the depleted disc model by running a large number of *N*-body simulations with different initial conditions and including the effects of a dissipating gas disc during the first few Myr of the simulations. We found that the model outputs planets that are less massive than the current terrestrial planets if we assume a MMSN surface density for the solids in the protoplanetary disc, but the model is successful nevertheless in producing planets with low mass in the region near Mars' orbit. Increasing the initial surface density of
 the solids in the protoplanetary disc by 1.5 to 2 times the MMSN value will resolve the deficit
 in the terrestrial planets' mass.

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

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

## **4** Summary and future work

#### **4.1** The thesis in brief

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

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

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

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

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

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

#### **Future directions** 4.21782

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

 Protoplanetary disc models: Since the construction of plausible planet formation mod-1785 els is dependent on the current understanding of protoplanetary disc models, it would 1786 be useful to delve into the study of protoplanetary discs. A good understanding of 1787 protoplanetary discs could for example aid in understanding how, when and where 1788 planetesimals form in the disc and the expected size-frequency distribution of the plan-1789 etesimals (e.g., Chambers, 2010; Johansen et al., 2014). 1790

• High-resolution simulations: N-body simulations run on graphics processing units 1791 (GPU) could achieve higher resolution with shorter computing time. Re-examining 1792 the current terrestrial planet formation models with N-body codes written for GPUs 1793 (e.g., GENGA; Grimm and Stadel, 2014) could push the current limits and perhaps re-1794 veal new information (e.g., Woo et al., 2021). 1795

1766

Cosmochemistry data: The building blocks of the Earth remain an unresolved puzzle.
 Accurate determination of isotopic anomalies and elemental abundances of a wide variety of meteorite samples with high-precision equipment coupled with modelling of geochemical and geophysical processes could help in cracking the code.

 Stellar/Galaxy cluster evolution: On a larger scale, the abundances of short-lived radionuclides (SLR) in our Solar System obtained from models of the evolution of the Sun's birth cluster (e.g., Fujimoto et al., 2018; Portegies Zwart et al., 2018) can be compared to the measured abundances of the daughter isotopes that are radioactive decay products of the SLRs. These models could perhaps be employed to study the distribu-

tion of nucleosynthetic isotopes in different regions of the protoplanetary disc.

#### Monte Carlo mixing model Α

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

#### A.1 Model inputs 1815

TABLE A.1: Measured  $\Delta^{17}$ O,  $\varepsilon^{50}$ Ti,  $\varepsilon^{54}$ Cr,  $\varepsilon^{62}$ Ni and  $\varepsilon^{92}$ 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  $\varepsilon^{62}$ Ni which we source from the compilation of Burkhardt et al. (2017).

	$\Delta^{17}O$ $\epsilon^{50}Ti$		$\epsilon^{54}Cr$	$\epsilon^{62}$ Ni	$\epsilon^{92}$ Mo
Mars	$0.27 \pm 0.03$	$-0.54\pm0.17$	$-0.19 \pm 0.04$	$0.040\pm0.022$	$0.20 \pm 0.53$
EL	$-0.01\pm0.07$	$-0.28\pm0.06$	$0.06 \pm 0.04$	$-0.025 \pm 0.044$	$0.30\pm0.74$
EH	$-0.03\pm0.10$	$-0.10\pm0.02$	$0.04\pm0.08$	$0.026 \pm 0.021$	$0.36\pm0.43$
Н	$0.72 \pm 0.05$	$-0.61\pm0.17$	$-0.38 \pm 0.03$	$-0.065 \pm 0.044$	$0.78 \pm 0.26$
L	$1.03\pm0.04$	$-0.63\pm0.02$	$-0.39\pm0.07$	$-0.051 \pm 0.020$	$0.61\pm0.62$
LL	$1.19\pm0.06$	$-0.65\pm0.04$	$-0.43\pm0.04$	$-0.076 \pm 0.013$	$0.87 \pm 1.13$
CI	$0.39 \pm 0.10$	$1.83\pm0.09$	$1.57\pm0.03$	$0.198 \pm 0.057$	$0.82 \pm 0.41$
CO	$-4.32\pm0.26$	$3.76\pm0.66$	$0.75\pm0.21$	$0.113 \pm 0.018$	$2.00 \pm 1.40$
CV	$-3.62\pm0.48$	$3.64 \pm 0.29$	$0.87\pm0.04$	$0.103\pm0.038$	$2.59\pm0.67$
СМ	$-2.92\pm0.04$	$3.01\pm0.09$	$1.10\pm0.18$	$0.095 \pm 0.030$	$5.71\pm0.94$
CR	$-1.48\pm0.55$	$2.35\pm0.04$	$1.32\pm0.08$	$0.095\pm0.035$	$3.00 \pm 1.80$
Angrites	$-0.11\pm0.11$	$-1.15\pm0.02$	$-0.41\pm0.09$	$0.028 \pm 0.082$	$-0.14\pm0.75$

<sup>1816</sup> 

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

	O (mg/g) Ti ( $\mu$ 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	
СМ	432	580	3.05	12.0	1500	
CR	420	647	3.75	13.6	1210	
Н	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.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).

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).

	0		Ti		Cr		Ni		Мо	
	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

three distinct stages. The inputs for our mixing model are summarised in Tables A.1, A.2 and A.3.

### **A.2** Governing equations

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

$$\varepsilon_{\text{mantle,comp}} = \sum_{j} X_{j} \frac{\sum_{i} f_{i,j} C_{i} \varepsilon_{i}}{\sum_{i} f_{i,j} C_{i}}, \qquad (A.1)$$

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

In our model, Eq. A.2 is decomposed into two parts, representing the contribution
 by EL chondrites, and all reservoirs other than EL chondrites. The corresponding equations

1835 are

$$\varepsilon_{\rm EL} = \sum_{j} X_{j} \frac{f_{j,\rm EL}C_{\rm EL}\varepsilon_{\rm EL}}{f_{j,\rm EL}C_{\rm EL} + (1 - f_{j,\rm EL})\sum_{i} f_{i,j,\rm nEL}C_{i,\rm nEL}},$$

$$\varepsilon_{\rm nEL} = \sum_{j} X_{j} \frac{(1 - f_{j,\rm EL})\sum_{i} f_{i,j,\rm nEL}C_{i,\rm nEL}\varepsilon_{i,\rm nEL}}{f_{j,\rm EL}C_{\rm EL} + (1 - f_{j,\rm EL})\sum_{i} f_{i,j,\rm nEL}C_{i,\rm nEL}},$$
(A.2)

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

$$\sigma_{\varepsilon_{\rm EL}} = \sum_{j} X_{j} \frac{f_{j,\rm EL}C_{\rm EL}}{f_{j,\rm EL}C_{\rm EL} + (1 - f_{j,\rm EL})\sum_{i} f_{i,j,\rm nEL}C_{i,\rm nEL}},$$

$$\sigma_{\varepsilon_{\rm nEL}} = \sum_{j} X_{j} \frac{(1 - f_{j,\rm EL})\sum_{i} f_{i,j,\rm nEL}C_{\rm EL}}{f_{j,\rm EL}C_{\rm EL} + (1 - f_{j,\rm EL})\sum_{i} f_{i,j,\rm nEL}C_{i,\rm nEL}},$$
(A.3)

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

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

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

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

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

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

### 1844 A.3 Model algorithm

The first step of the computation concerns the initialisation of the isotopic compositions (Eq. A.2), their corresponding uncertainties (Eq. A.3 and A.4) and the chi-square values (Eq. A.5). 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  $f_{i,j,\text{nEL}} = 0$ . With these initial values we compute  $\varepsilon_{\text{mantle,comp}}$  or  $\varepsilon_{\text{mantle,comp}}$  and  $\chi^2_{\text{old}}$ .

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

$$f_{i,j,\text{new}} = f_{i,j,\text{old}} + 0.005z_1,$$
  

$$f_{i,j,\text{new}} = f_{i,j,\text{old}} + 0.005z_2,$$
(A.6)

where  $z_1$  and  $z_2$  are given by

$$z_1 = \sqrt{-2\log u} \sin(2\pi v),$$
  

$$z_2 = \sqrt{-2\log u} \cos(2\pi v).$$
(A.7)

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

$$0 \le f_{j,\text{EL}} \le 1,$$
  

$$0 \le f_{i,j,\text{nEL}} \le 1,$$
  

$$\sum_{i} f_{i,j,\text{nEL}} \le 1.$$
(A.8)

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

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

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

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



#### **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.

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

• Earth =  $(52 \pm 6)\%$  EC +  $(36 \pm 4)\%$  OC +  $(12 \pm 2)\%$  CC

• Mars =  $(53 \pm 9)\%$  EC +  $(45 \pm 8)\%$  OC +  $(2 \pm 1)\%$  CC

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

1880

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

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

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

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

## **B** Numerical methods

#### **B.1** Gas disc model

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

$$\dot{M}_* = 3\pi\alpha\Sigma_{\rm g}H_{\rm g}^2\Omega_{\rm K},\tag{B.1}$$

where  $\Sigma_{\rm g}$  is the gas surface density,  $H_{\rm g}$  is the disc scale height and  $\Omega_{\rm K}$  is the Keplerian frequency. The disc  $\alpha$ -viscosity  $\alpha$  was set to  $10^{-3}$  and assumed to be constant throughout (Shakura and Sunyaev, 1973). It is given by

$$\alpha = \nu / (c_s^2 \Omega_{\rm K}), \tag{B.2}$$

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

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

<sup>1914</sup> where the extra 0.1 Myr was added to avoid the logarithmic singularity (Bitsch et al., 2015).

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

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

where  $T_{0\nu}$  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

$$\alpha_3 \equiv \frac{\alpha}{10^{-3}},\tag{B.5}$$

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

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

$$h_{\rm g,vis} = 0.034 \left(\frac{T_{0\nu}}{200 \,\mathrm{K}}\right)^{1/2} \alpha_3^{-1/10} \dot{M}_{*8}^{1/5} \left(\frac{r}{1 \,\mathrm{au}}\right)^{1/20},$$

$$h_{\rm g,irr} = 0.029 \left(\frac{r}{1 \,\mathrm{au}}\right)^{2/7}.$$
(B.7)

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

$$\Sigma_{\rm g,vis} = 1320 \left(\frac{T_{0\nu}}{200 \text{ K}}\right)^{-1} \alpha_3^{-4/5} \dot{M}_{*8}^{3/5} \left(\frac{r}{1 \text{ au}}\right)^{-3/5} \text{ g cm}^{-2},$$
  

$$\Sigma_{\rm g,irr} = 1785 \alpha_3^{-1} \dot{M}_{*8} \left(\frac{r}{1 \text{ au}}\right)^{-15/14} \text{ g cm}^{-2}.$$
(B.8)

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

$$\left(\frac{\mathrm{d}\ln P}{\mathrm{d}\ln r}\right)_{\mathrm{vis}} = \frac{51}{20},$$

$$\left(\frac{\mathrm{d}\ln P}{\mathrm{d}\ln r}\right)_{\mathrm{irr}} = \frac{39}{14}.$$
(B.9)

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

$$r_{\rm vis/irr} = \left(\frac{T_{0\nu}}{150\,\rm K}\right)^{70/33} \alpha_3^{-14/33} \dot{M}_{*8}^{28/33} \\\approx 1.84 \,\alpha_3^{-14/33} \dot{M}_{*8}^{28/33} \,\rm{au}.$$
(B.10)

#### **B.2** Disc-induced orbital evolution

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

$$\frac{\gamma\Gamma}{\Gamma_0} = \frac{\Gamma_{\rm C}}{\Gamma_0} F_{\rm C} + \frac{\Gamma_{\rm L}}{\Gamma_0} F_{\rm L} \tag{B.11}$$

where  $\Gamma_{\rm C}$  and  $\Gamma_{\rm L}$  are the corotation and Lindblad torques respectively (Paardekooper et al., 2011) and

$$\Gamma_0 = \left(\frac{M}{M_*}\right)^2 h_{\rm g}^{-2} \Sigma_{\rm g} \Omega_{\rm K}^2 \tag{B.12}$$

is a normalisation constant. The factors  $F_{\rm L}$  and  $F_{\rm C}$  are defined as (Cresswell and Nelson, 2008; Fendyke and Nelson, 2014)

$$\ln F_{\rm C} = -\frac{e}{e_{\rm f}},$$

$$\frac{1}{F_{\rm L}} = P_e + \text{sign}(P_{\rm e})(0.07\hat{I} + 0.085\hat{I}^4 - 0.08\hat{e}^2\hat{I}^2),$$
(B.13)

where  $e_{\rm f} = 0.01 + \frac{1}{2}h_{\rm g}$ ,  $\hat{e} = e/h_{\rm g}$ ,  $\hat{I} = \sin(I)/h_{\rm g}$  and

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

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

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

<sup>1943</sup> where the wave timescale is (Tanaka and Ward, 2004)

$$t_{\rm wav} = \left(\frac{M_*}{M}\right) \left(\frac{M_*}{\Sigma_{\rm g} R^2}\right) h_{\rm g}^4 \Omega_K^{-1}.$$
 (B.15)

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

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

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

$$\tau_{\rm mig,1} = -\frac{t_{\rm wav}\Gamma_0}{h_g^2\Gamma},\tag{B.17}$$

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

$$\tau_{\rm mig,2} = \frac{2R^2}{3\nu} \max\left(1, \frac{M}{2\pi\Sigma_{\rm g}R^2}\right). \tag{B.18}$$

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

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

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

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

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

$$au_{\rm KH} = 10^9 \left(\frac{M}{M_{\rm E}}\right)^{-3} \,{\rm yr.}$$
(B.20)

This process of runaway gas accretion is bounded by the gas accretion rate throughout the disc  $\dot{M}_*$ . Gas accretion ceases when the Hill radius of the planet is approximately equal to that of the disc scale height. Taking all these effects into account, the gas accretion rate ontothe planetary core is written as

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

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

$$\dot{M}_{\rm g,B} = \frac{4\pi \rho_{\rm g} G^2 M^2}{c_{\rm s}^3},$$
 (B.22)

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

# C Depleted disc model simulations with higher solid surface density

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

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

As the planets are now more massive on average, we observe an increase in the values of  $S_{\rm m}$  and  $S_{\rm H}$  (top panel of Fig. C.3). The results for the concentration parameter  $S_{\rm c}$  and AMD of the terrestrial planet systems are, however, similar to the outcomes for simulations with MMSN surface density (bottom panel of Fig. C.3).

We also find the same trend of correlated feeding zones with semi-major axis for the Venus and Earth analogues and a large variation in the feeding zones of Mars analogues (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  $S_{\rm m}$  versus the mean spacing parameter  $S_{\rm H}$  in units of the mutual Hill sphere. Bottom panel: Mass concentration parameter  $S_{\rm c}$  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 an 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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