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# Sensitivities of Earth's core and mantle compositions to accretion and differentiation processes

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#### ABSTRACT

The Earth and other terrestrial planets formed through the accretion of smaller bodies, with their core and mantle compositions primarily set by metal-silicate interactions during accretion. The conditions of these interactions are poorly understood, but could provide insight into the mechanisms of planetary core formation and the composition of Earth's core. Here we present modeling of Earth's core formation, combining results of 100 N-body accretion simulations with high pressure-temperature metal-silicate partitioning experiments. We explored how various aspects of accretion and core formation influence the resulting core and mantle chemistry: depth of equilibration, amounts of metal and silicate that equilibrate, initial distribution of oxidation states in the disk, temperature distribution in the planet, and target:impactor ratio of equilibrating silicate. Virtually all sets of model parameters that are able to reproduce the Earth's mantle composition result in at least several weight percent of both silicon and oxygen in the core, with more silicon than oxygen. This implies that the core's light element budget may be dominated by these elements, and is consistent with  $\leq 1-2$  wt% of other light elements. Reproducing geochemical and geophysical constraints requires that Earth formed from reduced materials that equilibrated at temperatures near or slightly above the mantle liquidus during accretion. The results indicate a strong tradeoff between the compositional effects of the depth of equilibration and the amounts of metal and silicate that equilibrate, so these aspects should be targeted in future studies aiming to better understand core formation conditions. Over the range of allowed parameter space, core and mantle compositions are most sensitive to these factors as well as stochastic variations in what the planet accreted as a function of time, so tighter constraints on these parameters will lead to an improved understanding of Earth's core composition.

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## 1. Introduction

The metal-silicate differentiation of the Earth, which occurred simultaneously with accretion, was the primary determinant of the Earth's modern-day core and mantle compositions. During the planet's formation, accretion of material occurred through energetic impacts, causing large-scale melting on the Earth and generating a partial or global magma ocean. Metal from impactors equilibrated with molten silicate at high pressures (P) and temperatures (*T*) before being segregated into the growing core. These high *P*-*T* reactions set the compositions of the core and mantle, which today provide geochemical and geophysical signatures of the core formation process.

One signature of this process is Earth's core density, which is  $\sim$ 10% lower than that of iron under the same *P*-*T* conditions, due to the presence of lighter elements such as Si, O, S, C, and/or H (e.g., Birch, 1952; Poirier, 1994; McDonough, 2003) that primarily entered the core during its formation. Density and sound velocity measurements of Fe alloys can be compared to the core's properties to put upper bounds on its light element abundances, such as ~8 wt% O or ~11 wt% Si (e.g., Fischer et al., 2011, 2014; Sata et al., 2010; Zhang et al., 2014; but also cf. Badro et al., 2015, and references therein), but the relative proportions of light elements in the core remains an open question. The core's light element composition relates to the devolatilization and redox history of the planet's interior, as well as Earth's bulk elemental and isotopic composition. These elements influence the core's thermal structure, crystal structures and anisotropy, thermal conductivity, and





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convection and magnetic field generation (e.g., Fischer et al., 2013; McDonough, 2003; Nimmo, 2007).

To constrain the relative proportions of light elements in the Earth's core and gain insight into the core formation process on terrestrial planets, here we combine N-body accretion simulations with experimental metal-silicate partitioning data to model core formation. Previous studies have combined N-body simulations with condensation models to calculate bulk planetary compositions (Bond et al., 2010; Elser et al., 2012) without consideration of core formation, or modeled core formation using a prescribed growth scenario to describe Earth's accretion (e.g., Badro et al., 2015; Rubie et al., 2011), which is less realistic than using accretion simulations due to the highly stochastic nature of accretion and which may not be representative of Earth's formation. Many studies imposed a constant or variable oxygen fugacity  $(fO_2)$  instead of allowing it to evolve as a consequence of partitioning (e.g., Badro et al., 2015; Siebert et al., 2012, 2013; Wade and Wood, 2005; Wood et al., 2014). Rubie et al. (2015) were pioneering in their fusion of accretion simulations and core formation modeling, utilizing six simulations run under the Grand Tack paradigm (Walsh et al., 2011) and allowing planetary oxygen fugacity to evolve selfconsistently. They predicted a core composition of 8-9 wt% Si and 2-4 wt% O, and varied the initial compositions of planetary building blocks to best reproduce the composition of the Earth's mantle.

Here we take a different approach, using forward modeling to explore how different aspects of Earth's accretion and core formation influence the resulting core and mantle compositions. We take advantage of recent advances in metal-silicate partitioning experiments to higher pressures and temperatures (e.g., Bouhifd and Jephcoat, 2011; Fischer et al., 2015; Siebert et al., 2012, 2013) and in N-body simulations, utilizing a large number of simulations (Fischer and Ciesla, 2014) to statistically analyze the results. Our goal is not to find one set of model parameters that best reproduces the Earth, due to the many inherent uncertainties involved, but rather to explore these uncertainties by assessing the effects of accretion and differentiation on the resulting planetary composition. In this way, we can evaluate which of these processes exert the most influence on planetary chemistry and are the least well-constrained, so that future experimental and numerical studies may be better targeted.

We begin by describing the numerical methodology (Section 2), then the resulting core and mantle compositions (Section 3) and the effects of different aspects of accretion and core formation (Section 4). These results are discussed in terms of tradeoffs, constraints, and sensitivities to various processes; limitations of the modeling; and future directions (Section 5), followed by concluding remarks (Section 6).

### 2. Methods

From the 100 N-body simulations of Fischer and Ciesla (2014), 73 Earth analogues were identified, defined as planets with final semimajor axes of 0.75-1.25 AU and masses within a factor of 1.5 of an Earth mass  $(M_{\oplus})$ . These high-resolution simulations were run with Jupiter and Saturn on either their modern-day orbits (Eccentric Jupiter and Saturn, EJS) or more circular orbits, as predicted by the Nice Model (e.g., Tsiganis et al., 2005) (Circular Jupiter and Saturn, CJS). The initial conditions were similar to those of previous studies (e.g., Raymond et al., 2009). For more details on these simulations, see the Supplemental Text or Fischer and Ciesla (2014). Fischer and Ciesla (2014) reported a lack of correlations between most Solar System observables, indicating that any simulations that form a realistic Earth analogue can provide a plausible accretion history for the Earth, even if they do not match every other aspect of the Solar System. Fig. 1 illustrates the types of information about Earth's accretion history that can be gleaned from these sim-



**Fig. 1.** Examples of information about the Earth's accretion history that can be obtained from *N*-body simulations. Bottom panel: Mass evolution of the Earth analogue as a function of time from three example simulations (dotted black, solid medium gray, and dashed light gray lines correspond to different simulations). Top panel: Initial semimajor axis of each body accreted by the Earth analogue in two of the same simulations (black and medium gray); the third simulation is not shown for clarity. Large filled circles: Moon- to Mars-mass planetary embryos. Small open circles: planetesimals (~0.001  $M_{\oplus}$ ).

ulations, showing the Earth analogue's mass (bottom panel) and the initial semimajor axis of everything it accretes (top panel) as a function of time in a few simulations chosen as illustrative examples.

Each body in every simulation was assigned an initial composition based on its initial semimajor orbital axis. These compositions were calculated by equilibrating a CI chondrite enriched in refractory elements at 0.1 GPa and 2000 K, with the oxygen content varied to reach a specified  $fO_2$ . Starting compositions are presented in Table S1. With each impact that the Earth analogue experienced, its pressure distribution was recalculated. The incoming metal and silicate were equilibrated by first calculating their major element compositions, then their trace element compositions, then the resulting metal and silicate were added to the core and mantle. This process was repeated for each body that the Earth analogue accreted.

Equilibration occurred at a fixed fraction of the target's coremantle boundary (CMB) pressure at the time of impact and the mantle liquidus temperature at that pressure (Andrault et al., 2011). The methodology for the chemical model was inspired by that of Rubie et al. (2011), in which oxygen fugacity evolved selfconsistently as the Earth grew as a consequence of metal-silicate partitioning, as opposed to being imposed. Partitioning was based on experimentally-determined metal-silicate partition coefficients (Fischer et al., 2015, and references therein), including new fits to data from P < 5 GPa (Supplemental Text; Table S2). Equilibrated metal and silicate compositions were calculated using mass balance equations and equations of the form:

$$\log_{10}(K_D^i) = a_i + \frac{b_i}{T} + \frac{c_i P}{T}$$
<sup>(1)</sup>

for each element *i*, where *T* is in Kelvin, *P* is in GPa, and  $a_i$ ,  $b_i$ , and  $c_i$  are fitting parameters from Fischer et al. (2015) (Table S2).

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