BRIEF FOLLOW-UP ON RECENT STUDIES OF THEIA’S ACCRETION
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ABSTRACT

Kaib and Cowan (2015) recently used terrestrial planet formation simulations to conclude that the moon-forming impactor (Theia) had only a ~5% or less chance of having the same oxygen isotope composition as Earth, while Mastrobuono-Battisti et al. (2015) used seemingly similar simulations and methods to arrive at a higher value of ~20% or more. Here we derive the results of both papers from a single set of simulations. Compared to Kaib and Cowan (2015), the analysis of Mastrobuono-Battisti et al. (2015) systematically yields more massive Theia analogs and imposes flatter $\Delta^{17}O$ gradients across the original protoplanetary disk. Both of these effects diminish isotopic differences between Earth and Theia analogs. While it is notoriously difficult to produce systems resembling our actual terrestrial planets, the analysis of Kaib and Cowan (2015) more often selects and analyzes Earth and Mars analogs at orbital locations near the real planets. Given this, we conclude that the greater isotopic differences between Earth and Theia found in Kaib and Cowan (2015) better reflect the predictions of terrestrial planet formation models. Finally, although simulation uncertainties and a terrestrial contribution to Moon formation enhance the fraction of Theia analogs consistent with the canonical giant impact hypothesis, this fraction still remains in the 5–8% range.

1. BACKGROUND

The canonical giant impact formation scenario for Earth’s moon predicts that a Mars-mass body, Theia, struck the proto-Earth in a glancing blow which threw material into orbit around Earth and eventually coalesced into the Moon (Hartmann and Davis 1975; Cameron and Ward 1976). Hydrodynamical modeling of this collision has since shown that the Moon should consist of ~60–90% of material from Theia, with the rest coming from the proto-Earth (Canup 2004; Reufer et al. 2012). Yet the Moon’s oxygen isotope composition is virtually identical to Earth ($\Delta^{17}O \lesssim 0.015\%$) even though the isotopic compositions of nearly all meteorites differ significantly from the Earth (Wiechert et al. [2001]; Herwartz et al. 2014). In particular, Mars has a $\Delta^{17}O$ of 0.32%. Because simulations of terrestrial planet formation predict that each large rocky body has a wide and stochastic feeding zone, it has been suggested that terrestrial planet formation is unlikely to produce an Earth and Theia that are isotopically similar if other bodies (i.e. Mars) are isotopically distinct (Pahelevan and Stevenson 2007).

Terrestrial planet formation simulations are an excellent tool to verify whether we should expect a large compositional difference between Earth and its major impactors. These simulations model the assembly of systems of terrestrial planets via the accretion of ~100–1000 km-sized objects in orbit about the Sun (Raymond et al. 2014). Two recent independent works used suites of these simulations to statistically quantify compositional differences between Earth analog planets and their last major impactors (Theia analogs) (Kaib and Cowan 2015; Mastrobuono-Battisti et al. 2015). While very similar simulations were used, they arrived at significantly different probabilities that Theia’s isotopic composition was similar to that of the Earth (and Moon). Kaib and Cowan (2015) (hereafter referred to as KC15) concluded that there was a $\lesssim 5\%$ chance that Theia’s isotopic composition was similar enough to the Earth’s to yield a Moon that had the Earth’s observed isotopic composition. On the other hand, Mastrobuono-Battisti et al. (2015) (hereafter referred to as MPR15) found a probability of $\gtrsim 20\%$.

In this brief follow-up work, we report the cause of this discrepancy. The main differences between the assumptions used in KC15 and MPR15 are: (1) the criteria used to select Earth and Mars analog pairs used to calibrate the initial $\Delta^{17}O$ distribution in each simulation, and (2) the criteria employed to select Earth and Theia analog pairs used to determine the oxygen isotopic difference between Earth and Theia in each simulation. In KC15, Earth analogs are required to have masses over 0.5 $M_{\oplus}$ and orbits between 0.8 and 1.2 AU, while Mars analogs are assumed to be the next planet outward with a mass larger than 0.05 $M_{\oplus}$. Once the Earth-Mars analog pair is selected, the accretion history of the inner planet (the Earth analog) is searched for an impactor with a mass larger than 0.1 $M_{\oplus}$. If such an impactor exists, the last of these is designated a Theia analog, and this body’s feeding zone is compared against the Earth analog. The isotopic composition of the Earth and Theia analogs is then calculated by imposing a $\Delta^{17}O$ gradient on the original planetesimals that yields a $\Delta^{17}O$ of 0.32% between the Earth analog and the Mars analog.

Meanwhile, MPR15 place more emphasis on planet ordering than orbital elements or planet mass to select Earth-Mars analogs. In systems that form 4 or more planets, the 3rd and 4th planets are assumed to represent Earth and Mars, respectively, while in 3-planet systems, Earth and Mars are taken to be the 2nd and 3rd planets. These Earth-Mars pairs are selected regardless of their masses or orbits. These planet pairs are then used to set the primordial $\Delta^{17}O$ gradient just as in KC15. Next, any planet in the system is searched

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The separations of the mean formation distances for Earth and Mars analog pairs are always fixed at 0.32 AU, the $\Delta^{17}O$ gradient imposed on the initial disk of planetesimals is completely dependent on the separation between the mean formation distance of the Mars analog and the mean formation distance of the Earth analog. A larger separation will produce a flatter gradient, which will in turn yield a smaller difference between the Earth’s and Theia’s isotopic composition (they are identical if the gradient is completely flat). In many instances, the 4th planet of simulated systems (the Mars analog under the MPR15 criteria) orbits well beyond 2 AU. This often leads to orbital separations of over $\sim1$ AU between the Earth and Mars analogs used to set the $\Delta^{17}O$ gradient in MPR15.

If these widely separated planets also have widely separated mean formation distances, we might expect that some of the success cases of MPR15 come from systems with unusually flat $\Delta^{17}O$ gradients. In fact, MPR15 explored the effects of employing steeper $\Delta^{17}O$ gradients in their Extended Data Table 2 and found a significant decrease in the fraction of isotopically Earth-like Theia analogs if the disk $\Delta^{17}O$ gradients were increased by 25%. In addition, we find a correlation coefficient of 0.72 when we compare the mean formation separations with the final orbital separations for the MPR15 Earth-Mars pairs. Given this, we may expect that the widely separated Earth-Mars pairs of MPR15 will in fact have widely separated mean formation distances, resulting in flat $\Delta^{17}O$ gradients.

The separations of the mean formation distances for Earth-Mars pairs selected with the KC15 and MPR15 criteria are shown in Figure 2. As expected, we see that the Earth-Mars pairs selected by the MPR15 prescription have a long tail to very high separations not seen among
the Earth-Mars pairs selected with the KC15 criteria. As mentioned previously, performing the MPR15 analysis on our simulations yields 10 instances where Theia’s $|\Delta^{17}O|$ is less than or equal to the Moon’s. As Figure 2 shows, 6 of these 10 instances have Earth-Mars pairs that lie in the tail of very high Earth-Mars separations, which require flat $\Delta^{17}O$ gradients. This suggests that the different distributions of Earth-Mars analog formation distances is a primary reason for the increased likelihood that Theia has an Earth-like isotopic composition in MPR15.

The large separations between the mean formation distances of Earth analogs and Mars analogs seem to only occur in systems where at least one of the two analog planets has a very small mass. In Figure 3 we plot the formation distance separation against the minimum planet mass of each Earth-Mars pair. Here we see that the separation between Earth’s and Mars’ formation distance is only above 1 AU if at least one of the analog planets has a mass well below 0.1 $M_{\oplus}$. These very low mass planets are comprised of one to a few particles, and it has been shown that individual particles can migrate very large distances during terrestrial planet formation. This causes the large formation distance separations and the flat $\Delta^{17}O$ gradients that are consequently imposed. If we only consider cases where both Earth and Mars analogs have masses above 0.06 $M_{\oplus}$ (approximately the smallest planetary mass seen in our Solar System) then the fraction of MPR15 Theia analogs with $|\Delta^{17}O| < 0.015\%$ drops to just 3% (1 out of 31 cases), nearly the same as the KC15 results.

It should be noted, however, that Mars analogs should in fact be substantially smaller than the Earth analogs, and no such requirement was made in KC15. If we use the KC15 Earth-Mars pairs and now require that the Earth analog is at least twice as massive as the Mars analog, our usable sample of simulations drops from 53 to 18. Of these 18 systems, we still only have one Theia analog with $|\Delta^{17}O| < 0.015\%$ (a 5.5% success rate), and the median value of $|\Delta^{17}O|$ actually increases slightly (0.16% vs. 0.18%). Thus, the results of KC15 do not seem to be due to having selected Mars analogs that are unrealistically massive.

### 2.1. Simulation Uncertainties

The stochastic nature of planet formation is well captured by numerical experiments: if a simulation is repeated with virtually identical initial conditions, planets form at different locations and have different feeding zones. This introduces an uncertainty in the results of any individual simulation, and is precisely the reason that KC15 and MPR15 ran large ensembles of simulations to quantify the likelihood of the Moon-forming impact.

The “granular” nature of N-body simulations also introduces an uncertainty in the planetary composition. Our simulations contain 1000 planetesimals to represent small bodies, but the real number may have been orders of magnitude higher during Solar System formation. The feeding zone of each simulated protoplanet is likely constructed from a much smaller number of planetesimals than in the actual solar system.

Granularity is a consequence of computational limitations and can artificially skew our results. Even if the true feeding zones of a Theia analog and an Earth analog were identical, our simulations could result in a non-zero $|\Delta^{17}O|$ due to the small number of simulated planetesimals. Alternatively, the coarse mass resolution of our simulations could produce two planets with nearly identical compositions where a higher-resolution simulation would have shown that they have significantly different feeding zones.

Disentangling granularity error from natural stochasticity is difficult. MPR15 estimate the uncertainty in each simulated major body’s mean formation distance using the standard error of the mean (SEM). The SEM values for Earth and Theia analogs are then added in quadrature and translated to a $\Delta^{17}O$ uncertainty. When simulated $|\Delta^{17}O|$ values are below 0.015%+ the SEM uncertainty, MPR15 deem that the simulation successfully explained the Moon’s isotopic composition. This only makes sense, however, if one presumes that the feeding zones of Earth and Theia are inherently identical and that simulation granularity artificially increased compositional differences.

We instead estimate the granularity error of our sim-
ulations by resampling each major body’s planetesimal distribution via bootstrap. If a simulated planet accreted $N$ planetesimals from different semi-major axes, then we draw $N$ times from that planetesimal distribution, with the possibility of repeated selections. This produces a new distribution of $N$ planetesimals. By repeating this process 1000 times for each body, we generate a distribution of feeding zone locations for each simulated body. Bodies made of a few planetesimals from disparate semi-major axes will have higher variance than bodies built from many nearby planetesimals. The standard deviation of the feeding zone location for each body is an estimate of the granularity uncertainty, and is typically within a few percent of the SEM value.

We only perform bootstrapping and SEM for distributions of planetesimals, which are all equal-mass particles. The number of simulated embryos is comparable to expected number in the real solar system, so our embryo population should not suffer from the granularity issues. It is not clear whether or not MPR15 make a distinction between embryos and planetesimals in their SEM calculations.

We use bootstrap resampling to predict—for each simulation—the probability that the feeding zones yield a Theia analog with $|\Delta^{17}O| \leq 0.015\%$. For each individual set of Earth-Mars-Theia feeding zones, we use bootstrap resampling to generate a distribution of 1000 $\Delta^{17}O$ gradients and $\Delta^{17}O$ values for each individual simulation. We then sum up the total probability that $|\Delta^{17}O| < 0.015\%$ for our ensemble of simulated Theia analogs. Unlike the raw simulation results, these results will account for the coarse mass resolution of our simulations. This analysis predicts a $\sim 4.8\%$ probability that Theia will have $|\Delta^{17}O| < 0.015\%$. This number is 2.5 times larger than the predictions of our raw simulation results, but still significantly smaller than the prediction of MPR15.

Finally, it is worth noting that both SEM and bootstrap resampling implicitly assume that each accreted object represents an independent sample of a protoplanet’s “true” underlying feeding zone. During accretion, however, small bodies often merge with each other before being accreted onto even larger bodies. Since much of a protoplanet’s feeding zone is derived from conglomerations of associated bodies, the initial locations of accreted planetesimals are likely correlated. It is therefore possible that neither SEM nor bootstrapping properly quantifies the uncertainty arising from using too few planetesimals.

2.2. Earth’s Contribution to the Moon

In KC15, it was assumed that lunar material is almost entirely derived from Theia instead of the Earth. In reality, Earth always contributes some fraction of material toward the Moon’s assembly. In the canonical giant impact hypothesis, the Earth fraction is typically around 15–25% ([Campl 2004]). In alternative scenarios, such as hit-and-run collisions, high velocity impacts, or very massive impactors, the terrestrial fraction of the Moon’s material can exceed 40% ([Reufer et al. 2012], [Cuk and Stewart 2012]). Considering a significant terrestrial contribution to the Moon’s mass allows Theia analogs with larger $|\Delta^{17}O|$ values to explain the Moon’s isotopic composition since the $|\Delta^{17}O|$ will be scaled down by the compositional fraction that Theia provides (1 minus the terrestrial fraction) when Theia material is incorporated into the Moon. In Figure 4, we examine how the fraction of Theia analogs that successfully explain the lunar isotopic composition varies as we consider greater contributions from the Earth. Using our $|\Delta^{17}O|$ values generated from bootstrap resampling, we find that our Theia success rate moves from 4.8% to 8.4% as we consider Earth contributions up to 40% of the Moon’s mass. When looking at the raw simulation data instead of our resamplings, one finds an increase from $\sim 2\%$ with no terrestrial contribution up to $\sim 0.5\%$ if the Earth supplies 40% of the Moon’s material.

Unlike KC15, MPR15 did consider scenarios in which the Moon had a significant terrestrial component and found that a terrestrial contribution of 40% could increase the success rate of Theia analogs up to 25% or 55%, depending on whether their SEM-derived uncertainties were being considered. As shown in Figure 4C, KC15 finds success rates that are significantly lower than either of these values. We attribute this difference to the Earth, Mars, and Theia analog selection criteria employed in KC15 vs MPR15.

3. DISCUSSION AND CONCLUSIONS

Although recent terrestrial planet formation models have shown more promise in producing Martian analogs ([Walsh et al. 2011], [Izidoro et al. 2014]), many of the simulations employed in KC15 and MPR15 have difficulty reproducing the low mass of Mars ([Raymond et al. 2009]). Because of this, it is not obvious how to designate Earth and Mars analogs. However, we believe the KC15 criteria are more self-consistent for several reasons. First, the target of the moon-forming collision is always required to be the same planet used in calibrating the initial $\Delta^{17}O$ of simulation particles, whereas the target planets selected under the criteria of MPR15 often orbit inside Venus’ orbit. In addition, to minimize simulation resolution effects, MPR15 require Theia analogs to be accreted from at least 50 particles, while the median Theia analog in KC15 is comprised of 33 particles. However, this 50-particle limit forces Theia analogs to always have larger
masses than that predicted in the canonical giant impact hypothesis. Finally, although the masses of Mars analogs are often too large in KC15, all of the simulations that are used in this work have a planet orbiting near 1.5 AU, just as the Solar System does, and this is used to calibrate the initial $\Delta^{17}$O distribution. Meanwhile, the Earth-Mars pairs selected with the MPR15 criteria can often orbit in the 2-3 AU region and have masses similar to or less than Mercury, something unseen in our Solar System. Flawed as these simulations may be at replicating the detailed structure of the inner Solar System, they do predict that the last major impactor on a massive planet near 1 AU is quite unlikely to have the same isotopic composition as the planet itself, when there is also a planetary mass body near 1.5 AU with a Mars-like composition.

MPR15 correctly point out that the feeding zones derived from terrestrial planet formation simulations are artificially influenced by the mass resolution of simulations. This increases the uncertainty in feeding zone locations, and hence $\Delta^{17}$O values. When we account for this uncertainty, the fraction of Theia analogs capable of explaining the Moon’s isotopic similarity to the Earth increases from 2% to 4.8%. Accounting for the possibility that the Moon could contain up to 40% terrestrial material further increases the successful fraction of Theia analogs to 8.4%. However, this is still well below the ~50% success rates reported by MPR15. Given this, we conclude that standard models of the final assembly of terrestrial planets predict there is a ~5% chance that the canonical giant impact hypothesis can account for the isotopic composition of the Moon.

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