Driven by Affect to Explore Asteroids, the Moon, and Science Education

by

Jude Viranga Dingatantrige Perera

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Graduate Supervisory Committee:

Erik Asphaug, Co-Chair
Steven Semken, Co-Chair
Ariel Anbar
Linda Elkins-Tanton
Mark Robinson

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ABSTRACT

Affect is a domain of psychology that includes attitudes, emotions, interests, and values. My own affect influenced the choice of topics for my dissertation. After examining asteroid interiors and the Moon's thermal evolution, I discuss the role of affect in online science education. I begin with asteroids, which are collections of smaller objects held together by gravity and possibly cohesion. These "rubble-pile" objects may experience the Brazil Nut Effect (BNE). When a collection of particles of similar densities, but of different sizes, is shaken, smaller particles will move parallel to the local gravity vector while larger objects will do the opposite. Thus, when asteroids are shaken by impacts, they may experience the BNE as possibly evidenced by large boulders seen on their surfaces. I found while the BNE is plausible on asteroids, it is confined to only the outer layers. The Moon, which formed with a Lunar Magma Ocean (LMO), is the next topic of this work. The LMO is due to the Moon forming rapidly after a giant impact between the proto-Earth and another planetary body. The first 80% of the LMO solidified rapidly at which point a floatation crust formed and slowed solidification of the remaining LMO. Impact bombardment during this cooling process, while an important component, has not been studied in detail. Impacts considered here are from debris generated during the formation of the Moon. I developed a thermal model that incorporates impacts and find that impacts may have either expedited or delayed LMO solidification. Finally, I return to affect to consider the differences in attitudes towards science between students enrolled in fully-online degree programs and those enrolled in traditional, in-person degree programs. I analyzed pre- and post-course survey data from the online astrobiology course Habitable Worlds. Unlike their traditional program counterparts, students enrolled in online programs started the course with better attitudes towards science and also further changed towards more positive attitudes during the course. Along with important conclusions in three research fields, this work aims to demonstrate the importance of affect in both scientific research and science education.

DEDICATION

To all wanderers who are striving to find their way home

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Chapter 1

INTRODUCTION

> We shall not cease from
> exploration...
>
> *T. S. Eliot*

Why do we explore? When the word “we” is used to mean human beings in general, one could argue that “we” are naturally inquisitive and collectively seek out the unknown as suggested by T.S. Elliot. But why do “we” as individuals explore? What is our motivation? What gets us started? Of course the answers to those questions will vary from person to person. Yet, I assert that those answers will often be grounded in affect (a domain of psychology that includes attitudes, emotions, interests, and values). Here, while introducing my research topics I will also describe how affect largely influenced my decision to pursue those lines of research.

Chapter 2 examines how the interiors of asteroids, the leftover small bodies from the early planet formation process, may evolve over time. Most asteroids are likely “rubble-piles” (i.e. a collection of objects held together by gravity and possibly cohesion). Due to their considerable age and orbital evolution, asteroids would have experienced many impacts that broken them apart. When that occurred, mutual gravity between constituent particles would have re-accumulated the particles that did not escape. Thus, their rubble-pile nature is the result of the repeated break up and re-accumulation process. The degree to which a particular asteroid is a rubble-pile may vary depending on its bombardment history, with some consisting of a monolith along with rubble, while others may be completely rubble. Interestingly, the rubble-pile nature of asteroids would mean that they should behave like granular materials. Granular material, such as sand, have many interesting properties. For instance, we know that sand can behave like a solid when we lay down on the beach but it can also flow like a liquid when poured out of a bucket.

One effect of granular material that is particularly pertinent to asteroids is the Brazil Nut Effect (BNE). The BNE is when a collection of contained particles, of nearly the same density but of different sizes, sort themselves by size due to repeated shaking or a series of jolts. The effect is named after Brazil nuts, which, generally being larger than other nuts, are often found at the top of a can of mixed nuts. The effect is that smaller objects migrate parallel to the local gravity vector, while larger objects migrate in the opposite direction. Though a consensus has not been reached, there are two proposed mechanisms that explain why the BNE occurs. One is that repeatedly shaking a collection of objects creates voids that are more easily filled by the smaller particles. Thus, over time this allows the smaller particles to migrate parallel to the local gravity vector. The other mechanism explains that repeatedly shaking a collection of particles will set up granular convection cells that trap larger particles away from the local gravity vector. It is possible that one mechanism is more prominent in certain situations or that both occur simultaneously. Regardless of the mechanism, it is plausible that the BNE may occur on asteroids. This is further supported by large boulders seen on the surfaces of asteroids. Nevertheless, past experiments and computer simulations have mainly focused on studying the BNE in vertical containers. Those conditions are rather different from that of asteroids particularly since particles on asteroids are not interacting with a wall but rather other particles. Thus, for a more realistic demonstration of the BNE as it applies to asteroids, in this work I ran computer simulations to show the BNE on an asteroid-like simulated body. I find that while the BNE is plausible on asteroids, it is likely limited to the outer layers. For asteroids that are mostly or completely made of rubble, this would leave asteroids with an interior region that has a mixture of particles sizes and an exterior that is sorted with larger objects near the surface.

This project began incidentally while I was working on a different project related to asteroids. At that time Erik Asphaug had suggested that I use the Discrete Element Modeling (DEM) code, PKDGRAV, for that work. PKDGRAV models spherical particles that can bounce, experience friction and be drawn to each other due to gravity. It is a code that is often used for asteroid research since it is suitable to model asteroids that are made of rubble.

During my research, I found past works to often cite the BNE as a possibility on asteroids. When I first started learning about the BNE, it was clear that though a number of previous works had studied it in detail, no one had simulated it using a three-dimensional self-gravitating collection of particles. I was intrigued. Since I knew that PKDGRAV was capable of doing such a simulation, I set off exploring if the BNE would actually happen on such a simulated body. When I first saw the movie of the BNE taking place on the simulated asteroid, I was captivated. It worked! It had begun with "I wonder what would happen if..." and it had produced an interesting result. I was not following particular instructions that said such a simulation would be beneficial. I was simply exploring on my own because I was interested in what would happen. Affect helped get the rubble shaking.

Chapter 3 discusses the thermal evolution of the Moon. The Moon likely formed from the debris generated after a giant impact between the proto-Earth and another planetary body. The accretion of the Moon would have occurred rapidly, which resulted in most of the Moon being molten. Thus, a 1000 km deep Lunar Magma Ocean (LMO) would have existed right after the Moon formed. The first 80% by volume of the LMO would have solidified rapidly (in about 1,000 years according to previous work). Afterwards, some of the solidifying material would have been low-density anorthosite, which would have floated to the surface and formed a conductive lid. That conductive lid would have considerably slowed solidification of the remaining 20% of the LMO. Though the first 80% of the LMO would have solidified in about 1,000 years, due to the conductive lid that formed after that, previous work showed that complete solidification of the LMO would have taken 10 million years (Myr). Impacts onto the Moon during the cooling of the LMO is an important aspect, but it has not previously been considered in detail. Specifically, in this work I consider impacts due to some of the debris that escaped the Earth-Moon system after the giant impact. That debris would have been on heliocentric orbits and subsequently re-impacted the Moon over a period of 100 Myr. Particularly after the conductive lid formed, these re-impacts could have punctured holes. Compared to areas of the conductive lid that did not have holes, the areas with holes would have had a higher thermal flux.

As such the more holes that were punctured into the lid, the more rapid the LMO solidification would have been. Nonetheless, re-impacts also contained significant kinetic energy, which upon impacting the lunar surface would have been converted to thermal energy. If the impacts were efficient at delivering thermal energy to the Moon, then that would have countered the effect of holes by helping to prolong LMO solidification. In this work, I developed a model that thermally evolves the LMO, while at the same time, allowing impacts to puncture holes into the surficial lid and to deliver thermal energy. By varying model input parameters over reasonable ranges, I give a range of possible LMO solidification times and discuss implications for the lunar surface, interior, and orbital evolution.

For years, I have had a particular fixation about the Moon. It started as a child when I saw the movie Apollo 13 and ever since then I have the persistent hope of getting the opportunity to fly there one day. Growing up in a chaotic world, I suppose it is sensible to want to escape to the quietness of the lunar surface. Unfortunately, we have seen that human journeys to the Moon do not happen very frequently, with the last Apollo mission having taken place nearly 45 years ago. Nonetheless, I eventually realized that I need not wait for an opportunity to travel to the Moon. I could explore the Moon with modest resources, often with a pencil, some paper, and a computer. My master's degree research had pertained to the Moon and as I was starting my dissertation research, I could not help but wonder how I may again go back to researching the Moon. Thus, when Alan Jackson mentioned working on research regarding the LMO, almost innately I leaped at the opportunity. It was the Moon. The answer was: of course! Much like my research on asteroid interiors, it was a strong interest about the Moon that got me started with my lunar research. Affect helped start hole puncturing.

Chapter 4 evaluates attitudes towards science of two student populations: those who are enrolled in fully online degree programs and those enrolled in traditional, in-person degree programs. As mentioned earlier, attitudes are a component of affect (a domain of psychology that includes attitudes, emotions, interests, and values). Learning takes place within three domains: affect, cognition, and behavior.

Thus, it is important to learn how students' affect (particularly attitudes in this work) may influence their cognition and behavior as a learner. Past work has often had mixed results when linking the three domains with one another due to the complex ways they interact with each other. One example is the link between positive attitudes and better course grades. While there are a number of studies that show a positive correlation between attitudes and course grades, there are many that do not find a correlation, and even one study showing a negative correlation. Since we know students are influenced by their affect, it is still important to assess those characteristics and to consider which specific aspects of their learning may be influenced by their affect. In this regard, students enrolled in online programs are particularly interesting to study since they are novel. As such it is important to consider how those learners may be similar to and different from their traditional program counterparts. In this work, I analyzed pre- and post-course survey data from three semesters of the online, introductory astrobiology course Habitable Worlds. Using a factor analysis, survey items were placed into latent variables. It was found that online program students started the course with more positive attitudes towards science and they also changed towards more positive attitudes at the end of the course. I consider the implications of this finding and others while making recommendations for future online courses.

This project started due to the requirement that Ph.D. students in our department pursue two distinct research projects. As I was exploring the different research areas of the School of Earth and Space Exploration, I noticed that a few professors were involved with science education research. I was intrigued mainly due to my past experiences with non-scientists' relationships with science. Being a person who adores the field in general, I had been perplexed by the number of people I met who did not understand the scientific process or certain scientific principles. Perhaps worse was meeting people who plainly denied basic scientific principles. Thus, doing research in the process of understanding how I can be a more effective science educator was very appealing to me. While exploring the data generated by the Habitable Worlds course, I was particularly draw towards the work on affect.

My past experiences informed me that people's affect should have some effect on their willingness to learn science. Seeing that further research was needed in that area, I started focusing on students' attitudes towards science. Affect helped me understand its role in science education.

A process that organizes constituent particles of asteroids by their sizes, debris impacting onto the early molten Moon, and attitudes that students hold towards science may appear to be a gallimaufry of research topics. Nevertheless, they are all tied together by affect. I pursued all three topics because of my own interests and inclinations. Like me, I suspect that most researchers pursue research topics that they are passionate about. As such the topic of students' attitudes towards science takes that notion into science education. Much like research is often directed by the affect of researchers, student learning is undoubtedly influenced by their own attitudes, emotions, interests, and values. Therefore, I argue that affect is instrumental both in driving researchers to explore the unknown and driving students towards science education.

Chapter 2

THE SPHERICAL BRAZIL NUT EFFECT AND ITS SIGNIFICANCE TO ASTEROIDS

> If finished planets are the loaves of bread, asteroids are the scraps on the floor of the bakery.
>
> *Erik Asphaug*

Many asteroids are likely rubble-piles that are a collection of smaller objects held together by gravity and possibly cohesion. These asteroids are seismically shaken by impacts, which leads to excitation of their constituent particles. As a result it has been suggested that their surfaces and sub-surface interiors may be governed by a size sorting mechanism known as the Brazil Nut Effect. I study the behavior of a model asteroid that is a spherical, self-gravitating aggregate with a binary size-distribution of particles under the action of applied seismic shaking. I find that above a seismic threshold, larger particles rise to the surface when friction is present, in agreement with previous studies that focused on cylindrical and rectangular box configurations. Unlike previous works I also find that size sorting takes place even with zero friction, though the presence of friction does aid the sorting process above the seismic threshold. Additionally, I find that while strong size sorting can take place near the surface, the innermost regions remain unsorted under even the most vigorous shaking.

2.1 Introduction

Asteroids are small bodies that are remnants of the early planet formation process (Asphaug, 2009). Space missions have imaged certain asteroids and as a result have greatly helped the understanding of asteroid surface properties. However, due to the lack of seismic data, it has been difficult to definitively constrain the internal structure of asteroids.

The understanding of their internal structures is important for planetary science, for future asteroid exploration and mining (Hatch and Wiegert, 2015), and for deterring potential Earth impact hazards (Shapiro *et al.*, 2010).

Previous works have inferred that asteroids 150 m to 10 km in size are likely rubble-pile objects that are a collection of smaller objects held together by gravity and possibly cohesion (Michel *et al.*, 2001; Richardson *et al.*, 2002; Pravec *et al.*, 2002; Sánchez and Scheeres, 2014). This characterization arises from several key observations:

1. Craters on their surfaces and the dynamical evolution of asteroids indicate that asteroids have undergone many impacts over their lifetimes that will have left disrupted, reaccumulated objects (Asphaug *et al.*, 1998; Richardson *et al.*, 2004).
2. Low bulk densities and high macroporosities of asteroids indicate the presence of large internal voids (Carry, 2012).
3. The limited spin rates of asteroids possibly point to loosely held aggregates (Scheeres *et al.*, 2015).
4. Spacecraft images have shown that some asteroids have large boulders that seem to be protruding from their surfaces such as Eros (Asphaug *et al.*, 2001) and Itokawa (Miyamoto *et al.*, 2007; Tancredi *et al.*, 2015).

As a rubble-pile asteroid is being seismically shaken by impacts, its constituent particles should undergo granular flow once frictional forces are overcome. Particularly, the Brazil Nut Effect where larger constituent objects rise to the top against gravity may occur on these rubble-pile asteroids (assuming the constituent objects are approximately the same density). Past work has shown that when a collection of particles of varying sizes is excited, over time larger particles will accumulate at the top given gravity is downward (Rosato *et al.*, 1987). Some large boulders on asteroids could be the result of the Brazil Nut Effect, though this may not be the only mechanism for producing large surface boulders (e.g. Thomas *et al.*, 2001).

The Brazil Nut Effect is a complex phenomenon, but it has been proposed to be mediated through two primary mechanisms:

1. Smaller particles may fill in and pass through spaces created by excitations while larger particles do not (Williams, 1976). If the direction of gravity is downward, this results in smaller particles migrating to the bottom while larger particles are ratcheted upwards.
2. Depending on boundary conditions, excitation of particles may set up granular convection that brings larger particles to the top but prevents them from moving downward (Knight *et al.*, 1993).

The Brazil Nut Effect has been studied in a terrestrial context through computer simulations using hard spheres (i.e. simulated spheres do not deform when forces are applied to them) (Rosato *et al.*, 1987), using soft spheres (i.e. simulated spheres deform when forces are applied to them) (Kohl and Schmiedeberg, 2014), and through experiments in cylindrical columns (Knight *et al.*, 1993). Additionally, in the context of the low-gravity environments of asteroids, simulations have been done using a soft spheres method in rectangular and cylindrical box configurations (Tancredi *et al.*, 2012; Matsumura *et al.*, 2014) and parabolic flight experiments have been done in a cylindrical configuration to momentarily obtain equivalent low-gravity conditions of the Moon and Mars (Güttler *et al.*, 2013).

Previous preliminary work in two-dimensions has suggested that size sorting can occur in self-gravitating aggregates (Sanchez *et al.*, 2010); however, the Brazil Nut Effect has not been studied in a fully three-dimensional configuration. Here I conducted simulations using a spherical, self-gravitating configuration of particles since that configuration is more representative of asteroids. In Section 2.2, I discuss the N-body gravity code that was used (Section 2.2.1) and the initial conditions along with a short discussion of how I created the aggregate that was used for the simulations (Section 2.2.2). In Section 2.2.3 I describe the simulations that were conducted and the section concludes with a discussion of how I compare the simulations to asteroids (Section 2.2.4).

In Section 2.3, I state my results while focussing on the central region of the aggregate (Section 2.3.1), the effect of friction (Section 2.3.2), and the time evolution of particle distributions (Section 2.3.3). In Section 2.4, I discuss the results considering asteroid surface processes (Section 2.4.1), the central region of the aggregate (Section 2.4.2), and the driving mechanism of the Brazil Nut Effect (Section 2.4.3). Finally, I summarize and discuss future work in Section 2.5.

2.2 Method

2.2.1 PKDGRAV

For this work I used PKDGRAV, a parallel N-body gravity tree code (Stadel, 2001) that has been adapted for particle collisions (Richardson *et al.*, 2000; Richardson *et al.*, 2009; Richardson *et al.*, 2011). Originally collisions in PKDGRAV were treated as idealized single-point-of-contact impacts between rigid spheres. I use a soft-sphere discrete element method (SSDEM) to model the collisions of particles. In SSDEM, particles are allowed to slightly overlap with one another. Particle contacts can last many time steps, with reaction forces dependent on the degree of overlap (a proxy for surface deformation) and contact history. The code uses a second-order leapfrog integrator to solve the equations of motion, with accelerations due to gravity and contact forces recomputed each step.

The spring/dashpot model used in PKDGRAV's soft-sphere implementation is described fully in Schwartz *et al.* (2012) and is based on Cundall and Strack (1979). Two overlapping particles feel a Hooke's law type reaction force in the normal and tangential directions determined by spring constants (k_n and k_t). I chose a normal spring constant (k_n) that kept particle overlaps $<1\%$. The choice of a linear spring was made during the original implementation of the soft-sphere code. While a Hertzian spring contact may provide benefits in certain circumstances, the linear spring is adequate for the problem at hand, with the added advantage of simplicity.

In particular, the coefficient of restitution of meter-scale granite spheres has been experimentally found to have no dependence on impact speed for low-speed impacts (Durda *et al.*, 2011), which is suggestive of a linear contact response. User-defined normal and tangential coefficients of restitution used in hard-sphere implementations, ϵ_n and ϵ_t, determine the plastic damping parameters (C_n and C_t), which are required to resolve a soft-sphere collision (see Eq. 15 in Schwartz *et al.* 2012). Frictional forces can also be imposed on the interaction by adjusting static, twisting, and rolling coefficients.

This SSDEM implementation has been validated through comparison with laboratory experiments (e.g., Schwartz *et al.* (2012) and Schwartz *et al.* (2013)). In addition, Ballouz *et al.* (2015) used this SSDEM to model the collisions of rubble-pile asteroids made up of 40 m spheres, and showed that the outcomes of binary collisions were consistent with scaling laws for low- and high-speed collisions. Furthermore, Matsumura *et al.* (2014) studied the classical Brazil Nut Effect for centimeter-sized grains in a cylindrical container using this method.

2.2.2 Initial Conditions

The initial spherical aggregate used in the following simulations was made by creating 500 particles of radius 40 m (colored yellow) and 500 particles of radius 80 m (colored red) that were randomly positioned inside a cubic space of 4 km per side. All particles had a density of 3 g/cm^3. Particles were then allowed to gravitationally collapse due to self-gravity with the coefficients of friction set to zero to form a mixed aggregate and left to settle for 75 simulation hours. The maximum free-fall time of the initial cubic distribution of particles (i.e. from the corners) is around 3 hours.

The aggregate that was created in the process had a mass of 3.62×10^{12} kg, a bulk radius of about 800 m, and a bulk density of about 1.7 g/cm^3. The aggregate properties are representative of common asteroids. The escape speed of the aggregate was 75 cm/s.

In order to properly resolve particle collisions, I use a normal spring constant of

$$k_n = m_p \left(\frac{v_{\max}}{x_{\max}} \right)^2 \tag{2.1}$$

where m_p is the typical particle mass, v_{max} is the maximum expected particle speed, and x_{max} is the maximum expected fractional overlap, which I set to 1% of the typical particle radius. This chosen value of k_n allows all the kinetic energy of the particle collision to be stored in a single spring that compresses to $x_{\max}$. Furthermore, in order to ensure that a collision is properly resolved, I require that particle overlaps last at least 12 time steps for the smallest particles. The length of a single time step can be estimated by considering the oscillation half-period of a spring with normal spring constant k_n (see Eq. 36–38 in Schwartz *et al.* 2012). Using the typical particle sizes, masses, and expected speeds I find that a spring constant of $k_n \sim 4.856 \times 10^9$ kg/s^2 and a time step of 8.523×10^{-2} s are required to properly resolve the collisions in the simulations. The tangential spring constant, k_t, is taken to be equal to $\frac{2}{7} \times k_n$. Tests with one half and one quarter of the chosen time step showed no deviation in behavior demonstrating that the chosen time step is adequate.

Since Matsumura *et al.* (2014) found that the Brazil Nut Effect is largely insensitive to the choice of the coefficients of restitution and since I wanted to focus on the magnitude of seismic shaking and the coefficients of friction, I set the normal coefficient of restitution to 0.2 and the tangential coefficient of restitution to 0.5 for all the simulations. I will further examine the effect of these damping coefficients on the Brazil Nut Effect in a future study.

In Figure 1 I show the likelihood that radial distributions of larger (red) and smaller (yellow) particles were drawn from the same parent population as a function of settling time. A higher probability indicates that it is more likely that the two particle groups were drawn from the same parent population, and thus that their radial distributions are more similar to each other. Probabilities were calculated using a two-sample Kolmogorov-Smirnov (K-S) test. The two-sample K-S statistic quantifies the distance between the cumulative distributions of the two samples (here the number of particles within a radius r), which determines the probability that the two samples are drawn from the same underlying distribution.

The utility of the K-S test lies in the fact that it is a non-parametric test, and so allows me to make no assumptions about the shape of the underlying distribution. The thick black line shows the initial aggregate used in this study. I also show five additional two-size aggregates (dashed lines) and an aggregate with equal-sized particles (solid gray line). The trial aggregates have largely settled by 5 hours and all have completely stabilized by 30 hours.

Since the particles in the equal-size case are identical aside from a randomly assigned color, it is expected that the colors to be well mixed and so I can use this as the ideal case. By comparison it is clear that the aggregate used for this study (solid black line) displays a statistically significant difference between the two particle groups. Nevertheless, the aggregate used for this study shows less of a difference than the other two-sized particle aggregates (dashed colored lines), which enabled me to more easily distinguish further Brazil Nut Effect size sorting during the later simulations.

I attribute the statistically significant difference to the occurrence of the Brazil Nut Effect during the formation of the two-sized particle aggregates. When particles collapsed due to self-gravity during the formation of the aggregate, their mutual kinetic energies imparted a seismic shock that size sorted the particles. During the collapse process, the coefficients of friction were set to zero to ensure that the aggregate would be approximately spherical in shape. Using higher coefficients of friction could possibly reduce the effect of the initial size sorting; however, it would also introduce the issue of a misshaped aggregate that would complicate the analysis of the motion of the particle distributions. An alternative method would be to create the aggregate particle by particle; however, that would have been very computationally intensive.

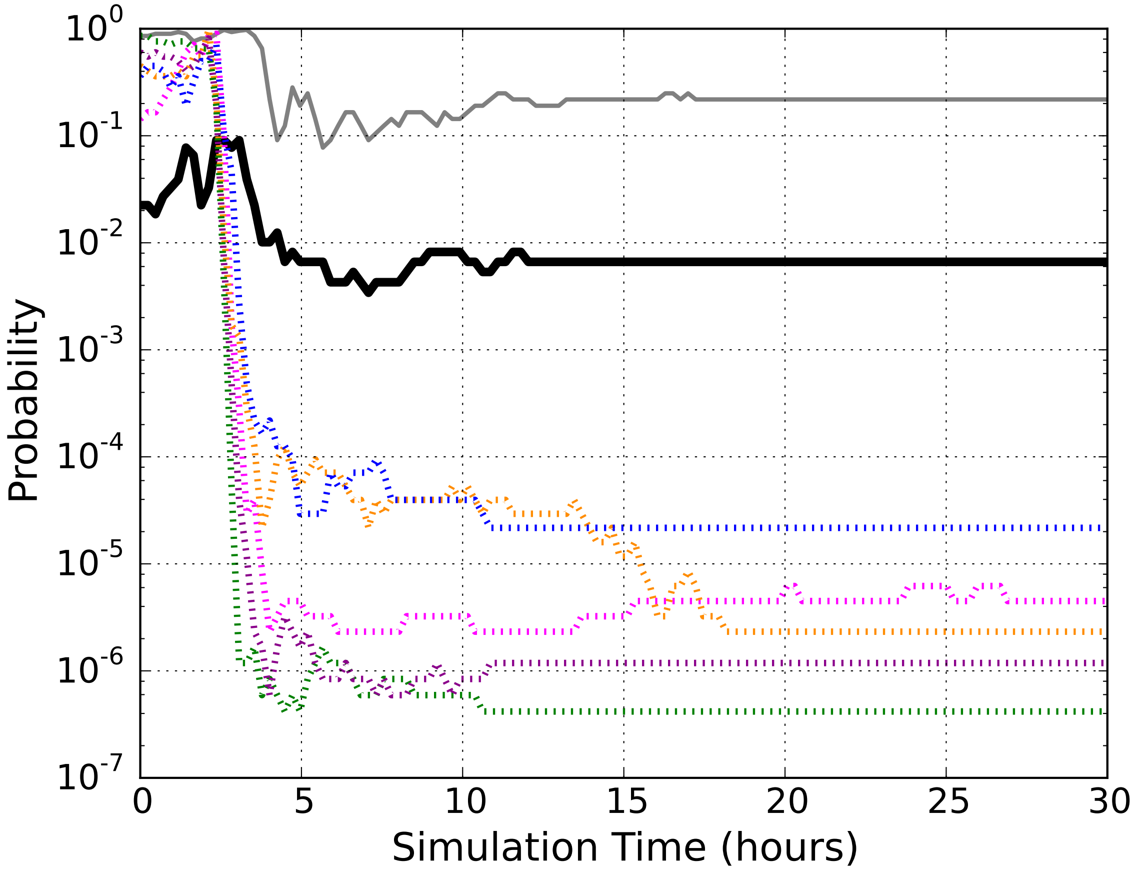

Figure 1: Probabilities that larger (red) and smaller (yellow) particles were drawn from the same parent distribution for seven initial aggregates. Probabilities shown as a function of initial aggregate formation/settling time and were determined using the K-S test. For all seven initial aggregates the friction coefficients were set to zero (to ensure aggregates that were formed were spherical) and the coefficients of restitution were 0.2 and 0.5 for the normal and tangential directions respectively. The solid black line shows values for the aggregate composed of particles of two sizes used for this work. Colored dotted lines show other trial aggregates composed of particles of two sizes. The solid gray line shows an aggregate that was composed of particles of the same size but were randomly assigned either a color of red or yellow for comparison.

2.2.3 Simulations

All simulations started with the same original aggregate (black line in Figure 1). This ensured that all of the numerical results began from the same initial distributions, aiding comparison of the results. The parameters varied for this study were the magnitude of the shaking and the coefficients of friction. In the first set of simulations particles did not have friction (i.e. friction coefficients were set to zero) and in the second set of simulations I assigned each particle a static friction coefficient of 0.7 and a rolling friction coefficient of 0.1 similar to nominal values used in Matsumura *et al.* (2014). They showed that the set of friction parameters listed above would lead to the Brazil Nut Effect occurring for a range of seismic and gravitational environments in a cylindrical box configuration.

At the beginning of each simulation each particle was independently assigned a random velocity drawn from a distribution of velocities that ranged from 0 to v_{max}. The values of v_{max} prescribed for the run are given in Table 1. The directions of the velocities were isotropically distributed with respect to the particle. After this 'shaking,' particles were allowed to gravitationally settle for a period of 4.7 simulation hours (200,000 time steps). Figure 1 shows that $\sim$5 hours is sufficient for the aggregate to have largely settled after the initial collapse and that the initial collapse is more violent than any individual shake in any of the simulations as well as having a longer lead time before settling can begin ($\sim$3 hours). After settling, all particles were again assigned new random velocities that were again no larger than the predefined maximum magnitude. For each run, the 'shaking' and settling process was repeated for 102 simulation days for a total of 516 'shakes' to mimic a prolonged period of seismic shaking. Each simulation run took approximately 15 days to complete.

For each of the friction and no friction sets, there were six simulations each for six different maximum magnitudes of velocity. Six speeds were chosen initially to be a percentage of the aggregate's estimated escape speed (1%, 10%, 25%, 30%, 40%, and 50%). These speeds were later converted to be a percentage of the aggregate's true escape speed (0.92%, 9.24%, 23.10%, 27.73%, 36.97%, and 46.21%).

Table 1: Simulation runs

Run	Static Friction	Rolling Friction	Max Speed (cm/s)	Max Speed (escape speed)
1	0	0	0.692	0.92%
2	0	0	6.95	9.24%
3	0	0	17.4	23.10%
4	0	0	20.9	27.73%
5	0	0	27.8	36.97%
6	0	0	34.7	46.21%
7	0.7	0.1	0.692	0.92%
8	0.7	0.1	6.95	9.24%
9	0.7	0.1	17.4	23.10%
10	0.7	0.1	20.9	27.73%
11	0.7	0.1	27.8	36.97%
12	0.7	0.1	34.7	46.21%

These values have no special significance other than to have a range of speeds to explore the parameter space. Friction coefficients and maximum magnitudes of velocity used for each run are listed in Table 1.

2.2.4 Considerations for comparisons with asteroids

There are several aspects to consider when comparing these simulations to asteroids. Rubble-pile asteroids are believed to be composed of self-gravitating particles and have friction and restitution, much like the simulated aggregates. In a rubble-pile asteroid however the constituent particles will be non-spherical and the friction and restitution parameters will likely be complex. To a certain degree, the asphericity of the particles can be considered as a source of large scale friction due to interlocking, and so this can be partly accounted for by the coefficient of friction.

While asteroids, like these aggregates, are self-gravitating, they are typically not spherical, but rather have a variety of odd shapes (Durech *et al.*, 2015). While these simulations may not be exactly representative of the typical non-spherical asteroid, the important aspect lies in the fact that these aggregates are three-dimensional and self-gravitating.

A corollary to this, which I believe is important, is that unlike simulations that involve box configurations these simulations do not have walls. Therefore, any size sorting that takes place can only be due to particle-particle interactions, and not due to particle-wall interactions.

2.2.4.1 The size distribution

An important aspect for comparing these simulations (or any other model of the Brazil Nut Effect) with asteroids is the size distribution. The constituent particles of a rubble-pile asteroid will form part of a likely largely continuous size distribution, however the shape of this distribution is poorly understood. As such it is preferable to adopt a simple assumption that allows me to make inferences about the behavior without being reliant on highly uncertain details of the size distribution. The simplest such assumption is that of a binary size distribution with two populations of particles. Like many works before them, Matsumura *et al.* (2014) focused on the intruder model. In intruder models, there is only one or a few large particle(s) in comparison to the quantity of small particles. Matsumura *et al.* (2014) argue that since the internal structures of asteroids are poorly understood, that assumption is valid. Though the intruder model might be applicable in the case of a single or a few large boulders buried beneath the surface of an asteroid, it is not clear that the model is suitable to study granular flow of all constituent particles of an asteroid. Rather than an intruder model, I chose to adopt a different implementation of a binary size distribution, with equal numbers of large and small particles, which I believe may be a better representation of a bulk asteroid.

2.2.4.2 The shaking model

The main seismic input for most asteroids is most likely from impacts, though other sources are possible, such as unloading of tidal stresses during close-encounters.

In an impact the seismic impulse will have a discrete source on the surface of the asteroid from which the seismic waves will propagate outwards, attenuating with distance travelled. This is clearly rather different from the method I use here, in which the seismic impulse is equally applied throughout the body. One important point here is that while an individual impact is a localized source I am not interested here in the effects of a single impact, but rather in the collective effect of many impacts over time. Individual impacts will occur at random locations on the surface, as such the bulk effect of many impacts over time will be uniformly distributed across the surface. In the interior I note that the seismic shock waves will reflect off the far side of the asteroid and off interior flaws within the body. Since asteroids are irregularly shaped these reflections will be chaotic and will likely lead to unpredictable foci and dead zones. As such it is unclear how attenuation into the interior of the asteroid should be handled, and so I choose to use my model of applying the seismic impulse uniformly throughout the interior for simplicity. I also note than any non-impact source of seismic disturbances, such as unloading of tidal stresses, would likely result in a more distributed source located below the surface, and that for any given shaking velocity my shaking model can be expected to give the maximum effect in the interior.

2.3 Results

In Figure 2, I show three time steps from Run 6 (no friction) on the left and three time steps from Run 12 (with friction) on the right. Progressive random shaking, in this case with a maximum magnitude of 46.21% of the escape speed (34.7 cm/s), resulted in the mixed aggregate becoming sorted. Over time, larger (red) particles can be observed rising to the surface while smaller (yellow) particles that were on the surface submerged. In the final cut-through views, there are larger particles on the surfaces with smaller particles beneath them. The innermost regions remain well mixed however. These size sorted and well mixed regions are also discernible on the histograms of particle radial distance (bottom panels of Figure 2).

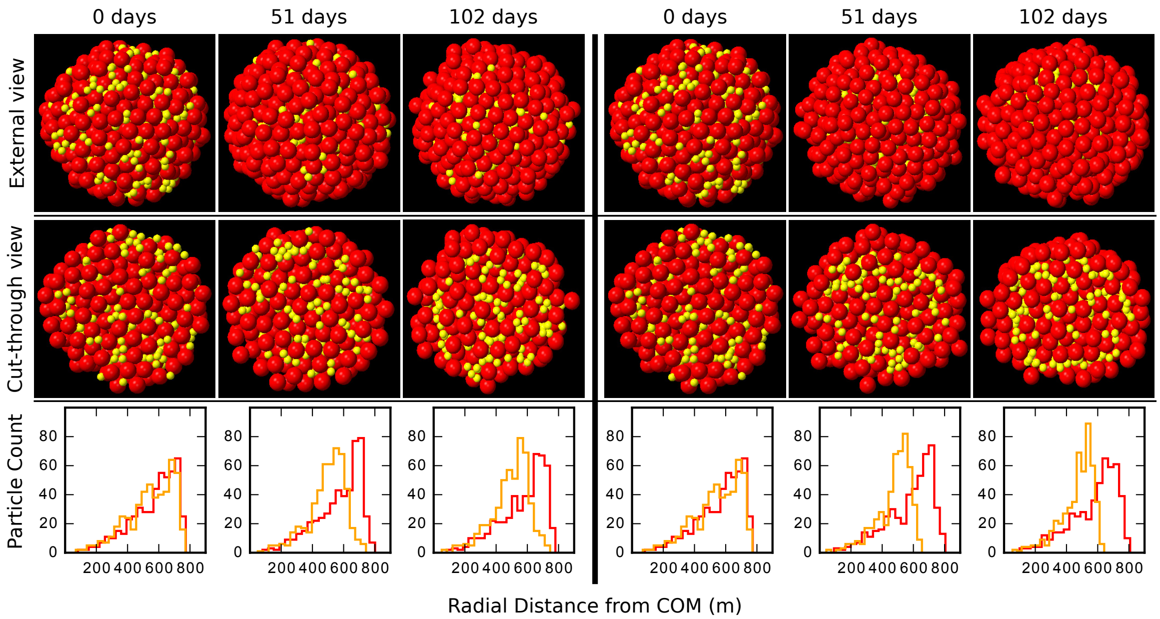

Figure 2: Two simulation runs shown without friction on the left and with friction on the right. Larger particles (radius 80 m) are colored red and the smaller particles (radius 40 m) are colored yellow. For both the runs (i.e. Runs 6 and 12), the maximum magnitude of shaking was 46.21% of the escape speed (34.7 cm/s). Each panel shows three stages (0, 51, and 102 days) of the simulations. Top row: external views. Middle row: cut-through views. Bottom row: histograms using a radius bin size of 20 m where particle radial distance is measure from the aggregate's center of mass. The yellow and red curves represent the smaller and larger particles respectively.

2.3.1 The well mixed central region

To explore this well mixed region further, I divided the aggregate into ten shells of 100 particles each. The first shell consisted of the first 100 particles from the center of mass, the second shell the next 100 particles and so forth. I chose to define the shells in this manner, rather than for example by defining them according to fixed radii, as this ensured that the shells always contained the same number of particles. This made comparisons between the simulation runs more straightforward.

Figure 3 lists percentages change, from initial and final stages of the simulations, of the number of smaller (yellow) particles present inside each of the ten shells.

The depletion of smaller particles from the outer part of the aggregate is again clear from the negative percentages listed. It is also apparent that for Shells 1 and 2 (the innermost shells) there is little change in the number of smaller particles (and thus also larger particles) present for any of the simulation runs. It should be noted that preliminary work by Sanchez *et al.* (2010) also found a well mixed central region with a rather different simulation setup.

2.3.2 The effect of friction

Friction first hinders size sorting due to particle interlocking. Row 7 of Figure 3 shows the case with friction and with a maximum shake speed of 0.92% of the aggregate's escape speed (0.692 cm/s). Unlike its no-friction counter part (Row 1), when friction is present there are no changes in the number of smaller (yellow) particles for the smallest shake magnitude in any of the shells. When friction is present, there is a seismic activation threshold that needs to be exceeded before particles can move past each other. In the 0.92% with friction case (Run 7), shake velocities are not large enough to overcome the frictional threshold. This suggests that there is likely a lower energy limit to impacts that are effective at triggering the Brazil Nut Effect on asteroids.

Once the threshold is met however, friction aids in the sorting process. This is likely a result of particle ratcheting. When friction is present the uppermost shell (Shell 10) is fully depleted of smaller (yellow) particles when constituent particles are shaken at a maximum magnitude of 27.73% of the aggregate's escape speed (20.9 cm/s) or higher. By comparison, in the no friction runs the uppermost shell is not fully depleted of smaller (yellow) particles even at the largest shake magnitude used for this study (46.21% of the aggregate's escape speed).

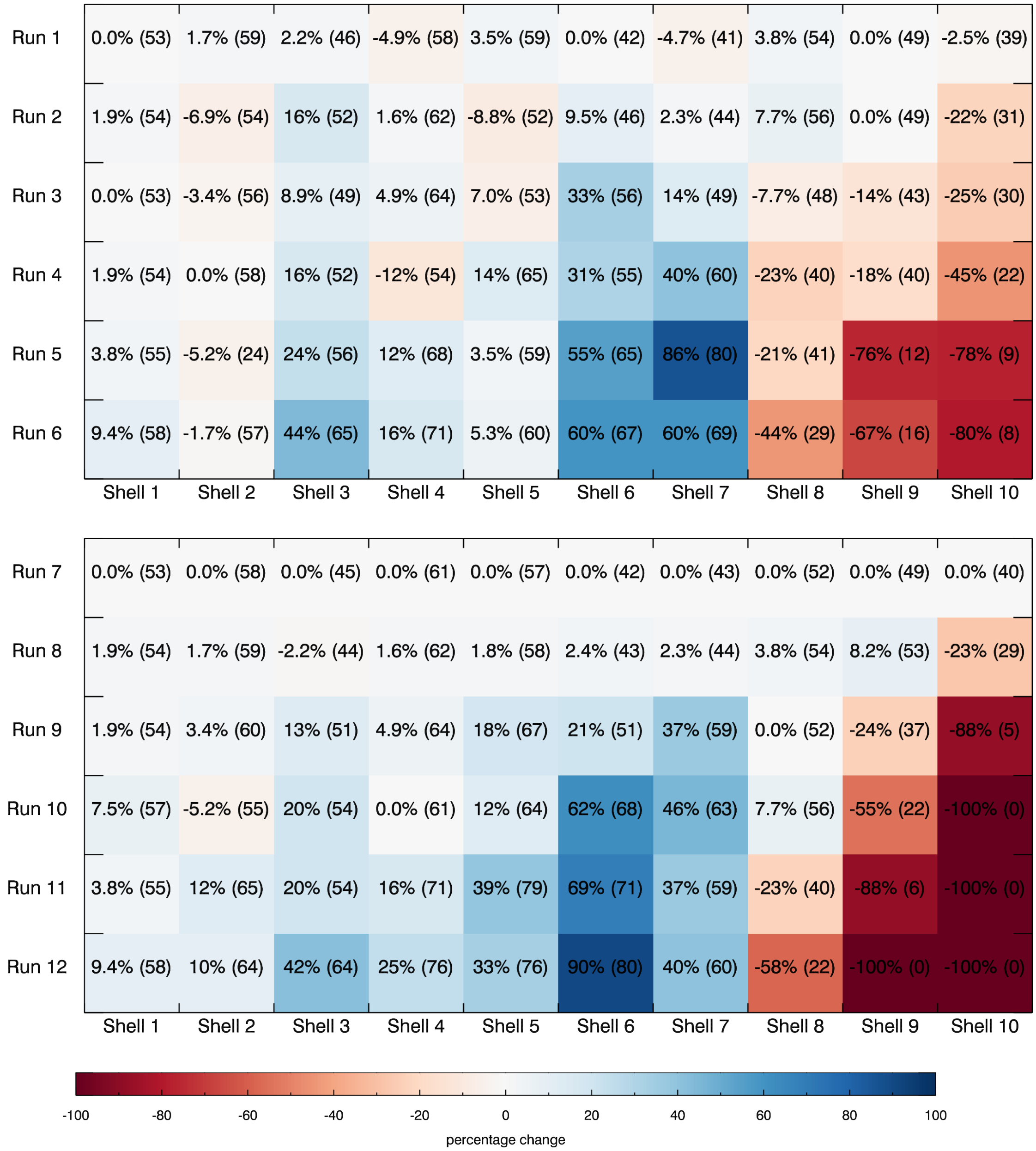

Figure 3: Percentage change of the number of smaller (yellow) particles present inside defined spherical shells from beginning to end of the simulations. Shell 1 contains the first 100 particles from the center of the aggregate while each of the following shells has the next 100 particles. Shell 10 contains the last 100 particles from the center of the aggregate. The coloring indicates whether smaller particles are being depleted (red coloring) or whether they are being augmented (blue coloring). Number of smaller (yellow) particles present at the end of the simulations are listed in parenthesis for each shell. Runs 1 to 6 have no friction (top) and Runs 7 to 12 have friction (bottom). For each of the no friction and with friction sets, progressive run numbers have increasing shake magnitudes.

2.3.3 Statistical analysis and time evolution

Figure 4 shows K-S test results for both the no friction and friction sets. The cases with maximum speeds that are 9.24% of the escape speed (Runs 2 and 8) are not shown as they are very similar to the 0.92% cases. In the left-hand column I show the comparison of the large and small particle distributions, while in the center and right-hand columns I show the comparison of each of the larger and smaller distributions respectively over time with their initial distributions. Comparing the distributions over time with their initial values allows me to fully account for the minor size sorting that occurred during the formation of the aggregate ensuring I am only analyzing additional size sorting that occurred after formation. While the K-S statistic shown in the left-hand column starts from a position of significant difference between the distributions due to the size sorting during formation, these plots allow me to see whether changes in the shape of each of the individual larger and smaller particle distributions are driving the distributions to greater or lesser dissimilarity.

When considering the left column plots in Figure 4, there are several cases that show substantially increased size separation. For the no-friction set, three aggregate cases show size separation (the 27.73% [green], 36.97% [orange], and 46.21% [red] cases). For the with-friction set, four aggregate cases show size separation (the 23.10% [blue], 27.73% [green], 36.97% [orange], and 46.21% [red] cases). The K-S statistic illustrates that the differences between larger particle and smaller particle distributions are highly significant in these cases. When comparing the middle column plots to the right column plots in Figure 4, they indicate that smaller particle distributions are changing significantly, while the larger particle distributions are remaining largely unchanged in shape. Even though larger particles are migrating outward, they are moving outward uniformly such that the shape of the distribution does not change dramatically while the smaller particles are filtering inwards.

Previous works have shown that the timescale for the Brazil Nut Effect to take place is either proportional to $1/g$ (Güttler *et al.*, 2013) or to $1/\sqrt{g}$ (Matsumura *et al.*, 2014).

Though both of these works focused on the intruder model and the exact inverse factor of g is uncertain, I expect that size sorting would take longer in the interior of my aggregate (and similarly in the interiors of asteroids) due to decreasing gravity towards the center of the body. It could thus be argued that if my simulations were run for a longer period of time, even innermost regions of the aggregate would be size sorted. However, Figure 5 shows that it is not the case. In Figure 5 the number of smaller particles in each of the 10 shells over time are plotted for Run 12 (the most vigorous case with friction). Changes that occur initially can be seen to plateau off even before the simulations have reached the halfway stage. Although at lower shake speeds the simulations take longer to reach a plateau, in all cases this is still reached before the end of the simulation run. The plateauing of the number of smaller particles in each shell indicates that particles have reached an equilibrium state for the given shake speed.

2.4 Discussion

My simulation results show that the Brazil Nut Effect occurs in these aggregates. To the extent that the simulated aggregates are representative of rubble-pile asteroids, I also expect the Brazil Nut Effect to occur in rubble-pile asteroids. While the effects of moving to a continuous size distribution from a binary one are not entirely clear, I expect larger boulders to rise to the surface of an asteroid over time as the asteroid experiences impacts or other seismic shaking events. These shaking events will be subject to an activation threshold since I expect the constituents of rubble-pile asteroids to have friction, and possibly cohesion.

2.4.1 Asteroid surfaces

The number of asteroids with sufficiently high resolution imaging of the surface to make any inferences about the size distribution of the surface material is rather small.

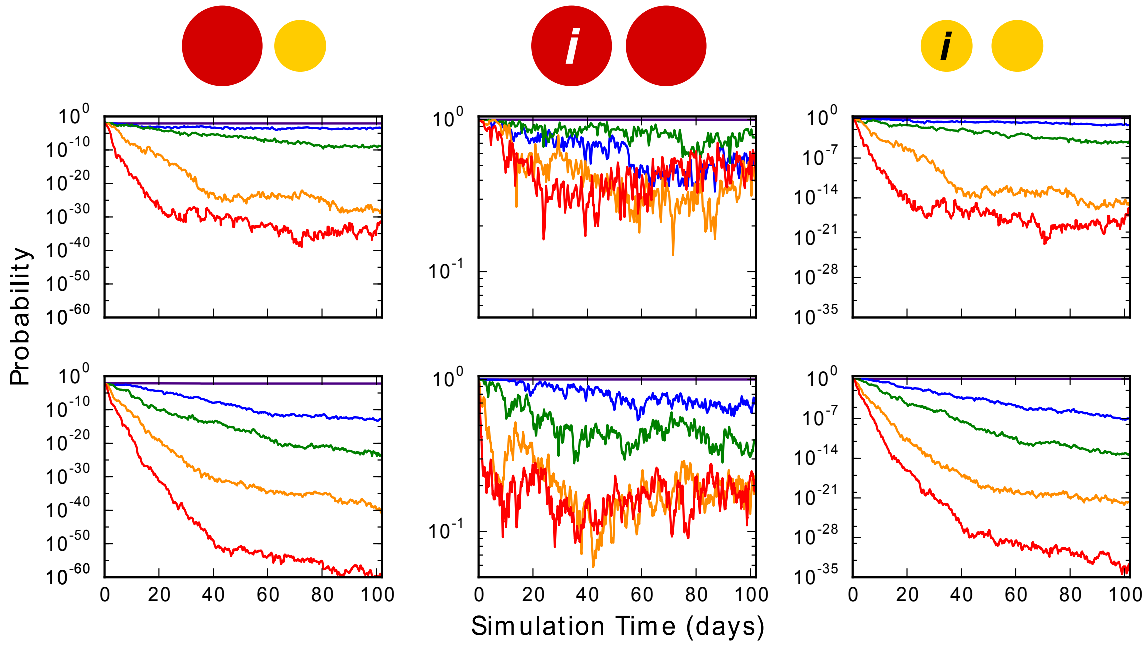

Figure 4: Probabilities that particles are drawn from the same distribution as determined by the K-S test. Top row: no friction sets (Runs 1 and 3–6). Bottom row: with friction sets (Runs 7 and 9–12). Runs 2 and 8 are not shown to reduce confusion since the lines are very similar to Runs 1 and 7 respectively. Left column: probability that larger and smaller particles were drawn from the same distribution as a function of time. Middle column: comparison between the distribution of larger particles over time and the initial distribution of larger particles. Right column: comparison between the distribution of smaller particles over time and the initial distribution of smaller particles. Line colors represent maximum magnitude of shaking as a percentage of the aggregate's escape speed (indigo = 0.92%, blue = 23.10%, green = 27.73%, orange = 36.97%, and red = 46.21%). All plots have been smoothed using a 50-point moving average.

One asteroid that does have such imaging is the small (535 m x 294 m x 209 m) near-Earth asteroid (25143) Itokawa. The surface of Itokawa displays regions that have substantially different ratios of larger boulders to smaller material, and Tancredi *et al.* (2015) compared these with gravity maps to suggest that there is a systematic trend for lower surface gravity ('higher') regions to have greater amounts of larger boulders. They argued that this is evidence that the Brazil Nut Effect has indeed been at work on Itokawa and resulted in size sorting.

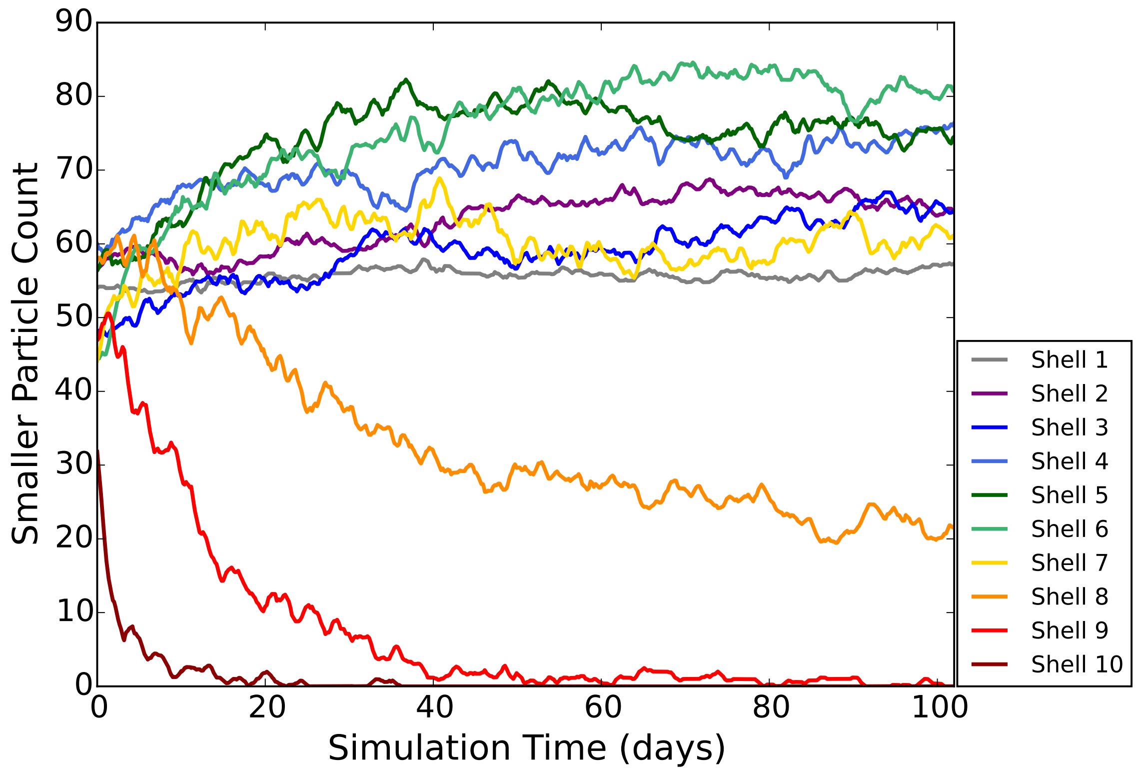

Figure 5: Smaller particle count inside each of the ten shells as a function of simulation time. Shown are particle counts for the with friction case that was shaken with a maximum magnitude of 46.21% the escape speed. All lines have been smoothed using a 100-point moving average.

In this way the irregular shape of Itokawa and other asteroids may be beneficial since the presence of regions with substantially different surface gravities can allow the observation of size sorting with only surface images, whereas for my spherical aggregates the only way to distinguish an aggregate in which the Brazil Nut Effect has brought larger material to the surface from one that is only made up of larger material is with information about the sub-surface.

While Itokawa may show evidence for size sorting it does not display complete size separation, that is regions that have larger numbers of boulders still also have finer material. There are a number of reasons why this might be the case. It is possible that the size sorting process on Itokawa has not yet had time to run to completion.

While I showed that the aggregates reached a steady-state configuration in which maximal size separation had occurred, I have not attempted to match this with the expected frequency of impacts or other seismic events on rubble-pile asteroids to determine whether it would be expected that the Brazil Nut Effect on rubble-pile asteroids to have reached an end state. This comparison is not immediately straight forward since it is not only the number of impacts or other seismic events that matters, but how many of these exceed the activation threshold. In addition, when an asteroid undergoes a catastrophic impact and is broken up into smaller pieces, the size sorting on those fragments will likely be reset since what was formerly in the interior may now be on the surface. The time over which the Brazil Nut Effect can act is thus more likely to be the time since the last catastrophic impact rather than the age of the solar system. Detailed study of this issue is beyond the scope of this work, but I note that the Brazil Nut Effect may not have had time to reach a steady-state on all asteroids.

Additionally, an asteroid sits in the wider environment of the solar system and the seismic events that enable the Brazil Nut Effect are not occurring in isolation. Impacts that are below the seismic activation threshold, particularly micro-meteorite impacts, will gradually break up surface material into finer sizes (Basilevsky *et al.*, 2015), and thermal fatigue may also play a similar role (Delbo *et al.*, 2014). The size-distribution of material on the surface of an asteroid is thus likely to be influenced by a balance between the Brazil Nut Effect bringing larger material to the surface and other processes breaking this material down into regolith.

2.4.2 The well mixed central region

A plausible explanation for why the innermost region of my aggregate is not size sorted could be that the magnitude of the shake speed was not sufficiently large. I should note, however, that the largest shake velocity, 50% of the escape velocity, is already very large and such large shaking velocities may not be plausible in asteroids.

To address this, it should be considered that asteroids are seismically shaken from their surfaces due to impacts. When impacts impart kinetic energy to their surfaces it is sufficient to influence the entire body (Garcia *et al.*, 2015). However, as I discussed in Section 2.2.4.2, due to attenuation the innermost regions will only receive some fraction of that energy, with my simulations representing the maximal case of no attenuation. Therefore, the innermost particles attaining a high velocity (larger than the 50% of the escape speed used in the most vigorous cases) would mean the outer layers of the asteroid would have likely received velocities exceeding the escape speed. This would mean that the outer layers of an asteroid would be disrupted and removed, leaving a modified body that is smaller than the original. While some of what was previously the innermost regions will now have been size sorted in this scenario, they will now be closer to the surface of the asteroid. Therefore, I deduce that asteroids will only be size sorted in their outermost regions, retaining a well-mixed central region.

2.4.3 Examining the Driving Mechanism of the Brazil Nut Effect

That the distribution of larger particles remains largely unchanged while the distribution of smaller particles changes substantially is interesting and deserves closer attention. Part of this difference in the behavior of the larger and smaller particles may be a result of the greater volume occupied by the larger particles. A large particle occupies 8 times the volume of a small particle and so, clearly, when a large particle rises upwards, multiple smaller particles can move down to take its place. The precise number of small particles that can occupy the space vacated by the red particle will vary, however. The maximum packing efficiency for hexagonal close-packed spheres (of equal size) is 0.74, so 5–6 small particles could be placed within the volume of the large particle. This neglects the voids near the original large particle however, which the smaller ones will be better able to fill, and so the removal of a large particle would generally create space for more than 5–6 small particles.

The theoretical packing efficiency (of equal sized particles) is independent of particle size, and so completely replacing large particles with small particles would increase the number of particles per unit volume by a factor of 8. Thus, it can be expected that on average each rising large particle is replaced by around 8 sinking small particles, but this will vary somewhat on a case-by-case basis.

While the difference in volume between large and small particles can account for some of the difference in the changes in the large and small particle distributions, it is unclear if it can account for all of the difference. In particular, if this was the sole reason for the difference in behavior of the evolution of the large and small particle distributions, then I would expect the large particle distribution to follow the same trend as the small particle distribution in Figure 4 but with a reduced magnitude. If Runs 11 and 12 (orange and red lines in the lower panels of Figure 4) are considered, it can be seen that although the changes in the distribution of large particles are not statistically significant, those changes that occurred do so over a much shorter time than the changes in the distribution of smaller particles. This suggests that an additional factor may be required to explain the difference in the behavior of the large and small particle distributions.

Another reason for the difference in the behavior of the large and small particle distributions may lie in the mechanism that drives the Brazil Nut Effect in these simulations. As mentioned previously, there are two mechanisms that have been postulated to mediate the Brazil Nut Effect: percolation of smaller particles through gaps created by the excitation of larger ones, and granular convection. If granular convection were the primary mechanism at work here, I would expect the distribution of large particles to undergo similarly large changes to the distribution of small particles (moderated by the greater volume of the large particles). On the other hand, if the small particles are filtering through the large ones while the large particles rise in a relatively uniform fashion, I would expect to see much smaller changes in the large particle distribution than the small particle distribution.

The lack of changes in the large particle distribution could thus be an indication that percolation of the smaller particles is the primary mechanism at work in driving the appearance of the Brazil Nut Effect here.

To examine this further I look at the motions of individual particles in detail. Figure 6 shows the motions of 16 randomly selected particles (8 of each particle size) from the outer regions (400 m and further from the center of mass) of the aggregate in Run 11. I selected Run 11 since it has a reduced magnitude of the shakes imparted, which is shown in the plots as short, sharp upward spikes in the radial locations of the particles. Though the curves are quite noisy, two behaviors are apparent in the right-hand panel of Figure 6 (for the smaller particles): long-term oscillations in radial position and rapid drops to a new plateau level. The latter effect is the most prominent by a considerable margin, while the former is less easily discernible, but can be best seen in the red and purple curves. The left-hand panel has less evidence for any distinctive behaviors with the majority of those particles that show long-term changes in radial location showing relatively gradual rises. Long-term oscillations in location are the signature of granular convection as particles rise and fall in a convection cell. Percolation meanwhile has the signature of rapid falls inward for the smaller particles as gaps open between the larger particles allowing the smaller ones to filter down between them at stochastic intervals, while the larger particles would rise more gradually. Since both effects are seen, both mechanisms are operating; however, the sudden drops account for the majority of the inward motion of the small particles (confirmed by examining many iterations of Figure 6). It thus appears that percolation is the dominant mechanism at work in these simulations in driving the Brazil Nut Effect.

While this analysis is suggestive that percolation is the dominant mechanism, I must note several caveats. Firstly, since as I stated in Section 2.3.1 the inner region of the aggregate remains well mixed, the region in which the Brazil Nut Effect occurs, and thus in which its driving mechanisms operate, is confined to the surface layers. This surface layer is relatively shallow in comparison to the size of the constituent particles of the aggregate, especially the large particles.

While this is unlikely to be a hindrance to the operation of percolation, it may well inhibit the formation of convection cells and thus act to dampen granular convection. Secondly, by the same token since the surface layers in which the Brazil Nut Effect occurs are relatively shallow, the problem of small number statistics should be considered.

Though there are definite indications that percolation is the primary mechanism at work in these simulations, I am cautious about applying this result to asteroids as a whole. To investigate the driving mechanisms of the Brazil Nut Effect in more detail will require a dedicated study with higher resolution simulations. For the purposes of this work however I note that this does not change the primary results; that the Brazil Nut Effect occurs in self-gravitating rubble-pile aggregates when I account for their three-dimensional shape and that the central regions remain well mixed. If granular convection is being artificially damped in these simulations due to the thinness of the surface layers, then I expect the Brazil Nut Effect should be more vigorous on asteroids. I note that if damping is due to the presence of the well mixed central region, if convection becomes more vigorous with higher resolution (smaller particle) simulations, I would not expect it to influence the well mixed central region.

2.5 Summary and Outlook

I find that in the spherical configuration the Brazil Nut Effect occurs both with and without friction. Friction hinders the sorting process at low shake velocities; however, after the frictional energy threshold is exceeded, friction works to aid the sorting process. Above a certain vibrational threshold, cases with friction require a lower shake speed to achieve the same level of size sorting as cases without friction. To the extent that the simulated aggregates are representative of rubble-pile asteroids, my results indicate that size sorting likely occurs in the outer part of rubble-pile asteroids. They also indicate however that the innermost regions should consist of a mixture of particle sizes, since even a shake magnitude of nearly 50% of the escape speed was insufficient to sort the center.

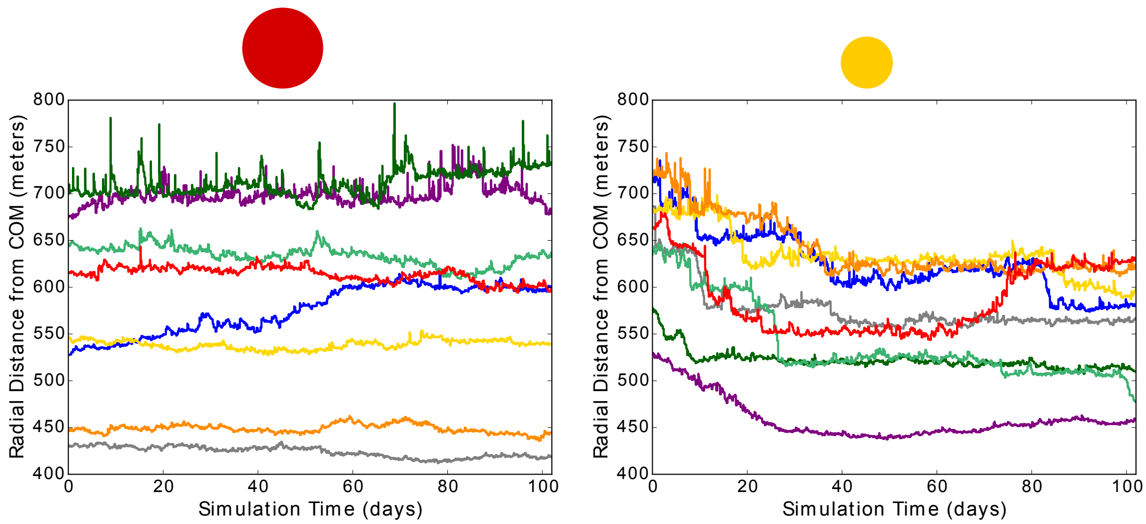

Figure 6: Radial distance with respect to the center of mass (COM) as a function of time for 16 randomly selected large and small particles (8 particles each) for Run 11. Larger (red) particles are shown on the left and smaller (yellow) particles are shown on the right. Only particles that started in the outer regions of the aggregate (i.e. 400 meters from the COM or further) were selected for these plots. The colors are used to distinguish between the different randomly chosen particles.

If an asteroid were to undergo an impact that resulted in the central particles acquiring a speed of 50% of the body's escape speed, then the surface of the asteroid is likely to be disrupted.

Percolation appears to be the dominant driving mechanism behind the Brazil Nut Effect in my simulations, with granular convection playing only a minor role. I note however that the shallow depth (in terms of particle radii) of the size sorted layer due to the presence of the well mixed central region may inhibit the formation of convection cells, thus damping granular convection.

I will further explore the layers of size sorting in the future by using a larger number of particles for finer resolution. Future work will also include exploring the Brazil Nut Effect in the spherical configuration for a range of aggregate sizes, constituent particle sizes, various rotational states of aggregates, coefficients of restitution, and coefficients of friction.

A spherical geometry is an idealization that I make to reduce invoking additional free parameters. Future modeling will also consider how the process would vary on bilobed asteroid shapes, and include better approximations for the input of seismic energy.

Chapter 3

EFFECT OF RE-IMPACTING DEBRIS ON THE SOLIDIFICATION OF THE LUNAR MAGMA OCEAN

> Guess what we just found! I think we found what we came for.
>
> ---
>
> *Dave Scott (Apollo 15 Commander after finding rock sample 15415 colloquially known as the "Genesis Rock")*

The anorthosites that comprise the bulk of the lunar crust are believed to have formed during the solidification of a Lunar Magma Ocean (LMO) in which these rocks would have floated to the surface. This early flotation crust would have formed a thermal blanket over the remaining LMO, prolonging solidification. Geochronology of lunar anorthosites indicates a long timescale of cooling of the LMO, or else re-melting and re-crystallization in one or more late events. To better interpret this geochronology, I model LMO solidification in a scenario where the Moon is being continuously bombarded by returning projectiles released from the Moon-forming giant impact. More than one lunar mass of material escaped the Earth-Moon system onto heliocentric orbits following the giant impact, much of it to come back on returning orbits for a period of 100 Myr. If large enough, these projectiles would have punctured holes in the nascent floatation crust of the Moon, exposing the LMO to space and causing more rapid cooling. I model these scenarios using a thermal evolution model of the Moon that allows for the production (by cratering) and evolution (solidification and infill) of holes in the flotation crust that insulates the LMO. For effective hole production, the solidification of the magma ocean can be significantly expedited, decreasing the cooling time by more than a factor of 5.

If hole production is inefficient, but shock conversion of projectile kinetic energy to thermal energy is efficient, then LMO solidification can be somewhat prolonged, lengthening the cooling time by 50% or more.

3.1 Introduction

The Moon likely coalesced from debris in the aftermath of a giant impact between the proto-Earth and another planet-sized body (Daly, 1946; Hartmann and Davis, 1975; Cameron and Ward, 1976). This Giant Impact Model explains the high angular momentum of the Earth–Moon system, the iron depletion of the Moon relative to the Earth, and the Moon's volatile depletion (Wolf and Anders, 1980; Taylor *et al.*, 2006b; Taylor and Wieczorek, 2014). After several iterations, a Canonical Giant Impact Model of a low-velocity, glancing impact by a Mars-sized body developed (see Canup, 2004, for a review). In the Canonical model, the Moon is predominantly composed of material from the impactor; however, recent geochemical analyses show that the Earth and the Moon have nearly identical isotopic signatures (e.g. Touboul *et al.*, 2007; Spicuzza *et al.*, 2007; Zhang *et al.*, 2012). As a result, several works have proposed modifications to the Giant Impact Model to account for the isotopic similarities (e.g. Pahlevan and Stevenson, 2007; Canup, 2012; Ćuk and Stewart, 2012; Reufer *et al.*, 2012; Mastrobuono-Battisti *et al.*, 2015; Ćuk *et al.*, 2016; Rufu *et al.*, 2017). Though the Giant Impact Model will undoubtedly continue to be revised and improved, it still is the accepted mechanism for the formation of the Moon (Asphaug, 2014; Barr, 2016).

3.1.1 Initial Thermal State of the Moon

The initial thermal state of a newly formed planet is primarily determined by how long it takes to form and how efficient accretionary impacts are at depositing thermal energy. Formation time is particularly important for two reasons.

First, it will determine how much of gravitational potential energy is thermally radiated away and how much is used to heat constituent material. Second, it will determine if hot disk material will be accreted quickly (e.g. silicate material in the debris disk were likely between 2,500 to 5,000 K after the Giant Impact (Canup, 2004)). Thus, the Moon would have been initially molten if it accreted rapidly. In that case, the debris would have been hot and the Moon's gravitational binding energy, which, per unit mass, is comparable to the latent heat of silicates (Pritchard and Stevenson, 2000), would have been used to melt constituent material. Though the Moon likely accreted rapidly, accretionary models vary in their estimates as to how long the Moon took to acquire the majority of its mass. For the Canonical model, that period is generally thought to be between a month to a year (Ida *et al.*, 1997; Kokubo *et al.*, 2000b; Takeda and Ida, 2001). Additionally, how efficient accretionary impacts are at depositing thermal energy is subject to considerable uncertainty. Past works have assumed that a certain fraction of the accretion energy was deposited into the planet as thermal energy (e.g. Kaula, 1979; Ransford and Kaula, 1980; Squyres *et al.*, 1988; Senshu *et al.*, 2002; Merk and Prialnik, 2006); however, the temperature of the planet at the end of accretion is strongly dependent on those assumptions (Stevenson *et al.*, 1986). Given these uncertainties, while dynamics suggests that an early Lunar Magma Ocean (LMO) is likely, it is currently not possible to be definitive regarding the initial thermal state of the Moon from a purely dynamical perspective.

An alternative, yet complementary, approach to characterizing the initial thermal state of the Moon is by geochemical analyses of lunar samples. Early work on Apollo samples found ferroan anorthosite (FAN) rock fragments (Wood *et al.*, 1970a). From that observation it was inferred that the early lunar crust was made from anorthositic rocks that floated to the surface of a LMO (Wood *et al.*, 1970b). Anorthosite rocks were buoyant due to the low density of its primary mineral plagioclase feldspar. Recent reflectance spectral data are consistent with this scenario since they show the presence of pure anorthosite on a large fraction of the lunar surface (Yamamoto *et al.*, 2012). The europium (Eu) anomaly is further evidence for a past LMO.

Eu is drawn to plagioclase feldspar and as such is enriched in the lunar crust and depleted in the mantle (Philpotts and Schnetzler, 1970; Wakita and Schmitt, 1970). Additionally, incompatible KREEP elements (i.e. potassium [K], rare earth elements [REE], and phosphorous [P]) that exists on the lunar surface are likely from residual liquid of the LMO (i.e. ur-KREEP) (Warren and Wasson, 1979). Some works have questioned the existence of an LMO (e.g. Walker, 1983; Longhi and Ashwal, 1985; Longhi, 2003; Boyet and Carlson, 2007), but the amalgamation of evidence suggests that a LMO existed (for a review see Elkins-Tanton, 2012).

To understand the thermal evolution of the Moon, it is important to estimate the initial depth of the LMO and the time that it took to solidify. The initial depth has been estimated by starting with an estimate for the lunar crustal thickness and arguing that a LMO of a certain initial composition (viz. Al_2O_3) needed to have been a particular depth to have produced that crust by fractional crystallization (Warren, 1985; Yamamoto *et al.*, 2012). For that depth estimate, it is assumed that a percentage of the crust is anorthositic. An additional assumption is the fractionation of Al_2O_3 that went into various minerals that crystallized. Some works have assumed that all of the Al_2O_3 went into forming plagioclase feldspar (e.g. Warren, 1985), while others have assumed that some of the Al_2O_3 also went into forming spinel (Elkins-Tanton *et al.*, 2011). Due to the varying assumptions, the estimated LMO initial depths range from 100 to 1000 km (Hodges and Kushiro, 1974; Walker *et al.*, 1975; Solomon and Chaiken, 1976; Solomon, 1980; Kirk and Stevenson, 1989; Elkins-Tanton *et al.*, 2011; Andrews-Hanna *et al.*, 2013; Lin *et al.*, 2017b). Similarly, the solidification time also has a range of estimates. For thermal models, it ranges from 10 to nearly 300 Myrs (Solomon and Longhi, 1977; Minear, 1980; Meyer *et al.*, 2010; Elkins-Tanton *et al.*, 2011), while for geochemical analyses, it ranges from about 100 to 254 Myrs (Nyquist *et al.*, 1995; Rankenburg *et al.*, 2006; Boyet and Carlson, 2007; Nemchin *et al.*, 2009). To be consistent with the LMO model, it is important that the solidification time of the LMO is comparable to the time span of primordial lunar crustal ages. Yet, this does not seem to be the case.

Recent work suggested the LMO would have crystallized in 10 Myrs (Elkins-Tanton *et al.*, 2011), which is much faster than what is suggested by the range of crust sample ages of ~ 200 Myrs (Alibert *et al.*, 1994; Borg *et al.*, 1999). Further work is required to refine these ages to be consistent with each other.

3.1.2 Re-impacting Debris

Recent work has shown that a substantial amount of debris (about 10^{23} kg or ~ 1.3 lunar masses) had sufficient speed to escape the Earth–Moon system after the Moon forming impact (Kokubo *et al.*, 2000a,b; Marcus *et al.*, 2009; Jackson and Wyatt, 2012). That quantity of escaping debris is for the Canonical model, which is a rather gentle impact with an impact velocity only just above the escape velocity. For many of the newer, modified versions of the Giant Impact Model, the giant impacts are more violent, thus they tend to produce more escaping debris. Leinhardt and Stewart (2012) find that a typical giant impact releases around 3 to 5% of the colliding mass as debris, as compared to 1.6% for the Canonical model. For this work, I am making a conservative estimate by assuming the quantity of debris is that of the Canonical model.

While on heliocentric orbits, much of the debris would have subsequently re-impacted onto both the Earth and the Moon (Daly, 1946; Jackson and Wyatt, 2012). Jackson and Wyatt (2012) found that within a million years after the giant impact, debris would have accreted onto the Moon at an average rate of $\sim 9 \times 10^{13}$ kg/yr (with 50% loss to collisional grinding). Debris would have re-impacted the Moon while the LMO was solidifying. Impacts could have significantly altered the cooling rate when the Moon had developed a conductive lid (i.e. at the point of plagioclase stability). Impacts that punctured holes into a conductive lid would have increased the thermal flux by exposing magma that used to be thermally insulated. A similar scenario is expected on Europa when impacts puncture holes into its ice shell to expose liquid water beneath (Bauer and Cox, 2011).

Hartmann (1980) proposed that early impacts should have pulverized the nascent floatation crust and they may have sped up the LMO solidification; however, they did not quantify the LMO solidification time. Minear (1980) and Davies (1982) both argued that impacts should have sped up LMO solidification; however, their models were highly simplified.

3.1.3 Scope of this Work

In this work, I include the sustained bombardment of debris generated after the giant impact with the thermal evolution of the LMO. I am primarily interested in how re-impacting debris affects the thermal evolution of the LMO. For this work, I use a model that can thermally evolve the LMO while producing and thermally evolving holes generated in the lunar crust by re-impacting debris. In Section 3.2.1 I discuss numerical calculations of debris evolution and in Section 3.2.2 I discuss the details of my thermal evolution code. In Section 3.3 I show the results. In Section 3.4 I discuss consistency of my results with lunar crust sample ages, implications for the lunar surface and interior, and implications for the lunar orbital evolution.

3.2 Methods

Since I was interested in the bulk, rather than spatially resolved, properties of the LMO thermal evolution, for this work I use a 1-D spherically symmetric thermal model. Following a similar procedure to Elkins-Tanton *et al.* (2011), I use minute volume segments to iteratively solidify the modeled LMO and release the relevant energy through the modeled Moon's surface. Unlike previous work, here I consider the effect of re-impacting debris on the solidification of the LMO. In Section 3.2.2 and in following subsections I discuss the thermal evolution code in detail; however, I begin with Section 3.2.1 by discussing the expected quantity and evolution of debris after the Moon forming impact.

3.2.1 Re-impacting Debris Evolution

As noted above, the Canonical Moon-forming impact results in the release of around 1.3 lunar masses of material onto heliocentric orbits (Jackson and Wyatt, 2012). That mass is comparable to the mass that remains in Earth orbit as the proto-lunar disk (e.g. Canup, 2004). As it orbits the Sun this debris will encounter the terrestrial planets, especially Earth since it by definition must begin on Earth-crossing orbits, and will be re-accreted over time. Jackson and Wyatt (2012) conducted an extensive analysis of the dynamical evolution of the heliocentric Moon-forming debris using N-body simulations. I utilize the results of an improved N-body simulation that uses the same initial conditions and setup as Jackson and Wyatt (2012) and the same Mercury integrator (Chambers, 1999), but with an increased number of debris particles (10^5) and a longer integration time of 100 Myr rather than 10 Myr.

As described by Jackson and Wyatt (2012), it is not feasible to resolve the orbit of the Moon in a long term dynamical simulation and as such the Earth and Moon are treated as a single body. The debris accretion rate determined from the simulation is thus the accretion rate onto the Earth-Moon system as a whole. To separate them the ratio between the accretion rates for Earth and the Moon is required. Bandermann and Singer (1973) derive an analytic relation for the accretion ratio between the Earth and Moon, which they give as

$$\frac{A_E}{A_M} = \frac{R_E}{R_M} \frac{1 + u^2}{\frac{7}{6}\frac{R_E}{r} + 0.045 + u^2}, \tag{3.1}$$

where A_E and A_M are the accretion rates for Earth and the Moon, R_E and R_M are the respective radii, r is the Earth-Moon separation and u is the ratio of the relative velocity to the escape velocity of Earth, v_{rel}/w_E. Note that strictly this is a lower limit to the accretion ratio (or an upper limit to the lunar accretion rate) since it ignores the effect of shadowing by Earth, but this effect is small at all but the smallest Earth-Moon separations. The impact velocity, v_{imp}, of each impacting debris particle is provided by the N-body simulation and the relative velocity is then just $v_{rel} = \sqrt{v_{imp}^2 - w_E^2}$.

In addition to the relative velocity that can be determined from the N-body simulation, the accretion ratio also depends on the Earth-Moon separation, which is an independent parameter. Today the Earth-Moon separation is 60 R_E, however the Moon is migrating outwards over time and would likely have formed near the Roche limit at around 3 R_E. The timeline of the evolution of the lunar orbit is complicated however, especially at early times, and as the Moon crossed orbital resonances it likely went through high-eccentricity periods that further complicate the picture (e.g. Touma and Wisdom, 1998). Furthermore, the thermal state of the Moon and the rate of tidal evolution are somewhat coupled, as studied by Tian *et al.* (2017), such that if we expect the thermal evolution of the Moon to change as a result of re-impacting debris, this would also change the tidal evolution. Nonetheless, the Moon likely reached a separation of 10 R_E quite rapidly (e.g. Touma and Wisdom, 1994; Touma and Wisdom, 1998), and beyond this the accretion ratio changes fairly slowly (see Figure 7). As such I use a constant Earth-Moon separation of 10 R_E as being relatively representative of the early Moon.

While the N-body simulation in combination with Equation 3.1 provides the rate at which the massless N-body debris particles strike the Moon, that rate needs to be converted into a mass accretion rate. Individual bodies in the disk of heliocentric debris will collide with one another and gradually break up into ever smaller fragments until the resulting dust is small enough (roughly 1 μm) that it can be removed from the Solar System by radiation pressure. To calculate an accurate mass accretion rate, debris evolution needs to be accounted for through self-collision between debris fragments.

To compute the collisional evolution, the code developed by Jackson *et al.* (2014) was used. Jackson *et al.* (2014) improves on the work of Jackson and Wyatt (2012) by accurately accounting for the initial asymmetry in the debris disk and allowing the mass assigned to each N-body particle to evolve individually. The collisional evolution is dependent on the size-distribution of the debris fragments. The shape of the size-distribution is poorly constrained. Thus, following Jackson and Wyatt (2012) and Jackson *et al.* (2014), the size-distribution is assumed to be a single power law that follows $n(D)dD \propto D^{-7/2}dD$.

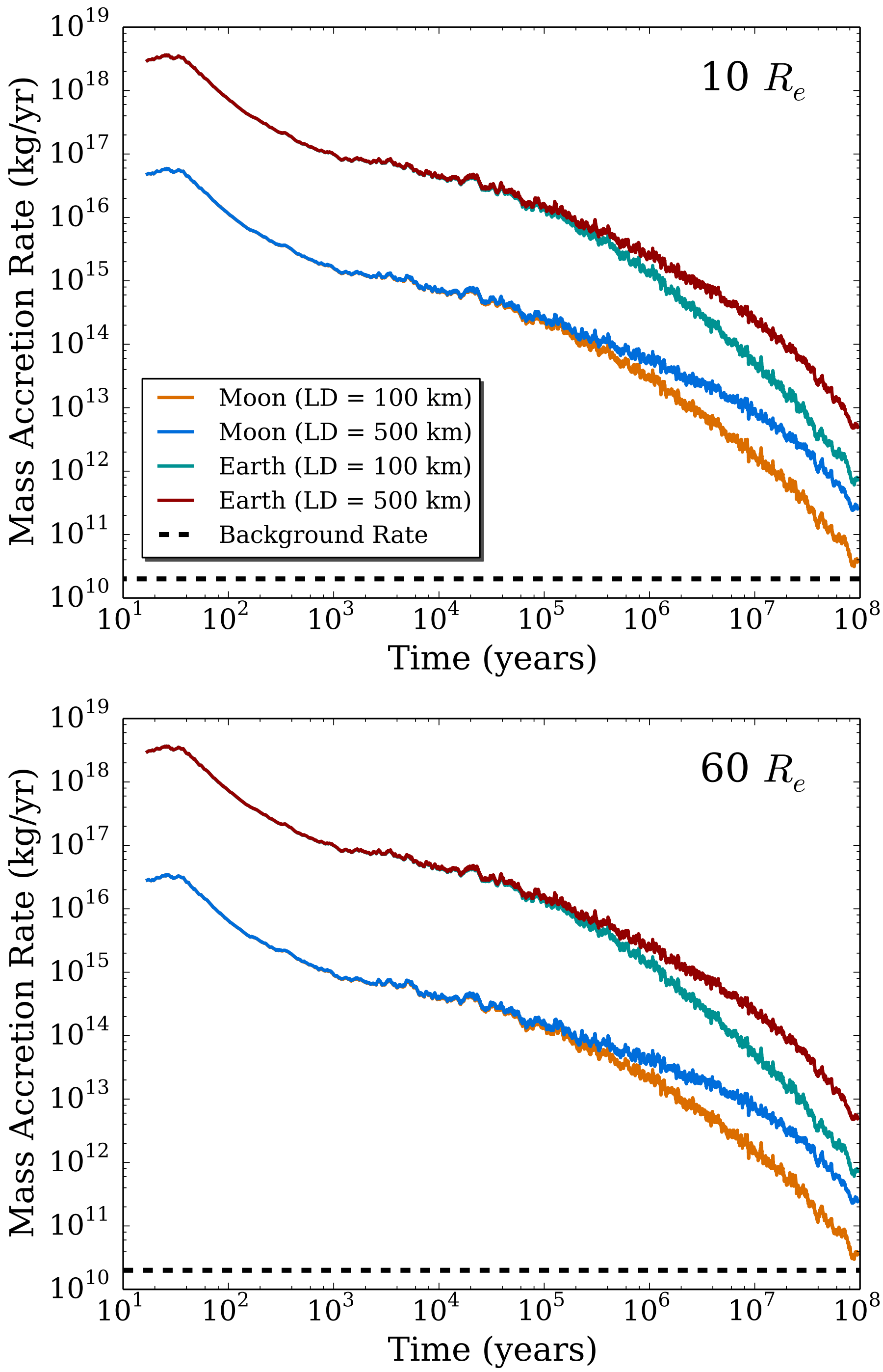

Figure 7: Mass accretion rate over time for the Earth (dark cyan and red lines) and the Moon (blue and orange lines) for two populations of re-impacting debris based on the size of the largest debris (LD). Top: Accretion rate when the Moon is at a distance of 10 Earth radii. Bottom: Accretion rate when it is at a distance of 60 Earth radii. An estimate for the accretion rate due to 'background' asteroidal impacts during the proposed Late Heavy Bombardment (Ryder, 2002) is shown by a black dashed line for comparison.

This is the slope to which a self-similar collisional cascade will relax over time (e.g. Dohnanyi, 1969; Tanaka *et al.*, 1996). Small fragments will have short collisional lifetimes and thus will rapidly evolve towards collisional equilibrium, where this slope will be a relatively accurate reflection of the reality (e.g. Wyatt *et al.*, 2011). Larger, longer lived fragments will evolve more slowly and so this assumption is less certain, however there is no evidence to support a different distribution and this is the simplest assumption.

For a size distribution that is in collisional equilibrium the evolution of the mass in the cascade is governed by the size of the largest fragments, since these are the longest lived, meaning that as these largest bodies break up their mass is redistributed down the cascade on timescales short compared with their lifetimes. Mass is ultimately lost from the cascade once it reaches micron sizes at which point Solar radiation pressure is sufficient to blow the dust out of the Solar System. This is a very useful property as it means that in addition to the assumption of the shape of the size-distribution only one other assumption is needed, which is the size of the largest objects in the debris. In Figure 7 I show the evolution of the mass accretion rate for two different values of the size of the largest object in the debris, 500 km and 100 km. Jackson and Wyatt (2012) chose 500 km as their fiducial estimate of the size of the largest objects in the debris from Moon-formation, and suggested that objects much larger than this are implausible. To be conservative I choose to use 100 km as the size of the largest object in the debris for this study. It is important also to note that while a certain size-distribution was assumed to determine the rate of collisional evolution of the debris, this only feeds into this work through the mass accretion rate, it does not influence any of the aspects of this study.

3.2.2 Thermal Evolution Code

As stated earlier, there are many estimates for the initial LMO depth; however, no geochemical modeling estimate has called for an entirely molten early Moon.

Additionally, Salmon and Canup (2012) have argued that a cold "parent body" (about 40% of lunar mass), which would not have undergone intense bombardment, would have formed shortly after the giant impact. Thus, here I assume that the Moon formed with a nearly solidified interior and a molten exterior (e.g. Solomon, 1986). I use a nominal LMO depth of 1000 km similar to Elkins-Tanton *et al.* (2011) for this work and in Section 3.3.2 I show that the LMO solidification time is rather insensitive to the initial depth. I recognize that the Moon could have a liquid outer core (Williams *et al.*, 2014; Matsuyama *et al.*, 2016); however, provided it is not undergoing significant solidification (and attendant heat loss), that should be inconsequential to the LMO's overall thermal evolution. I also ignore the lunar core formation process since Solomon (1980) showed that it only raised the average temperature of the Moon by 10 K.

Unlike, for example, Minear and Fletcher (1978) and Elkins-Tanton *et al.* (2011), I did not explicitly model the geochemical crystallization of the LMO. I am interested in how re-impacts affected the bulk thermal properties of the LMO (e.g. its overall solidification time), rather than the geochemical internal structure of the Moon. This choice simplified the code and made it faster, which allowed me to explore a wider parameter space to better understand the effect of re-impacts. This is further justified by Minear and Fletcher (1978), who found that the LMO solidification time is mainly dependent on the mode of heat transportation, crust thermal conductivity, and final crustal thickness. A limitation of not modeling the geochemical crystallization process is that there is not a natural prescription for what fraction of the solidified material should sink or float. To approximate how crystallizing material would partition according to density, initially, for each iterative step, all material that solidified is assumed to be denser than the LMO and thus is added to the top of the solid interior. To model floatation crust formation, when the LMO depth decreases to 100 km, instead of all crystallizing material sinking to the interior, a fixed fraction (viz. 45%) is directed to the surface to form crust. This is similar to Tian *et al.* (2017) who used a 40% fraction in the final 110 km of the LMO with the crust beginning with a thickness of 5 km.

I choose this partitioning fraction to closely replicate the geochemical evolution in Elkins-Tanton *et al.* (2011) and the current crustal thickness of the Moon (Wieczorek *et al.*, 2013).

My Python code iterates over a minute LMO volume segment, which is determined by dividing the initial LMO volume by a user defined number of segments. At each iteration, the total energy released through the modeled surface is the sum of energy released due to secular cooling and partial solidification of the LMO. The total energy is allowed to be released both via direct thermal radiation and conduction depending on the surface conditions. Unlike Elkins-Tanton *et al.* (2011), I do not assume that an early atmosphere would be capable of maintaining a free, liquid surface to the LMO. Instead, I allow quench crust to form if the conditions are suitable (see Section 3.2.2.1). Quench crust is a rapidly solidified layer of crust that is approximately the same composition as the liquid magma. Therefore, in this work, the LMO cooling is initially controlled by thermal conduction through the quench crust.

The temperature in the LMO is estimated by calculating the temperature at the solid-liquid boundary at the base of the LMO and using the adiabat slope to calculate the temperature at a given radial position. By definition, the temperature at the solid-liquid boundary will be the solidus temperature of the LMO at the relevant depth/pressure. I use the same solidus temperature equation (Equation 3.2) as in Elkins-Tanton *et al.* (2011). The solidus temperature (in Kelvin) is given by

$$T_s(r) = \Big(- 1.3714 \times 10^{-4} \Big) r^2 - 0.1724r + 2134.15 - \frac{4.4}{0.2L + 0.01}, \tag{3.2}$$

where r is the radial position from the Moon's center in km and L is the remaining liquid fraction of the LMO ranging from 1 to 0.

The surface temperature is calculated self-consistently by equating the conductive flux through the crust to the radiative flux on the surface as given by

$$\kappa_c \rho_c c_c \left(\frac{T_{bc} - T_{tc}}{d_c} \right) = \epsilon \sigma \left(T_{tc}^4 - T_e^4 \right), \tag{3.3}$$

where κ_c is the thermal diffusivity of the crust, ρ_c is the density of the crust, c_c is the specific heat capacity of the crust, T_{bc} and T_{tc} are the temperatures at the bottom and at the top of the crust respectively, d_c is the crustal thickness, ϵ is the emissivity, σ is the Stefan–Boltzmann constant, and T_e is the equilibrium temperature of the surface in the absence of internal heat sources. At each iterative step, I solve for the surface temperature (i.e. T_{tc}) that equates the conductive and radiative fluxes.

Whether quench or floatation crust is present on the surface, the simple conductive energy release is complicated by re-impacting debris, which may puncture holes into the crust. At each iteration, I consider the area of holes that are punctured by impacts (see Section 3.2.2.2). I calculate the equilibrium quench crust that would form in a particular hole and I account for the increased conductive flux (due to the thin layer of quench) in the energy release calculations.

Since I use increments of constant volume rather than constant time, it is necessary to calculate the time taken for each volume increment to solidify, which is simply the energy that must be released in that step divided by the net heat flux at the lunar surface. Note that the quantity of material accreted, and thus the area of holes produced during the solidification of a volume increment is dependent on the time taken, but that the area of holes produced will also influence the time taken. As such within the calculation for each volume increment an iteration is required to ensure consistency. While this adds to the computational cost of each volume increment calculation it converges quickly and the very large variation in solidification rates over a complete run makes this preferable to using increments of constant time.

The iteration is terminated when 1% by volume of the initial LMO remains.

Previous work, such as Elkins-Tanton *et al.* (2011), typically stop their calculations at that point since the remaining liquid consists of incompatible elements and is proposed to be the ur-KREEP layer (i.e. the hypothesized source region of KREEP elements on the lunar surface) (Warren and Wasson, 1979). I list the nominal values for the relevant parameters used for these calculations in Table 2.

During the thermal evolution of the LMO, it is likely that it had additional heat sources due to some or all of the following: secular cooling of the core (e.g. Zhang *et al.*, 2013), radiogenic heating (e.g. Meyer *et al.*, 2010; Elkins-Tanton *et al.*, 2011), tidal heating (Meyer *et al.*, 2010; Chen and Nimmo, 2016), and electrical induction heating (Herbert *et al.*, 1977). In this work, I do not explicitly consider individual heat sources but I allow for additional energy to be added to the LMO during its thermal evolution (see Section 3.4.1).

3.2.2.1 Quench Crust

Quench crust at the early stage of the LMO's thermal evolution has been considered inconsistently, with some works having included it (e.g. Minear, 1980), while others having disregarded it (e.g. Elkins-Tanton *et al.*, 2011). That choice has a dramatic effect on how long the LMO takes to solidify up to the point at which floatation crust formation begins. When quench crust is not considered, magma radiates directly to space and consequently, cooling of the LMO is extremely rapid. On the other hand, when quench crust is considered, thermal evolution of the LMO is always conductive. That makes the cooling slower since the conductive flux is only proportional to the temperature difference between the top and bottom of the quench crust. Quench crust has also been considered for Mercury (Riner *et al.*, 2009), which, like the Moon, may have also had a floatation crust form from a magma ocean (Vander Kaaden and McCubbin, 2015).

I argue that quench crust would have been present for two reasons. First, I compare the convective flux from the LMO to the radiative flux from the surface.

Table 2: Nominal Parameter Values

Symbol	Value	Units	Description	Reference
S_a	1.5×10^{-4}	K/m	Adiabat Slope	Zhang *et al.* (2013)
d_m	1000	km	LMO Initial Depth	Elkins-Tanton *et al.* (2011)
d_f	100	km	Floatation Crust Formation Depth	Elkins-Tanton *et al.* (2011)
f_p	0.45	–	Floatation Crust Partition Fraction	Set to match lunar crustal thickness
z_m	1%	–	Residual LMO	Warren and Wasson (1979)
H_f	4.187×10^5	J/kg	LMO Heat of Fusion	Elkins-Tanton *et al.* (2007); Piskorz *et al.* (2014)
α_m	3×10^{-5}	1/K	LMO Thermal Expansion Coefficient	Elkins-Tanton *et al.* (2007)
η_m	10^3	Pa · s	LMO Dynamic Viscosity	Bottinga and Weill (1972)
ρ_m	3.0	g/cm^3	LMO Density	Meyer *et al.* (2010)
ρ_c	2.7	g/cm^3	Crust Density	Gast and Giuli (1972)
ρ_q	2.7	g/cm^3	Quench Density	Set equal to crust value for quench floatation
c_m, c_c, c_q	1256.1	J/kg · K	LMO, Crust & Quench Specific Heat Capacity	Elkins-Tanton *et al.* (2007); Eppelbaum *et al.* (2014)
κ_m, κ_c, κ_q	10^{-6}	m^2/s	LMO, Crust & Quench Thermal Diffusivity	Elkins-Tanton *et al.* (2007); Eppelbaum *et al.* (2014)
d_q	10	m	Maximum Quench Thickness	Rathbun *et al.* (2002); Matson *et al.* (2006)
T_{melt}	1000	K	Quench Melting Temperature	Eppelbaum *et al.* (2014)
T_e	250	K	Equilibrium Radiative Temperature	Approximate lunar equilibrium temperature without an atmosphere
ϵ	1.0	–	Emissivity	Idealized perfect emitter
a_g	1.6	m/s^2	Acceleration Due to Gravity	Approximate surface value

If the LMO radiated directly to space with a surface temperature > 1000 K and an equilibrium temperature of 250 K, convection would not be able to deliver heat to the top of the LMO fast enough to balance the rate of heat loss by thermal radiation. As such, quench crust would form on the surface. This can be shown using the Nusselt number (Nu), which is the ratio of convective and conductive heat fluxes and is given by

$$Nu = a \cdot Ra^{\beta}, \tag{3.4}$$

where a and β are constants. I use a = 0.124 and β = 0.309 from experimental work by Niemela *et al.* (2000) (see Appendix B.1 for additional details). Ra is the Rayleigh number, which is given by

$$Ra = \frac{a_g \cdot \rho_m \cdot \alpha_m \cdot \Delta T \cdot d_m^3}{\eta_m \cdot \kappa_m}, \tag{3.5}$$

where a_g is acceleration due to gravity, ρ_m is the density of the LMO, α_m is the thermal expansion coefficient of the LMO, ΔT is the temperature difference, d_m is the depth of the LMO, η_m is the dynamic viscosity of the LMO, and κ_m is the thermal diffusivity of the LMO. Using an initial ΔT of 150 K (adiabatic temperature change over 1000 km) along with nominal values from Table 2, Ra is approximately 2×10^{22} and in turn, Nu is approximately 10^6. The conductive heat flux of the LMO is given by

$$Flux_{cond}^{m} = \kappa_m \rho_m c_m \frac{T_{mb} - T_{mt}}{d_m}, \tag{3.6}$$

where κ_m is the thermal diffusivity of the LMO, ρ_m is the density of the LMO, c_m is the specific heat capacity of the LMO, T_{mb} and T_{mt} are the temperatures at the bottom and at the top of the LMO respectively, and d_m is the thickness of the LMO. Using the nominal values along with initial values for T_{mb} equal to 1912 K (the solidus temperature at the initial solid-liquid boundary) and T_{mt} equal to 1400 K (the solidus temperature at the top of the LMO initially, which I thus expect to be the temperature at the base of the quench layer), the conductive flux is equal to $\sim 2 \times 10^{-3}$ W/m^2. By using Nu, I calculate the convective flux to equal $\sim 2 \times 10^3$ W/m^2.

This is about two orders of magnitude smaller than the radiative flux of a surface with a temperature of 1400 K and an equilibrium temperature of 250 K (i.e. $\sim 10^5$ W/m^2). Therefore, a substantial atmosphere would be required to decrease the radiative flux from the surface and thus to prevent quench crust formation.

I will now consider the plausibility of a thick early lunar atmosphere. It is possible that an early lunar atmosphere was generated by vapor outgassed by the LMO and/or water released by impacts. That was likely the case for the Earth, where an early steam atmosphere may have kept the surface from rapidly solidifying (i.e. forming quench crust) (Abe and Matsui, 1986). The Moon, however, is depleted in volatiles relative to Earth (Taylor and Wieczorek, 2014), and being less massive has a significantly larger surface area to mass ratio such that any atmosphere will be spread more thinly. Furthermore, the Moon formed at approximately the Roche limit (Canup, 2004). Thus, any initial atmosphere would have been highly susceptible to Roche lobe overflow (e.g. Repetto and Nelemans, 2014), especially considering the large scale height a hot early lunar atmosphere would have had. There are also other depletion mechanisms to consider including hydrodynamic escape (e.g. Pepin, 1991), impact removal (e.g. Melosh and Vickery, 1989) and charged particle interactions (e.g. Luhmann *et al.*, 1992). Thus, it seems unlikely that the Moon was able to retain a substantial atmosphere for at least 1,000 years (the approximate time required to start forming floatation crust according to Elkins-Tanton *et al.* (2011)). As such, I consider quench crust to have been present atop the LMO.

I use the work of Matson *et al.* (2006) for Loki Patera on Io as a model for quench crust formation and evolution. Their model considered Loki Patera to be a silicate 'magma sea' that is large enough to have negligible shore influence and deep enough to ignore floor effects. That model should be readily extensible to the LMO in which there were no shores and which was deep. Matson *et al.* (2006) also argued that though material that solidifies out of magma is generally denser than the magma itself and thus should sink (e.g. Walker *et al.*, 1980; Spera, 1992), solidified material should be buoyant due to trapped volatiles until it grows to a certain maximum thickness.

As solidified material gets thicker, additional material would be solidifying at greater depths meaning that the bubbles would be smaller and provide less buoyancy. As such Matson *et al.* (2006) argued at greater than approximately 7 m thickness (for magma on Io), the solidified layer should sink. Similarly, quench crust thicknesses have been estimated to be about 6 m for Hawaiian lava lakes (Rathbun *et al.*, 2002). This suggests that maximum quench crust thickness in the order of 10 m may be ubiquitous to silicate magmas on any planet. Hence, for this work, I allow quench crust to growth up to a nominal maximum thickness of 10 m.

Equilibrium quench crust thickness is calculated by equating the convective heat flux out of the LMO, the conductive heat flux through the quench crust, and the radiative flux from the top of the quench crust. Once the convective heat flux of the LMO has been calculated, I then calculate the temperature at the top of the quench crust by setting the convective heat flux from the LMO equal to the radiative heat flux from the quench crust surface using

$$T_{tq} = \Big(\frac{Flux^m_{conv}}{\epsilon\sigma} + T_e^4\Big)^{1/4}, \tag{3.7}$$

where T_{tq} is the temperature on top of the quench crust, $Flux^m_{conv}$ is the convective heat flux of the LMO, and T_e is the equilibrium temperature of the atmosphere. With the temperatures at the bottom and at the top of the quench crust defined, the thickness of the quench crust can then be calculating by setting the conductive flux through the crust equal to the convective flux of the LMO as given by

$$d_q = \kappa_q \rho_q c_q \frac{T_{melt} - T_{tq}}{Flux^m_{conv}}, \tag{3.8}$$

where d_q is the thickness of the quench crust, κ_q is the thermal diffusivity of quench crust, ρ_q is the density of quench crust, c_q is the specific heat capacity of quench crust, and T_{melt} is the melting temperature of quench crust.

Quench crust growth rate may be quantified using the Stefan problem (see Appendix B.2). However, since timesteps in this work are larger than the time required to form quench crust, I do not explicitly calculate quench growth at each iteration. Additionally, as stated above, an early lunar atmosphere may have affected quench crust stability.

Though I do not explicitly model an early lunar atmosphere, this formulation is sufficiently general to indirectly mimic an atmosphere (using emissivity and equilibrium radiative temperature).

3.2.2.2 Incorporating Re-impacts

At each iterative step, the code looks up the mass of debris that impacted onto the Moon during that timestep using the results mentioned in Section 3.2.1. As stated there, the mass of debris can be accurately quantified; however, the size distribution of the impactors is difficult to estimate due to the lack of constraints. In addition, even if a certain size distribution is assumed, it is unclear how hole diameter is related to the size and the velocity of an impactor. The diameter of a hole is also likely dependent on the crustal thickness and the strength of the crust, with both changing over time. As such, rather than attempting to model the production of individual holes at each timestep, I utilize a conversion factor, k, which is defined so that

$$A_{holes}(t_{step}) = \frac{M_{imp}(t_{step})}{k}, \tag{3.9}$$

where $A_{holes}(t_{step})$ is area of holes produced on the surface during a certain timestep and $M_{imp}(t_{step})$ is impacting mass during that same timestep. Thus, k has units of kg/m^2. This method allows me to characterize bulk properties of the thermal evolution of the LMO without making assumptions about the impactor size or velocity distributions or the process of hole production.

There are no true bounds for k, however very small values are unrealistic. For instance if $k = 10^3$ kg/m^2, that would mean that $\sim 4 \cdot 10^{16}$ kg of accreted mass (equivalent to a ~ 30 km object with a density of 3 g/cm^3) would produce an area of holes that is equivalent to the surface area of the Moon. For the lowest k value used in this work (i.e. $k = 10^5$ kg/m^2), $\sim 4 \cdot 10^{16}$ kg of accreted mass would produce an area of holes equal to about 1% of the lunar surface area or a single hole with a radius of about 360 km.

For this example, if the crustal thickness was 4 km, it means that impacting material is able to displace crustal mass about two orders of magnitude more than its own mass. On the other hand, larger values of k means that, though the Moon is accreting mass by impacts, the conditions are such that few to no holes are produced, with the no holes case represented by the limit where $k \rightarrow \infty$. This could be due to small impactors, low-velocity impactors, a thick crust, and/or a high strength crust. For the largest k value extremum I use $k = 10^9$ kg/m^2. In this case, only a small area of holes, equivalent to a single hole with a radius $\sim$ 4 km, is produced by my hypothetical 30 km impactor, which is again an unlikely scenario. To estimate what might be typical values, recall that the final lunar crust is around 45 km thick, and so thicknesses of around 10 km will be typical during LMO solidification. It seems reasonable to expect that a 10 km impactor could produce a hole of at least 10 km diameter in 10 km thick crust, which would correspond to $k \sim 10^7$. As such, the lower and upper bounds cover the range between a very intense bombardment that produces large hole areas and a very feeble bombardment that produces small hole areas, while I expect that values of k around 10^7 may be typical.

3.2.2.3 Distribution and Redistribution of Crustal Material

Though I do not explicitly model individual impacts, there are certain physical effects that need to be implemented in the code to make the calculations realistic. One such effect is to allow holes to be closed naturally by newly formed floatation crust. This is implemented by dividing newly formed floatation crust material between existing crust and holes according to the surface area covered by each. The other effects that need to be considered are allowing impacts to occur in both non-impacted and previously impacted areas of the Moon and the conservation of crustal material. To account for allowing impacts in both non-impacted areas and previously impacted areas, when a new hole area is generated it is divided between areas that do and do not contain holes according to the surface area of the Moon covered by each so that a uniform probability of impact at any point on the lunar surface is maintained.

To ensure conservation of crustal material, when new hole area is generated the volume of crust removed from the new holes is spread across the remainder of the lunar surface.

3.2.3 Convergence Tests

It is important to ensure that a sufficient number of volume segments (and equivalently sufficiently small timesteps) is used such that results are not dependent on the number of volume segments used. In particular, since the mass added to the Moon during any given numerical step is dependent on the timestep, too few volume segments (equivalently timesteps that are too large) will generate very large holes. The conservation and redistribution of crustal material will usually ensure that saturation, i.e. the total area of holes approaching the surface area of the Moon, is appropriately handled. If, however, the area of holes added in any time step is a large fraction of the surface area of the Moon there is a danger that this will break down and cause the total area of holes to exceed the surface area of the Moon. Since the conversion of impacting mass into hole area is governed by k the number of volume segments required for convergence will also depend on k. Therefore, I conducted a number of convergence tests by varying the impact intensity (i.e. k) and the number of volume segments to find the minimum number of volume segments required. For all convergence tests I used the nominal values listed in Table 2. Figure 8 shows the LMO solidification time for the convergence tests. Overall, the less intense the bombardment (i.e. higher k values which produce smaller hole areas) the fewer volume segments that are needed for convergence, as expected. When the largest debris is 100 km, for $k \geq 10^7$ kg/m^2, I find that 10^5 volume segments is sufficient. For $k = 10^6$ kg/m^2 I find that 3×10^5 volume segments is sufficient and for $k = 10^5$ kg/m^2 I find that 6×10^5 volume segments is sufficient. When the largest debris is 500 km, for $k \geq 10^7$ kg/m^2 I find that 1.5×10^5 volume segments is sufficient and for $k = 10^6$ kg/m^2 I find that 5×10^5 volume segments is sufficient.

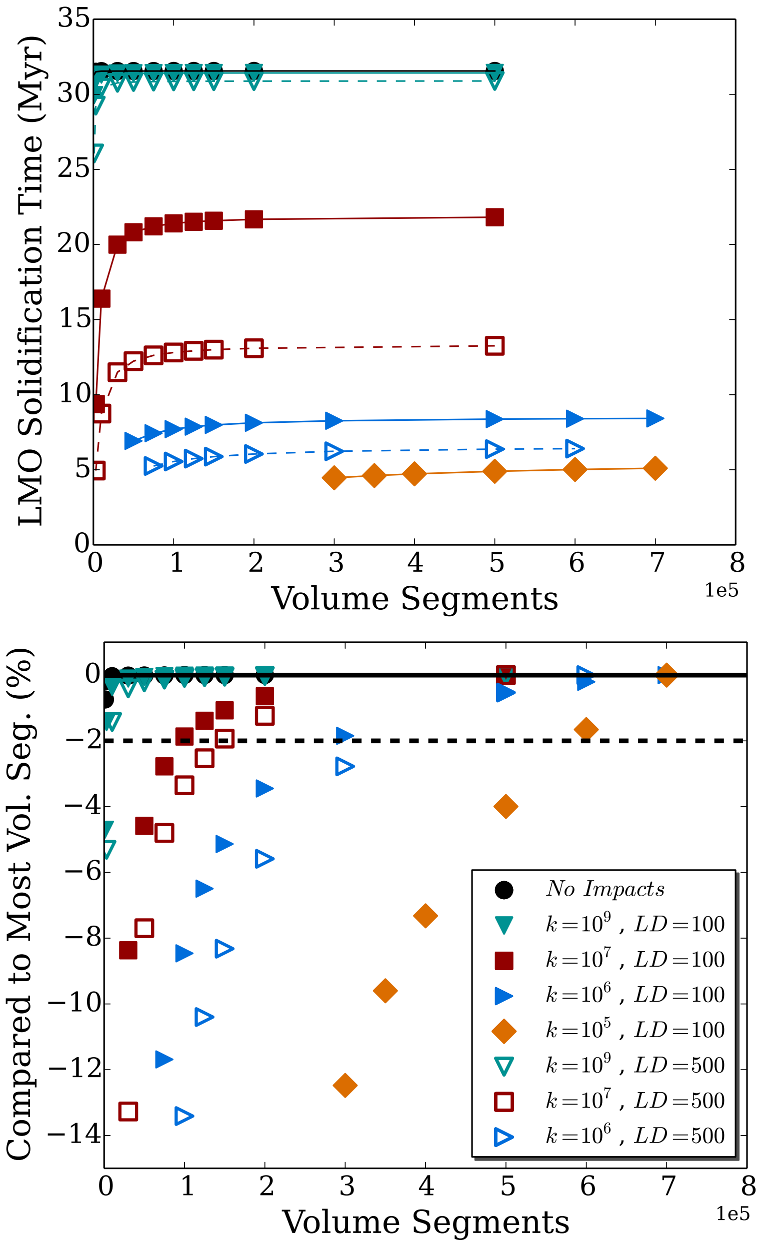

Figure 8: Convergence test of the LMO solidification time (on the top) for varying levels of impact intensity (i.e. k) as a function of the number of volume segments. Shown on the bottom is the difference between a solidification time and the solidification time with the most volume segments for a particular set. Colored markers and lines are used for the different k values. The filled markers and solid lines correspond to the case when the largest debris (LD) is 100 km. The open markers and dashed lines correspond to the case when the LD is 500 km. Black filled circles show the no impacts runs. Note that these are almost completely overlain by the $k = 10^9$ kg/m^2 points. The solid black line marks the 0% point and the dashed black line marks the -2% point (the point at which a particular k value is considered converged).

3.3 Results

3.3.1 Surface Area with Holes

In Figure 9 I show the effect of k on the percentage of the Moon's surface that has been impacted at the end of the iteration. For large values of k ($\sim 10^9$ kg/m^2), the percentage of the Moon with holes is close to zero and when k is small ($\leq 10^6$ kg/m^2), nearly all of the Moon's surface had holes after the LMO solidified. Since both newly formed crustal material and crustal material removed from newly formed holes are distributed equally across the lunar surface, the crust thickness of holes will not catch up to the crustal thickness of non-impacted areas. Therefore, holes should theoretically be identifiable at the end of the LMO solidification since their crustal thicknesses will be less than non-impacted areas. In Figure 9 I show results for two populations of debris, one with the largest object being 100 km in size (the nominal case) and one with the largest object being 500 km in size. For the 500 km case, the bombardment intensity does not decrease as rapidly as for the 100 km case (as shown in Figure 7), and as such, for a given k value, the 500 km case produces more holes. The runs for the various values of k had different numbers of volume segments to ensure convergence, as described in Section 3.2.3

3.3.2 Lunar Magma Ocean Solidification Time

In Figure 10 I show the fraction of the magma ocean remaining as a function of time for conditions matching those used by Elkins-Tanton *et al.* (2011), i.e. a 25 K equilibrium radiative temperature, which I refer to as the EBY11 cooling model. I find a similar, but slightly longer solidification time of 26 Myr for these conditions, compared with the $\sim$ 10 Myr found by Elkins-Tanton *et al.* (2011). This difference is likely because I did not explicitly model the fractional crystallization process like they did in their work.

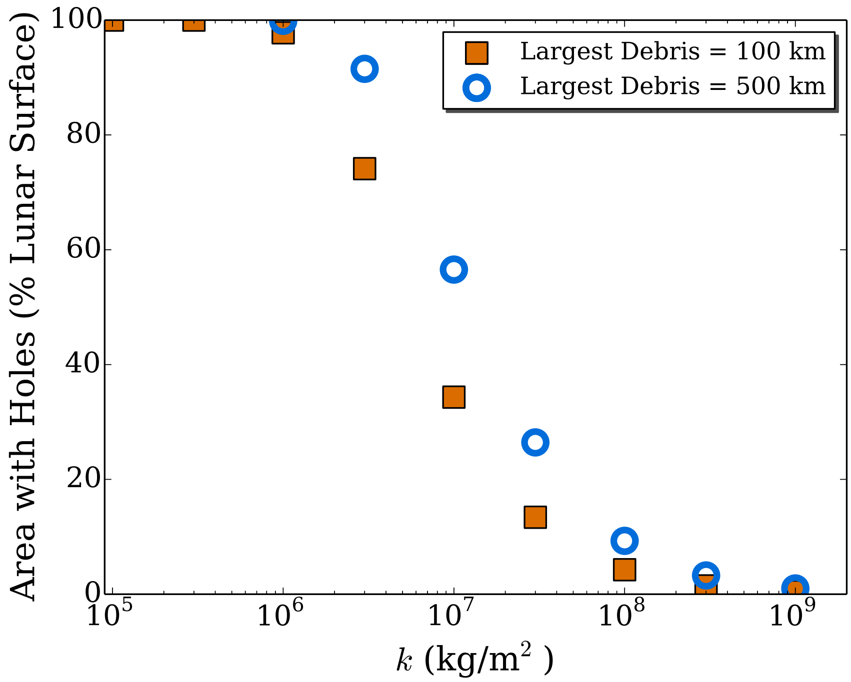

Figure 9: Surface area of the Moon that has holes at the end of the iteration as a function of k. Cases where the largest debris is 100 km in size is shown with closed orange squares, while cases where the largest debris is 500 km in size is shown with open blue circles.

That the difference is only a factor of $\sim$ 2-3 however reassures me that I am capturing the broad characteristics of the cooling process and that I can realistically explore the effect of re-impacts on the cooling process. Elkins-Tanton *et al.* (2011) does not consider quench crust, rather keeping the liquid surface of the magma ocean exposed to space until plagioclase formation begins. For the solid blue curve in Figure 10 I turn off the quench crust to replicate the fast early phase of Elkins-Tanton *et al.* (2011) in which the first 80% of the LMO solidifies, which here I find takes around 100 years. Though quench crust does not significantly alter the overall solidification time of the LMO, it prolongs the early, rapid cooling phase by $\sim 10^4$ years, as shown by the dashed orange curve in Figure 10.

In Figure 11 I show lunar crustal thickness over time as a function of k. As k is reduced, the time taken for the completion of crust formation (and solidification of the LMO) decreases substantially, from $\sim$ 32 Myr at $k \geq 10^9$ kg/m^2 to only $\sim$ 5 Myr at $k = 10^5$ kg/m^2.

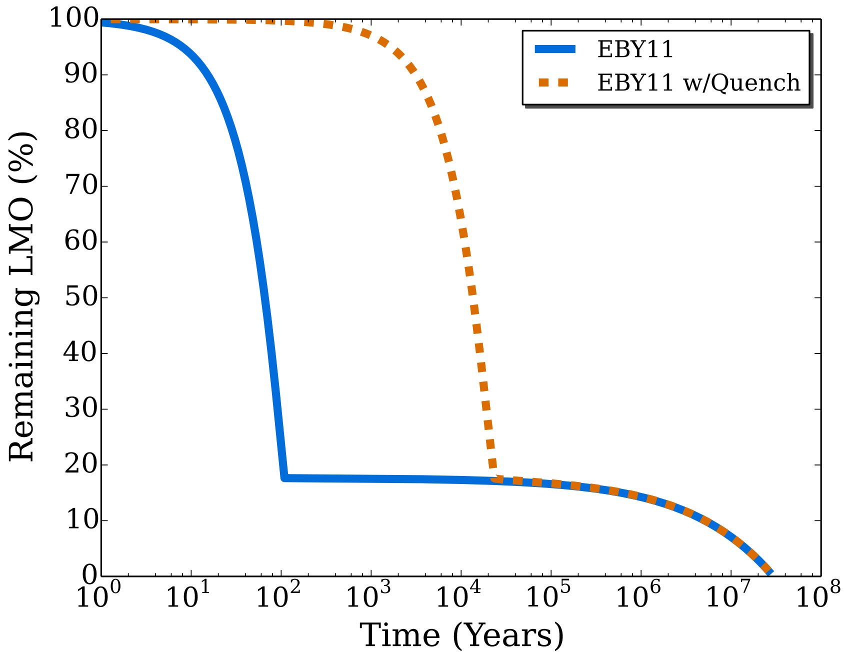

Figure 10: Fraction of magma ocean remaining over time. The EBY11 cooling model is shown by the solid blue curve and the EBY11 model with quench crust is shown by the dashed orange curve. In the EBY11 model, the initial rapid cooling is due to the thermally radiative global surface, while the slower cooling from $\sim$ 100 years onward is due to the presence of the thermally conductive global lid. The case with quench crust is similar to the EBY11 model, except the rapid cooling is delayed by $\sim 10^4$ years. Although nominally I used 250 K as the equilibrium radiative temperature, here I used a value of 25 K to approximate the temperature used in the EBY11 model.

For $k \gtrsim 10^9$ kg/m^2, the crust evolves as essentially identically to there being no holes generated by re-impacting debris. Nominally the number of volume segments used was 10^5; however, for $k = 10^6$ kg/m^2 and $k = 10^5$ kg/m^2 more volume segments (3×10^5 and 6×10^5 respectively) were used for convergence as noted above. Note that the difference between the 32 Myr here for large k values and the 26 Myr for the EBY11 model is due to the change from an equilibrium temperature of 25 K for the EBY11 model to my nominal equilibrium temperature of 250K.

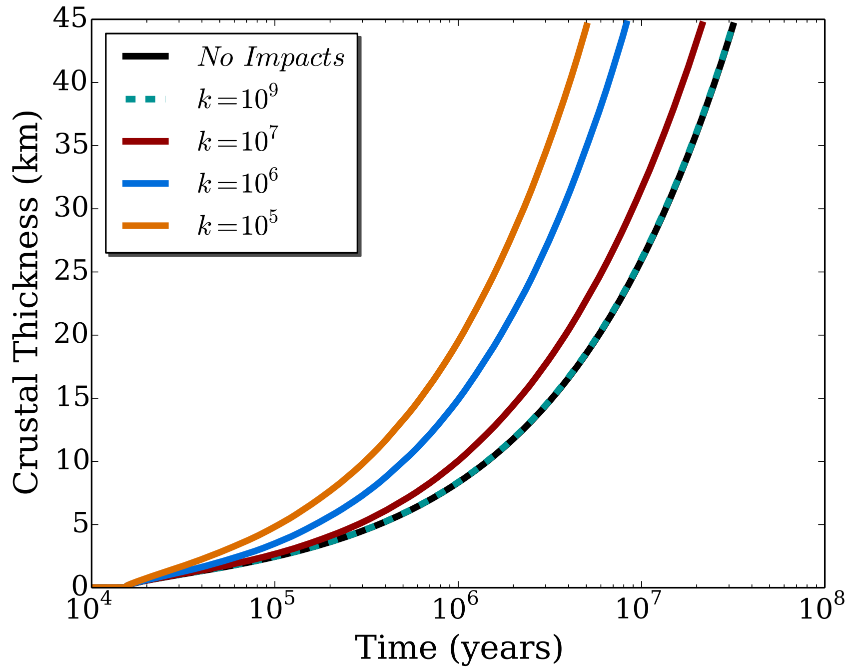

Figure 11: Crustal thickness over time for different k values (colored curves) compared to the no impacts case (black curve). The curve for the $k = 10^9$ kg/m^2 case is dashed so that the no impacts case is visible. All parameters aside from k are set at their nominal values as given in Table 2.

3.3.2.1 Model Parameter Sensitivity

Although I use the nominal input parameter values listed in Table 2 for the majority of this work, some of those parameters are subject to uncertainty. For example, estimates for the percentage by volume of the LMO that has to be solidified prior to plagioclase stability vary from 60% to 80% (Longhi, 1980; Snyder *et al.*, 1992; Elkins-Tanton *et al.*, 2011; Lin *et al.*, 2017b). Thus, it is important to evaluate the sensitivity of output parameters, particularly the solidification time of the LMO, to variability of input parameters. In Figure 12 I show the fractional change in LMO solidification time as a function of varying some of the model input parameters (with the exception of k and the LMO dynamic viscosity). Dynamic viscosity is not shown since it was varied over eight orders of magnitude.

Some input parameters have the same effect on the LMO solidification time whether impacts are or are not included. Three parameters, the maximum thickness of quench crust, the initial depth of the LMO, and emissivity have (nearly) no effect on the solidification time in either case. The insensitivity of the solidification time to the initial LMO depth is consistent with Solomon and Longhi (1977). This implies that having precise values for these three parameters is not vital. The equilibrium radiative temperature, depth at which plagioclase formation begins, and the heat of fusion and heat capacity of the LMO all correlate positively with the solidification time (i.e. increasing them increases the solidification time), which is as expected. Increasing the equilibrium radiative temperature, and increasing the depth at which plagioclase formation begins (which increases the final depth of the crust) both act to slow down the release of thermal energy from the LMO. Increasing the heat of fusion or the heat capacity of the LMO increases the total thermal energy that must be released during the solidification process. On the other hand, the heat capacity of the crust is negatively correlated with the solidification time. A higher heat capacity in the crust increases the conductive flux through the crust, and so I would expect it to decrease the solidification time.

Other parameters have different effects on the LMO solidification time depending on if there are impact generated holes or not. Dynamic viscosity and the melting temperature of quench crust have no effect on the solidification time when there are no impacts; however, when there are impacts dynamic viscosity is positively correlated and the melting temperature is negatively correlated with the solidification time. When there are impacts, varying dynamic viscosity from 1 to 10^8 Pa·s results in a -35% to 7% change in the solidification time. Lower dynamic viscosity values would increase Ra, which through Nu would lead to a thinner quench layer (see Section 3.2.2.1) and thus would decrease the solidification time by increasing the thermal flux. Lower values of the melting temperature of quench crust will have the opposite effect since it will reduce the conductive flux through quench crust by decreasing the temperature at the bottom of quench crust (i.e. its melting temperature).

The heat capacity of the quench crust and the slope of the adiabat also have no effect on the solidification time when there are no impacts but when there are impacts, they have a small correlation with the solidification time. The positive correlation of the quench heat capacity arises for exactly the same reason as the positive correlation with the heat capacity of the plagioclase floatation crust. On the other hand, the negative correlation of the adiabat slope is due to smaller values reducing the temperature difference between the bottom and top of the LMO and thus decreasing the thermal flux out of the LMO.

From Figure 12 it can be seen that the LMO solidification time is most sensitive to the depth at which plagioclase starts to form and the heat capacity of the crust. This is consistent with the work of Minear and Fletcher (1978). As mentioned previously, there is a range of estimated LMO depths at which plagioclase becomes stable. The depth could be about the nominal value used in this work (i.e. 100 km) or as deep as 250 km (Longhi, 1980; Snyder *et al.*, 1992; Elkins-Tanton *et al.*, 2011; Lin *et al.*, 2017b). Since I do not model the geochemistry, I limit the variable change of the plagioclase stability depth since varying it significantly changes the final crustal thickness. With or without impacts, when I set the depth to 70 km, the final crustal thickness was 31 km and when I set the depth to 130 km, the final crustal thickness was 58 km. It is plausible that the thickness of the primordial lunar crust was greater than the average crustal thickness today. However, I do not explore that possibility in this work. Overall, these results indicate that the LMO solidification is primarily governed by the conductive flux through the crust, which is both a function of its thickness and its thermal properties (i.e. specific heat capacity).

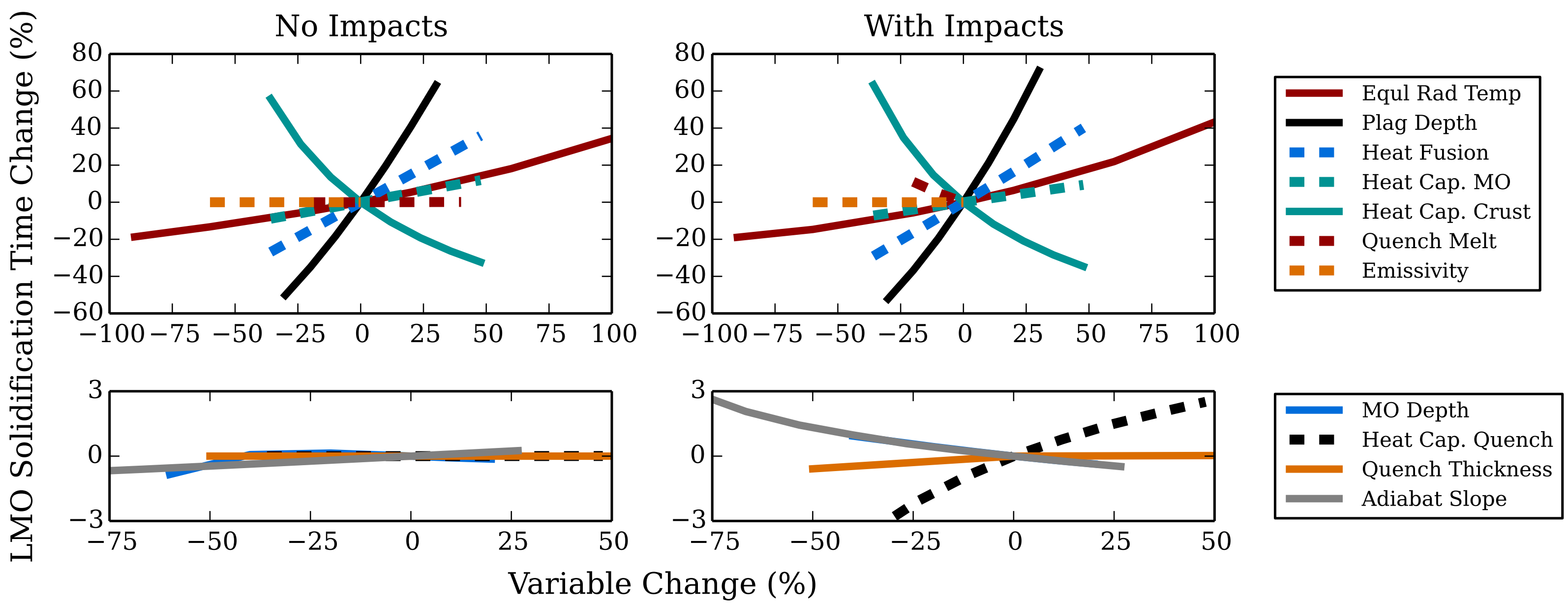

Figure 12: Sensitivity tests for the change of the LMO solidification time from the nominal value due to the variation of one input parameter at a time. The no impacts runs are shown on the left and the with impacts runs ($k = 10^7$ kg/m^2) are shown on the right. For clarity, the figure is split so that the larger changes in LMO solidification time are shown on the top panels and the smaller changes in LMO solidification time is shown on the bottom panels.

3.3.3 Kinetic Energy Imparted by Re-impacting Debris

As mentioned in Section 3.2.1, re-impacting debris will not only produce holes in the lunar crust but they will also impart thermal energy due to their kinetic energy (see Figure 13). Thus far I have only considered the effect of re-impacting debris producing holes. In Figure 14 I show the variation of the LMO solidification time as a result of different assumptions regarding the efficiency by which the impactors' kinetic energy is converted to thermal energy. I define that efficiency, λ_{KE}, to range from 1 (all of the kinetic energy is converted to thermal energy) to 0 (none of the kinetic energy is converted to thermal energy). When kinetic energy is not considered, the effect of re-impacting debris is to reduce the LMO solidification time from ~ 32 Myr ($k = 10^9$ kg/m^2) to ~ 5 Myr ($k = 10^5$ kg/m^2). Interestingly, when I consider both hole production and thermal energy impartment by re-impacting debris, the LMO solidification time may be longer or shorter than the no impacts solidification time (i.e. ~ 32 Myr). If fewer holes are produced (i.e. $k > 10^7$ kg/m^2) and impacts are efficient at delivering thermal energy (i.e. $\lambda_{KE} > 0.5$), the LMO solidification time is greater than its value when impacts are not considered. On the other hand, regardless of λ_{KE}, if impacts generate a larger number of holes (i.e. $k < 3 \times 10^6$ kg/m^2), the LMO solidification time is less than its value when impacts are not considered. Thus, there are particular values of k and λ_{KE} that balance the increased amount of heat out due to holes and the additional heat input due to the kinetic energy of impacts. This would mean that for those values of k and λ_{KE}, the LMO solidification time would be the same, with or without impacts.

The number of volume segments used for the different values of k are the same as mentioned early. However, for $\lambda_{KE} = 1$, $k = 3 \times 10^8$ kg/m^2 required 5×10^5 volume segments and $k = 10^6$ kg/m^2 required 6×10^5 volume segments for convergence. For $\lambda_{KE} = 0.5$, $k = 3 \times 10^8$ kg/m^2 required 5×10^5 volume segments, $k = 10^5$ kg/m^2 required 7×10^5 volume segments, and $k = 3 \times 10^5$ kg/m^2 required 10^6 volume segments. The larger number of segments required is a result of the increased amount of heat that must be lost from the LMO when impactor kinetic energy is considered.

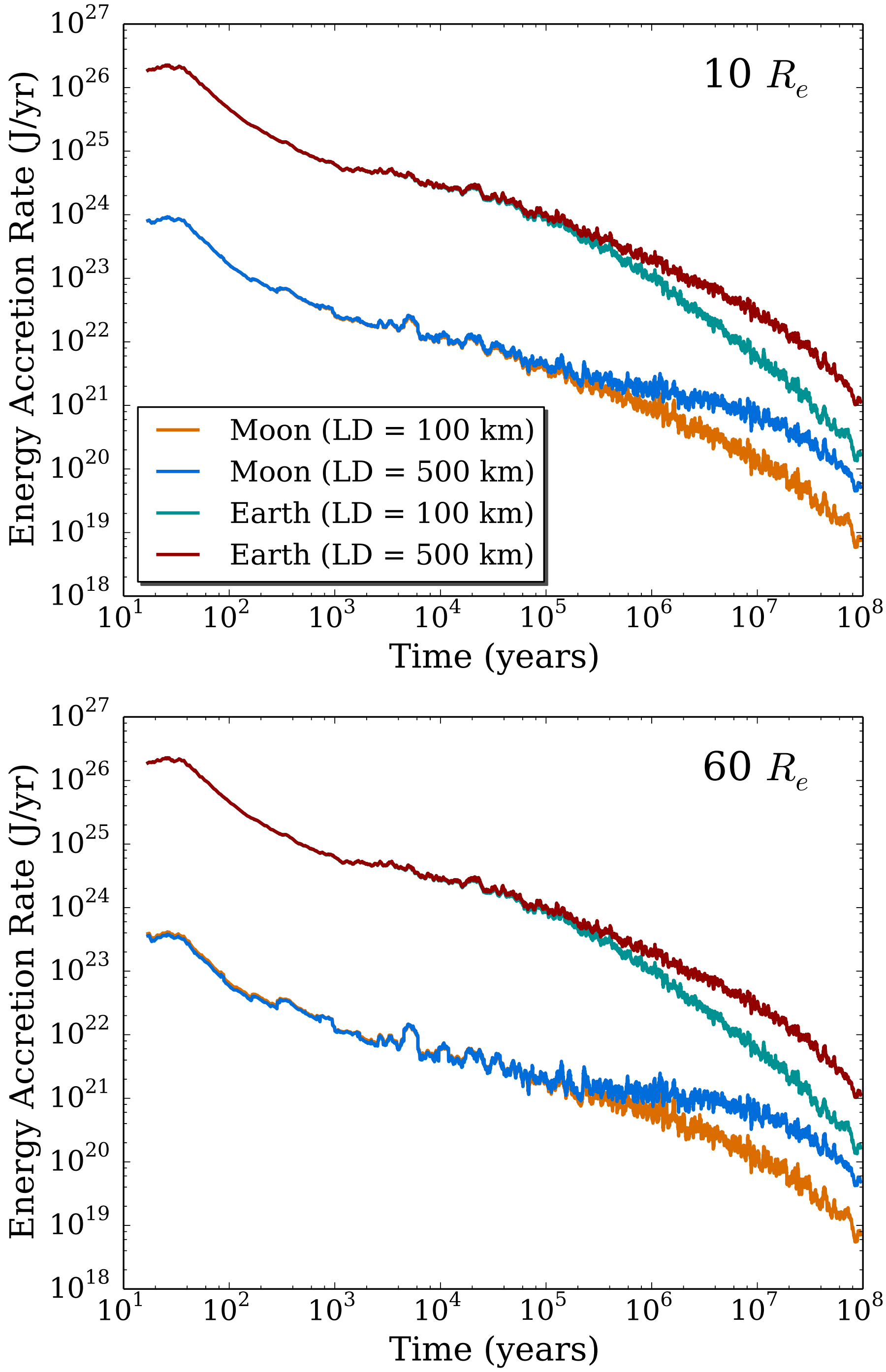

Figure 13: Energy accretion rate over time for the Earth (dark cyan and red lines) and the Moon (blue and orange lines) for two populations of re-impacting debris based on the size of the largest debris (LD). On the left is the accretion rate when the Moon is at a distance of 10 Earth radii and on the right when it is at a distance of 60 Earth radii.

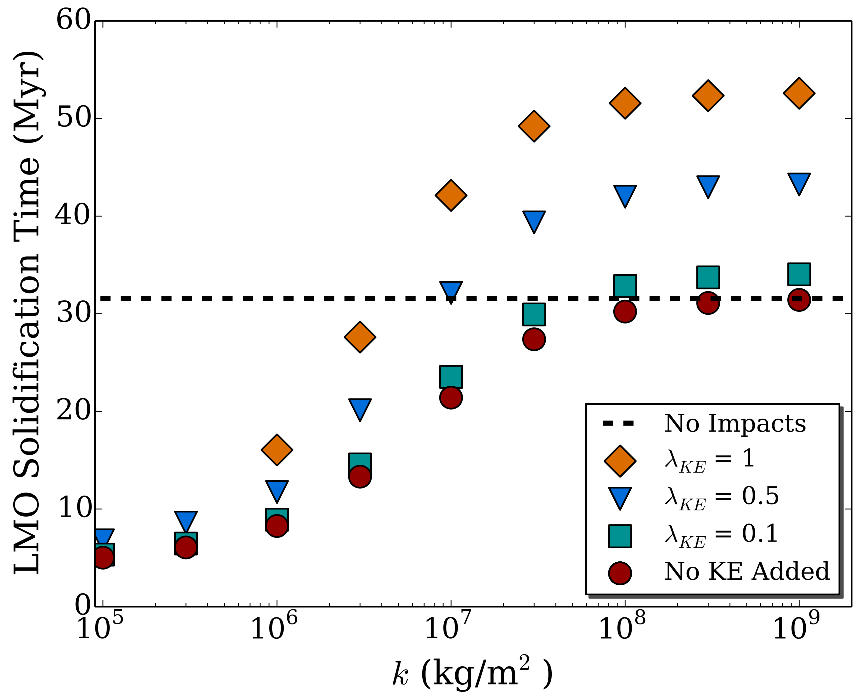

Figure 14: LMO solidification time as a function of k for different assumptions regarding kinetic energy imparted by re-impacting debris. λ_{KE}, kinetic energy efficiency, of 1 signifies that all of the kinetic energy of the impactors was imparted as thermal energy. The no impacts solidification time is shown with a dashed black line for reference.

3.3.4 Concentrating Floatation Crust into Holes

So far I evenly divided newly formed floatation crust between existing crust and holes according to the surface area covered by each. It may be expected that more of the newly formed plagioclase would be drawn to the holes for a number of reasons. Due to the increased thermal flux from the holes it is likely that convective upwellings would be located beneath them, which could concentrate new floatation crust into the holes. Additionally, in much the same way as a ball will tend to roll down a hill, since the holes represent highs in the topography of the base of the crust buoyant material will tend to roll towards the holes. The nominal case has an enhancement factor (f_e) of 1, such that equal amounts of new floatation crust per unit area go to both the holes and the rest of the crust, but I can vary f_e to force more floatation crust into the holes.

Using the nominal values with $k = 10^7$ kg/m^2 and $f_e = 1$, the LMO solidification time is ~ 21 Myr. LMO solidification time increases to ~ 27 Myr and ~ 29 Myr for $f_e = 3$ and $f_e = 10$ respectively, with even higher f_e values producing results that are very similar to the $f_e = 10$ case. Another outcome of interest is the surface area of the Moon that has holes at the end of the iteration. Holes are considered closed when their crustal thickness is equal to the non-impacted crustal thickness. Thus, in the nominal case, holes do not close since their crustal thicknesses will always be less than the non-impacted crustal thickness. If holes acquire an enhanced amount of floatation crust, they will close and thus reduce the area of the Moon that has holes at the end of the iteration. That area is 34% for the nominal case, while it is 3% and 0.7% when $f_e = 3$ and $f_e = 10$ respectively. Though floatation crust enhancement has a significant effect on the surface area of holes; overall, it has little effect on the LMO solidification time.

3.4 Discussion

3.4.1 Reconciling Crust Sample Ages with the Magma Ocean Solidification Time

The LMO model predicts that the ages of the primordial lunar crust will be determined by the LMO solidification time. Assuming that lunar crustal ages have not been reset, the crust that formed from the floating anorthosite rocks should have an age that decreases with increasing depth below the surface. I would expect the age difference between the top and bottom layers of the crust should approximately be the time that it took for the last 20% of the LMO to solidify. Age dating of lunar FAN samples have implied that the LMO may have taken over 200 Myr to solidify (Alibert *et al.*, 1994; Borg *et al.*, 1999). However, geochemical modeling work by Elkins-Tanton *et al.* (2011) showed that the LMO should have taken about 10 Myr to solidify, and I find a maximum solidification time of around 50 Myr with the probably somewhat unrealistic scenario of minimal hole puncturing and maximal impact energy deposition.

Therefore, there is a discrepancy between the lunar crust sample ages and cooling models of the LMO. The reasons for this discrepancy may be due to one or both of the following: misinterpretation of lunar crust sample ages or the presence of additional heat sources for the LMO. I will discuss each of these in turn.

It is possible that the primordial lunar crustal ages do not actually span 200 Myr. As discussed by Borg *et al.* (2011), some FAN samples, such as sample 60025 with an age of 4.360 ± 0.003 Gya, may have recorded more recent melting events rather than the formation time of the primordial lunar crust. If this is the case, then samples with older ages such as samples 67016c (4.53 ± 0.12 Gya, Shirley 1983), 67075 (4.47 ± 0.07 Gya, Nyquist *et al.* 2010), and Y-86032 (4.43 ± 0.03 Gya, Nyquist *et al.* 2006) may have recorded the crystallization time of the primordial crust, while the younger samples may have recorded more recent re-melting events. These melting evens may be due to both 'background' asteroidal impacts (Nyquist *et al.*, 2006; Rolf *et al.*, 2017) and re-impacting debris (Taylor *et al.*, 1993). Evidence to the recrystallization of some parts of the lunar crust is given by both Ogawa *et al.* (2011) and Yamamoto *et al.* (2015) who argue that high-calcium pyroxene material near young lunar craters was due to re-differentiation of the primordial anorthosite crust due to impacts. To help elucidate these ages, it may be possible to delineate ages by the crystallization time of ur-KREEP material, which is estimated to have taken place at 4.368 ± 0.029 Gya (Gaffney and Borg, 2014; Borg *et al.*, 2015). If ur-KREEP is identified with the final, incompatible remnant dregs of the LMO, the ur-KREEP crystallization time would represent an upper limit to the LMO solidification time since it must have solidified after the rest of the LMO. Hence, if I assume that the LMO solidification time is given by the difference between the ages of the oldest crust samples and the time of ur-KREEP crystallization, the crust samples would then indicate that the LMO solidification time was less than 160 Myr instead of 200 Myr. Taking the ur-KREEP crystallization time as an upper limit to the LMO solidification time improves the discrepancy between crustal age estimates and modelling, though it does not remove it completely.

That the ur-KREEP crystallization time is itself discrepant with some of the measured crustal ages is however suggestive that some re-examination of crustal age measurements may be in order.

As mentioned in Section 3.2.2, additional heat sources would have likely influenced the thermal evolution of the LMO. For example, Meyer *et al.* (2010) suggested that tidal heating may have extended the LMO solidification time to 272 Myr. To explore this effect on the LMO, my code allows for additional constant heating. I use that to estimate the effects of heat sources such as tidal and radiogenic heating. Such heating is often approximately constant for the time interval of interest (e.g. Meyer *et al.*, 2010). Using the nominal input parameter values, I varied this constant heating rate to see the result on the LMO solidification time. In Figure 15 I show the solidification time as a function of additional heating for the no impacts case and three impacts cases (with $k = 10^5$, 10^6 & 10^7 kg/m^2). For the no impacts case, a heat rate of about 2.4×10^{12} W is sufficient to increase the LMO solidification time to about 300 Myrs. When impacts are included, higher heat rates are required to increase the LMO solidification time to about 300 Myrs. For the case where $k = 10^7$ kg/m^2, the required heat rate is between 3.4 to 4.5×10^{12} W depending on λ_{KE}. For the case where $k \leq 10^6$ kg/m^2 the required heat rate is more than 1.2×10^{13} W. Meyer *et al.* (2010) suggested that the typical tidal heating rate is around 6×10^{11} W, lower than the roughly 10^{12} W provided by radiogenic heating. This would not be sufficient to significantly increase the solidification time of the LMO if impact generated holes play an important role. Calculations by Chen and Nimmo (2016) however suggest larger typical tidal heating rates of $\sim 4 - 8 \times 10^{12}$ W. Tidal heating at these rates would be sufficient to substantially extend LMO solidification provided that hole production is moderate ($k > 10^6$ kg/m^2). Tidal heating rates can be much higher than these typical values when the lunar orbit passes through resonances (e.g. Touma and Wisdom, 1998), however these very high rates are short lived and occur early in the tidal evolution of the Moon. Existing work thus suggests that tidal heating can only provide a large increase to the LMO solidification time if hole generation is not too vigorous.

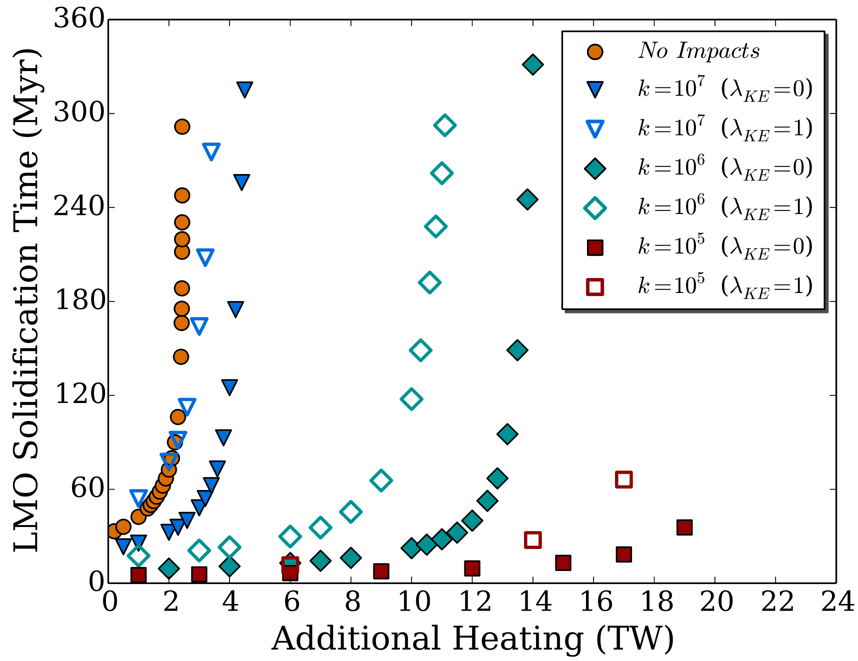

Figure 15: LMO solidification time as a function of additional constant heating. The without impacts case is shown with orange circles. The with impacts and with $\lambda_{KE} = 0$ cases are shown with filled markers: blue triangles ($k = 10^7$ kg/m^2), dark cyan diamonds ($k = 10^6$ kg/m^2), and dark red squares ($k = 10^5$ kg/m^2). The corresponding $\lambda_{KE} = 1$ cases are shown with unfilled markers. The impact rate decays inversely with time beyond 100 Myr.

When considering the lunar crust sample ages, a caveat is that those samples are likely from the upper layers of the lunar crust. This means that we may be measuring time periods that only partially cover the time that it took for the LMO to solidify. It may be possible to obtain crust samples from the bottom of the crust by sampling certain impact craters, such as Moscoviense and Crisium, which may have been excavated down to the mantle (Wieczorek *et al.*, 2013). However, such samples are unlikely to solve the discrepancy between the LMO solidification times estimated by sample ages and those estimated by modeling work. A partial sampling of the upper crust would mean that the estimates based on crust samples, which are already much longer than estimates from modeling, should be even longer.

3.4.2 Implications for the Lunar Surface

Re-impacting debris may have affected the primordial lunar crust by shock heating it, by puncturing holes into it, and by adding material onto it. While some of the changes to the crust caused by re-impacting debris may not be detectable today (such as crustal thickness variations due to refilled holes), there may be other effects that are recognizable. One potential effect, resetting of crustal ages by impacts, has already been mentioned in the previous section (Section 3.4.1). In the same manner, re-impacting debris may have produced feldspathic granulitic impactites (Simonds *et al.*, 1974; Warner *et al.*, 1977) and granulitic noritic anorthosites (McLeod *et al.*, 2016). Re-impacting debris may have also aided the enrichment of ^{37}Cl in lunar samples due to the degassing of ^{35}Cl (Sharp *et al.*, 2010; Boyce *et al.*, 2015) by breaching the primordial lunar crust (Barnes *et al.*, 2016). Another consequence of breaching the crust is that quench crust would form in newly created holes. If the lunar surface was saturated with holes (i.e. $k \leq 10^6$ kg/m^2), at the completion of the LMO solidification approximately $\sim 1 \times 10^{18}$ kg (0.02% of the lunar crust by mass) of quench crust would have formed and been incorporated into the primordial lunar crust. Lastly, re-impacting debris would have added material onto the lunar crust. As such, the early lunar crust should have comprised of largely anorthosite rock with some debris component, which had a similar composition to the original debris of the Moon-forming impact. I may assume that the LMO solidified in 60 Myr based on the average age differences between four samples (i.e. FAN sample 60025, norite samples 77215 and 78236/8, and troctolite sample 76535) that met all five of the reliability criteria identified in Borg *et al.* (2015). In that case, $\sim 2 \times 10^{18}$ kg of re-impacting debris (0.05% of the lunar crust by mass) would be added onto the crust after the solidification of the LMO, which would be higher if the LMO solidified faster and if some fraction of impacting material does not penetrate the crust, but remains on the surface.

3.4.3 Implications for the Lunar Interior and Orbital Evolution

Re-impacting debris that punctured holes in the crust would have made the LMO an open magmatic system (e.g. O'Hara, 1977) and thus may have altered its geochemical evolution. Periodically adding material that has the composition of the initial debris created during the Moon-forming impact may have altered the fractional crystallization process of the LMO. In this work, $\sim 2 \times 10^{20}$ kg of re-impacting debris would be added to the LMO. While this is a small fraction (0.33%) of the initial LMO mass, addition of external material would become more significant as the LMO mass decreases. Thus, future geochemical modeling should allow for open system behavior to consider what effect it may have, both in the addition of material from debris and in loss of volatiles through degassing. One possible result of this may be the considerable variability of zinc in lunar anorthosite samples (Kato *et al.*, 2015). Another may be the heterogeneous distribution of water in the lunar interior. If debris stored and periodically added water to, or allowed it to be selectively degassed from, hole regions it may explain the contradiction between works claiming the Moon to be hydrous (Saal *et al.*, 2008; Boyce *et al.*, 2010; McCubbin *et al.*, 2010) and works claiming it to be anhydrous (Taylor *et al.*, 2006a; Sharp *et al.*, 2010). Importantly, water content also controls the stability of plagioclase, with more water delaying plagioclase formation (Lin *et al.*, 2017a).

As discussed in Section 3.4.1, tidal heating is not only a possible external heat source for the LMO, but it may also be required to explain the range of lunar crust sample ages. Tidal heating is largely dependent on the eccentricity and the semi-major axis of the lunar orbit. Nonetheless, Tian *et al.* (2017) showed that the Moon's initial tidal quality factor, Q, and rigidity along with how those values change over time are important to its orbital evolution. Both Q and rigidity are linked to the internal structure of the moon, particularly the fraction that is liquid. As such the thermal evolution and the orbital evolution of the Moon are coupled. Previous work such as Meyer *et al.* (2010) and Chen and Nimmo (2016) considered this coupling but they did not include the effect of re-impacting debris.

Tides may also affect the holes themselves by producing cracks along lines of maximum stress. This should be more pronounced given that these surfaces are already weakened by impacts. Thus, tidal stress may make holes larger and prolong their closure, which can be explored in the future using finite element modeling.

3.5 Conclusions

The Moon likely formed after a giant impact. A large quantity of debris from that impact escaped the Earth-Moon system and subsequently returned over a period of 100 Myr. During that time, the Lunar Magma Ocean (LMO) would have been solidifying with an early quench crust, followed by an anorthositic crust on its surface. Re-impacting debris would have affected the thermal evolution of the LMO by puncturing holes into the crust and delivering thermal energy to the LMO. Holes that were produced would have increased the thermal flux that was initially limited by the conductive crust. While that would have sped up the solidification of the LMO, thermal energy imparted by impacts would have done the reverse, to an extent that is not yet clear. By investigating a wide range of possible values for the amount of hole generation and the efficiency of kinetic energy conversion by impacts, I suggest LMO solidification times ranging from $\sim$ 5 Myr to $\sim$ 50 Myr at the extrema. Given that the range of lunar crust sample ages may be 60 to 200 Myr, the lower estimates for the LMO solidification time would require one or more additional heat sources (e.g. tidal heating), potentially with very high heating rates to make the LMO solidification time consistent with the range of lunar crust sample ages. At the higher end, with moderate hole generation and efficient kinetic energy deposition, this work suggests that the amount of tidal heating required to bring the LMO solidification time into concordance with lunar crust sample ages may be less than previously thought, especially if the age span of samples that truly date LMO solidification is closer to 60 Myr rather than 200 Myr. With this simple model I have provided insight into how re-impacting debris influences the cooling time of the LMO.

Nonetheless, further work is still needed to integrate all aspects of the early thermal evolution of the Moon, including geochemistry, re-impacting debris, tides and crustal structure.

Chapter 4

STUDENTS IN FULLY-ONLINE PROGRAMS REPORT MORE POSITIVE ATTITUDES TOWARD SCIENCE THAN STUDENTS IN TRADITIONAL, IN-PERSON PROGRAMS

The mind is not a vessel to be
filled, but a fire to be kindled.

Plutarch

Following the growth of online, higher-education courses, academic institutions are now offering fully-online degree programs. Yet, it is not clear how students who enroll in fully-online degree programs are similar to those students who enroll in in-person ("traditional") degree programs. Since previous work has shown students' attitudes towards science can affect course performance, it is valuable to ask how attitudes towards science differ between these two populations. I studied students who completed a fully-online astrobiology course. In an analysis of 451 student responses to the Classroom Undergraduate Research Experience (CURE) survey, I found online program students began the course with a higher scientific sophistication and a higher sense of personal value of science than those in traditional programs. Pre-course attitudes also showed some predictive power of course grades among online students, but not for traditional students. Given established relationships between feelings of personal value, intrinsic motivation and, in turn, traits such as persistence, these results suggest that open-ended or exploration-based learning may be more engaging to online program students due to their pre-existing attitudes. The converse may also be true, that certain pre-existing attitudes among online program students is more detrimental than it is for traditional program students.

4.1 Introduction

Online courses have proliferated and are being offered by many colleges and universities as part of their broader distance education options. In the United States, 70.7% of all institutions of higher education and 95% of institutions with enrollment greater than 5,000 students offer distance education (Allen and Seaman, 2015). In addition, 28% of students in higher education use distance learning for some of their coursework (Allen *et al.*, 2016). While many students take only a few courses online, an increasing number are enrolling in fully-online degree programs (National Center for Education Statistics, 2014). A number of factors such as the wider availability of technology, difficult economic conditions, and changing perceptions of the quality of online education have contributed to increasing popularity of online platforms, by making learning more affordable, accessible, and personalized (Means *et al.*, 2014).

Research has been done to understand why students do or do not choose to take online courses instead of traditional courses (Jaggars, 2014). There are clear advantages to online courses, such as a more flexible schedule for those balancing family, work, and school. There are also potential disadvantages, such as the fact that some students are unwilling to enroll in fully-online degree programs out of a desire to maintain a connection to the campus (both the location and the people) and to have a better connection with the instructor (Jaggars, 2014). However, online students may be alleviating this disadvantage by traveling to the campus. Clinefelter and Aslanian (2017) found that 59% of respondents to their nationwide survey travelled to the campus in which they were enrolled (between one to five times per year). The process of weighing these advantages and disadvantages implies that there will be systematic differences in preferences, financial circumstances, and family considerations between students who ultimately choose to enroll in fully-online degree programs and those who do not.

The extent to which these differences extend to differences in attitudes toward academics in general, attitudes toward specific subjects, and the efficacy of specific strategies is unclear. Therefore, I focused on students' attitudes toward science and how those attitudes may affect their performance in science courses.

Attitude is an expansive topic in psychology (cf. Bohner and Dickel, 2011); nevertheless, for this work, I focus on explicit attitudes and use the definition for "attitude" from Eagly (1992): "a tendency or state internal to a person which biases or predisposes a person toward evaluative responses which are to some degree favorable or unfavorable." Attitudes, in the context of learning, fall within the broader characterization of affect. However, in the human brain, cognition (which includes attention, language, memory, planning, and problem solving) and affect (which includes attitudes, emotions, interests, and values) do not operate entirely separately from one another (e.g. Pessoa, 2008). If they were independent, it would be unnecessary to consider affect in the context of education. However, since cognition and affect are integrated and influence each other (e.g. Shiv and Fedorikhin, 1999; Dolan, 2002), it is not only vital to study how they interact with one another but also how they relate to behavior. All three–affect, cognition, and behavior–are important to learning.

Elements of student affect, such as interest in the subject and perceived value of the skills and content taught, have previously been argued to be important to learning (e.g. Koballa and Glynn, 2007; van der Hoeven Kraft *et al.*, 2011; McConnell and van der Hoeven Kraft, 2011; Fortus, 2014; Lin-Siegler *et al.*, 2016). However, the question may be asked as to how exactly student affect is linked to cognition and behavior. Previous works have, for example, considered how attitudes may be the cause of certain behaviors. However, there are alternative ideas such as attitudes following behaviors and attitudes and behaviors being reciprocal (Shrigley, 1990). There are a number of examples where attitudes do not seem to correlate with behavior (e.g. LaPiere, 1934; Kutner *et al.*, 1952). For example, in a study by Corey (1937) of sixty-seven university students who were taking an introductory educational psychology course, students who stated that cheating was wrong still changed their own exam responses when given the opportunity to grade their own work.

Additionally, it has been shown that attitudes towards biology were largely independent of whether or not a student majored in biology (Rogers and Ford, 1997), showing that the decision to major does not imply a particular attitude toward the subject. These studies may imply that human behavior is primarily unconscious and in turn that attitudes have little, if any, control over behavior. However, studies have shown that imagining oneself successfully completing a task can improve performance (e.g. Sanders *et al.*, 2004; McGlone and Aronson, 2007) and that even false memories can measurably change behavior (Geraerts *et al.*, 2008). Thus, a recent review concluded that human behavior is the result of both conscious and unconscious processes (Baumeister *et al.*, 2011).

Since the link between affect and behavior is complex, past research on student affect and behavior have yielded mixed and often contradictory results. For example, though Hough and Piper (1982) and Steiner and Sullivan (1984) found that students' attitudes towards the subject positively correlated with their performance, Rogers and Ford (1997) found a negative correlation between final course grade and attitude gain. Studying students' attitudes is further complicated by the fact that they are functions of the classroom environment (e.g. McMillan and May, 1979), discipline or topic (e.g. Ramsden, 1998), student's culture (e.g. Krogh and Thomsen, 2005; Ainley and Ainley, 2011), family background (e.g. Turner *et al.*, 2004), student's age or grade level (e.g. Prokop *et al.*, 2007) and student's gender (e.g. Simpson and Oliver, 1985; Weinburgh, 1995; Jones *et al.*, 2000; Miller *et al.*, 2006; Liu *et al.*, 2010). These complexities indicate that further research is necessary to better understand connections among student affect, cognition, and behavior.

The study described here compares the attitudes toward science of two groups of students: (1) those enrolled in fully-online degree programs and (2) those enrolled in traditional, in-person degree programs. Students in both groups were enrolled in an identical online, introductory astrobiology course. The intent was to contribute to the larger body of research on connections among affect, cognition, and behavior; and to the still-limited body of research into online science learning. From this work, I make recommendations to improve future online courses and programs for both types of students.

4.2 Methods

4.2.1 The course and the studied population

Habitable Worlds is a 7.5-week, fully-online course intended for non-science majors, which satisfies a general-education laboratory science credit requirement for graduation at Arizona State University (ASU). The course and its design are described in more detail by Horodyskyj *et al.* (2017). The course is open to enrollment for students in traditional degree programs (in which it is identified as an I-COURSE) and for students in fully-online programs (in which it is identified as an O-COURSE).

This study was conducted according to a research protocol approved by the Institutional Review Board at ASU (Study #00003679). A total of 774 out of 941 students who took the course in the Fall 2014, Spring 2015, and Fall 2015 semesters consented to having their survey responses and course data used for this study. I further limited the analysis to students who completed the course and responded to all of the survey items ultimately included in the analysis (see Section 4.3.1). This left 451 students as the main sample population for this study.

The sample population had a nearly equal number of I-COURSE students ($n_i = 232$) and O-COURSE students ($n_o = 219$). Student ages ranged from 18 to 58 years. Overall, the course not only had a higher percentage of self-identified White students than the university average, but also higher than the nationwide average of 63% self-identified White students reported by (Clinefelter and Aslanian, 2017). While the O-COURSE group had more females than the university average, the difference was not as great as in Clinefelter and Aslanian (2017) who found that 75% of online students identified as female. The demographic data (all self-identified) of the students are listed and compared to those of ASU as a whole in Table 3.

Table 3: Demographic data (as percentages) for the Habitable Worlds I-COURSE and O-COURSE students compared to the university as a whole (average data are for the Fall 2014 semester of all ASU undergraduates).

Demographic data (self-identified)		I-COURSE students (n_i = 232)	O-COURSE students ($n_o = 219$)	University Average (undergraduates)
Sex	Male	50.9%	45.2%	50.8%
	Female	49.1%	54.8%	49.2%
Ethnicity	American Indian/Alaska Native	1.7%	0%	1.6%
	Asian	3.4%	1.8%	5.8%
	Black/African American	3.4%	4.1%	5.0 %
	Hispanic/Latino	17.2%	16.4%	20.2%
	International	2.2%	1.4%	7.1%
	Native Hawaiian/Pacific Islander	0%	0%	0.3%
	White	69.0%	72.2%	55.4%
	Two or more races	3.0%	3.6%	3.9%
	Unknown	0%	0.5%	0.9%
Mean Age (years)		23	31	22

4.2.2 The survey

The learning design of Habitable Worlds emphasizes scientific practices and often asks students to figure out how a phenomenon works through observation and experiment. The use of this pedagogy guided the choice of survey instrument for this study. The instrument that was selected was the widely-used Classroom Undergraduate Research Experience (CURE) survey, which was originally developed to measure the effectiveness of small, in-person, course-based undergraduate research experiences in improving students' attitudes toward science (Lopatto, 2009). CURE items relate to student experience, career intentions, attitudes about science, and learning style (Denofrio *et al.*, 2007; Shaffer *et al.*, 2010). The survey is typically used to assess students' attitudes after the completion of a course with a research component (Lopatto *et al.*, 2008; Jordan *et al.*, 2014). Because of the shared emphasis on scientific practices between Habitable Worlds and course-based undergraduate research experiences, it is expected that many of the CURE survey items would be relevant to my study population and that the large existing CURE data set would offer meaningful comparisons to my results.

Other surveys of students' attitudes towards science exist, ranging from topic- or subject-specific to science in general. I considered topic-specific surveys (e.g. Thompson and Mintzes, 2002) and subject-specific surveys such as the Biology Attitude Scale (Russell and Hollander, 1975) and the Colorado Learning Attitudes about Science Survey for Biology (CLASS-Bio) (Semsar *et al.*, 2011) to be less applicable because of the interdisciplinary nature of Habitable Worlds. There are several surveys on attitudes towards science in general that could have been used, such as the Views About Sciences Survey (VASS) (Halloun and Hestenes, 1996) and the Views on Science and Education Questionnaire (VOSE) (Chen, 2006). I did not use these surveys due to their limited representation in the literature to date. The CURE survey has thus far been administered to more than 10,000 students at 122 different institutions nationwide; as noted above, this wide use affords a strong comparison with other courses and programs.

The CURE survey was originally designed for in-person students with a strong interest in science. In using the survey for an online course and with non-science majors, I could not assume its validity. For this reason, I included a factor analysis step in the analysis to help guide my interpretation of the survey responses.

For this work, I focused on two sections of the CURE survey. The Science Attitudes section focuses on students' attitudes towards science. The Benefits section focuses on students' perceived learning and development gains as a result of taking the course. The items used for this work are listed in Tables 2 and 3. The 22 Science Attitudes items are a subset of the 35 items of Wenk (2000), with the item in her work regarding intuition changed to an item pertaining to creativity in the CURE survey. These items are both positively and negatively worded (e.g., "I like studying science" vs. "I don't like studying science") according to Wenk (2000) to demonstrate complex thinking on the part of the students. The 21 Benefits items are derived from earlier survey work by Lopatto (2003).

For each of the 22 Science Attitudes items and the 21 Benefits items, the students responded on a five-point Likert response format plus an option to not respond. For the Science Attitudes items, the options presented were "strongly disagree," "disagree," "neutral," "agree," and "strongly agree." For the Benefits items, the options presented were "no gain," "small gain," "moderate gain," "large gain," and "very large gain." These responses were then numerically coded to 1, 2, 3, 4, and 5 respectively for analysis, with non-responses coded as "not applicable." It should also be noted that students were not required to respond to any of the items above. The Science Attitudes items were presented to the students both at the beginning and at the end of the course, while the Benefits items were only presented to the students at the end of the course, which follows the typical administration of the CURE survey. The pre- and post-course surveys each took approximately 10 minutes to complete.

Certain items from the original CURE survey were excluded from the final analysis because they were not relevant to the learning objectives of Habitable Worlds. For instance, the Science Attitudes item relating to writing was removed because there are no writing assignments in Habitable Worlds.

Additionally, 10 items were removed from the Benefits items since they pertained to learning outcomes that were not emphasized in the course. These changes were supported by the factor analyses (see Section 3). Additionally, items that were removed had substantially more not applicable responses, which further supported the decision to exclude those items.

4.2.3 Factor analysis

As noted above, I excluded one item from the Science Attitudes section and 10 items from the Benefits section as those were not applicable to the course (see Tables 2 & 3). This left 32 items for further analysis.

Gardner (1995) recommended that a scale should be internally consistent (using Cronbach Alpha values) and unidimensional (i.e., measures one attitude construct). A high Cronbach Alpha value can indicate high internal consistency but it can also mean that there are items that cluster together into multiple constructs. Therefore, in addition to calculating Cronbach Alpha values, factor analyses were used to ensure that the scales are unidimensional.

I conducted a maximum likelihood, oblique rotation exploratory factor analysis to identify latent factors in the data following recommendations of Preacher and MacCallum (2003). The 21 Science Attitudes items were analyzed separately from the 11 Benefits items because of their different response options (i.e., agreement or disagreement for the Science Attitudes items versus no to high gain for the Benefits items). Since I was interested in the effect the course had on students' attitudes towards science, I chose to use the change in response scores from pre- to post-course rather than pre- or post-course values for the factor analysis of the Science Attitudes items. The Benefits items were only administered post-course; therefore, I used those for the factor analysis. A confirmatory factor analysis was also performed for which the robust diagonally weighted least squares (WLSMV) estimator was used, which is recommended for use with Likert response format data (Flora and Curran, 2004; Brown, 2014; Li, 2016).

I calculated the exploratory factor analysis in R using the package psych (Revelle, W., 2016), while the confirmatory factor analysis was done with the lavaan package (Rosseel, Y., 2012). I identified the number of factors to extract through a combination of scree plot analysis and parallel analysis (Horn, 1965; Cattell, 1966). An oblique PROMAX rotation was used to allow inter-factor correlation, if present.

4.3 Results

4.3.1 Factor analysis

A two-factor solution was the most appropriate for the Science Attitudes items, while the Benefits items could be described by a single factor. I retained only items with loadings greater than 0.5 for the Science Attitudes items. All Benefits items loaded very strongly onto a single factor. The rotated solutions are shown in Tables 13 and 14 in the Appendix. I named the two Science Attitudes factors Scientific Sophistication (SS) and Personal Value (PV), while the Benefits factor was simply called Benefits. Table 4 shows the items that grouped into each of the Science Attitudes factors and Table 5 shows the items that grouped into the Benefits factor. Since the items that grouped into the SS factor were negatively worded, I reverse scored them so that a positive combined SS factor score would mean an increase in scientific sophistication. The internal consistencies were $\alpha = 0.85$ for the SS factor, $\alpha = 0.69$ for the PV factor, and $\alpha = 0.97$ for the Benefits factor.

Table 4: CURE Science Attitudes items and their factor alignments

Label	Full wording	Factor
No major	Students who do not major/concentrate in science should not have to take science courses.	Scientific Sophistication (SS)[2]
Figure out	There is too much emphasis in science classes on figuring things out for yourself.	
Just tell	I wish science instructors would just tell us what we need to know so we can learn it.	
Creativity	Creativity does not play a role in science.	
Not connected	Science is not connected to non-science fields such as history, literature, economics, or art. (Science is not connected to fields such as history, literature, economics, or art.)[1]	
Only experts	Only scientific experts are qualified to make judgements on scientific issues.	
Know before	Scientists know what the results of their experiments will be before they start.	
Statistics	Scientists play with statistics to support their own ideas. (Scientists are willing to falsify their data to support their favored ideas.)[1]	
Thinking skills	Even if I forget the facts, I'll still be able to use the thinking skills I learn in science.	Personal Value (PV)
Satisfaction	I get personal satisfaction when I solve a scientific problem by figuring it out myself.	
Do well	I can do well in science courses.	
Explain	Explaining science ideas to others has helped me understand the ideas better.	
True	You can rely on scientific results to be true and correct. (The purpose of science is to identify true facts.)[1]	

Continued on next page

[1] Beginning in the Fall 2015 semester, 9 of the 21 Science Attitudes items were reworded to clarify their meaning. The revised versions are in parenthesis.

[2] Items in this factor were reverse scored

Table 4 – Continued from previous page

Label	Full wording	Factor
Experience	When scientific results conflict with my personal experience, I follow my experience in making choices. (When scientific results conflict with my prior understanding, I favor my prior understanding in making choices.)[1]	None
Missing facts	When experts disagree on a science question, it's because they don't know all the facts yet. (Experts may reach different reasonable conclusions using the same information.)[1]	
All valid	Since nothing in science is known for certain, all theories are equally valid. (In science, all ideas are equally valid.)[1]	
Facts	Science is essentially an accumulation of facts, rules, and formulas.	
Experiment fail	If an experiment shows that something doesn't work, the experiment was a failure. (In science, something can be learned even when experimental results do not match the expected outcome.)[1]	
Straight line	Real scientists don't follow the scientific method in a straight line. (The scientific process operates along a straight line from hypothesis to fact.)[1]	
Work ourselves	The main job of the instructor is to structure the work so that we can learn it ourselves.	
Lab confirm	Lab experiments are used to confirm information studied in science class. (Experiments are usually used to confirm what we already know.)[1]	
Write	The process of writing in science is helpful for understanding scientific ideas.	Excluded

Table 5: CURE Benefits items and their factor alignment

Label	Full wording	Factor
Interpret	Skill in interpretation of results	Benefits
Obstacle tolerance	Tolerance for obstacles faced in the research process	
Demanding	Readiness for more demanding research	
Knowledge construction	Understanding how knowledge is constructed	
Integrate	Ability to integrate theory and practice	
Real scientists	Understanding of how scientists work on real problems	
Evidence	Understanding that scientific assertions require supporting evidence	
Analyze	Ability to analyze data and other information	
Science	Understanding science	
Scientists think	Understanding of how scientists think	
Independence	Learning to work independently	
Career	Clarification of career path	Excluded
Your field	Understanding of the research process in your field	
Ethical	Learning ethical conduct in your field	
Lab techniques	Learning laboratory techniques	
Self confidence	Self-confidence	
Learning community	Becoming part of a learning community	
Teacher	Confidence in your potential to be a teacher of science	

Continued on next page

Table 5 – Continued from previous page

Label	Full wording	Factor
Primary literature	Ability to read and understand primary literature	
Oral	Skill in how to give an effective oral presentation	
Writing	Skill in science writing	

I considered a three-factor solution for the Science Attitudes items; however, the third factor was considerably weaker and was roughly the result of splitting up the SS factor into two factors. Additionally, a scree plot analysis did not support a three-factor solution. Therefore, I decided against a three-factor solution for the Science Attitudes items. A confirmatory factor analysis using data from the Spring 2016 offering of Habitable Worlds further supports this specific factor solution. This independent sample included 203 complete and consented responses. The results indicate an acceptable fit (CFI = 0.95, TLI = 0.94, RMSEA = 0.03). Therefore, I am confident that the specified factors are robust.

4.3.2 Factor correlations

To calculate correlations between the factors listed above and the final course grade, I grouped the items within a single factor into one composite scale for each student. This was done by taking the mean of all items within a factor for each student. See Table 6 for Pearson correlation coefficients for the course grade in comparison to the three composite scales (two for the Science Attitudes items and one for the Benefits items).

Table 6: Correlation of the two Science Attitudes factors (difference of pre- and post-course responses), the Benefits factor (post-course responses), and the final course grade (numerically coded e.g. "A" = 4, "B" = 3, etc.) for the whole cohort (correlations with a p-value ≤ 0.05 are highlighted in orange).

	Course Grade	Scientific Sophistication (SS)	Personal Value (PV)
Scientific Sophistication (SS)	0.27		
Personal Value (PV)	0.17	0.06	
Benefits	0.16	0.07	0.52

The non-significant correlation between the SS factor and the PV factor illustrates that these two factors are independent measures of latent variables in the data.

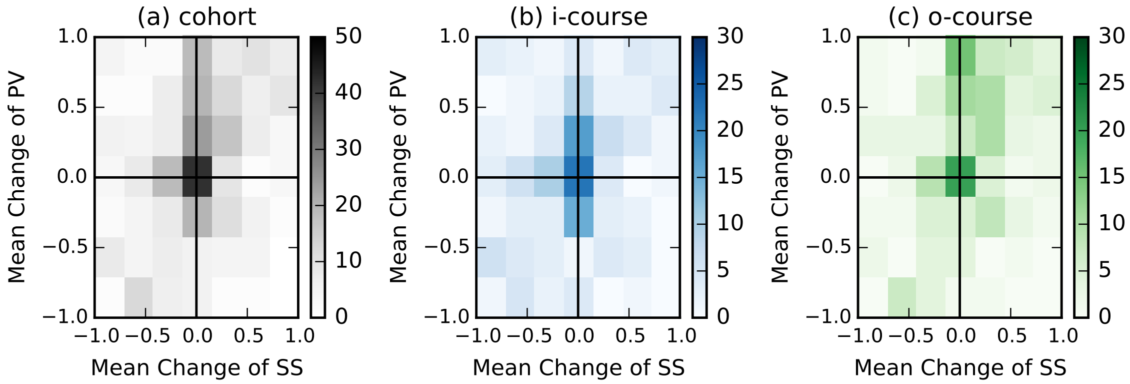

Figure 16: Two-dimensional histogram of the number of students as a function of mean changes in their responses to the SS factor items (horizontal axes) and their responses to the PV factor items (vertical axes). The whole cohort is shown on the left (black), i-course students in the middle (blue), and o-course students on the right (green).

To illustrate this further, I made two-dimensional histograms with the mean changes in PV versus SS factor scores serving as axes, and the number of students who had that particular change represented by color darkness (see Figure 16). The figure shows the results for the whole cohort (Figure 16a), the i-course students (Figure 16b), and the o-course students (Figure 16c). The desirable quadrant of the two-dimensional histograms is the top-right quadrant since I consider both a positive change in PV and a positive change in SS a desired outcome of the course.

4.3.3 Factor scores and factor score changes

To determine if the differences in Science Attitudes factor scores between i-course and o-course students were statistically significant, I conducted several simultaneous linear regressions (see Table 7 with additional models shown in Tables 15 to 20 in the Appendix). For the SS factor, pre-course scores predicted 24.5% of the post-course score variance for the whole cohort (Model SS1). When controlling for program type (i.e. i-course or o-course), the model predicted 26.4% of variance of the post-course scores (Model SS2).

Thus, there is a statistically significant effect of program type on post-course SS factor scores, with O-COURSE students having higher scores. For the PV factor, a model with pre-course scores as the independent variable and the post-course scores as the dependent variable was heteroscedastic (thus should not be considered), though the pre-course scores were statistically significant with the model predicting 23.5% of the post-course score variance (Model PV1). However, the model including program type was not heteroscedastic (Model PV2). That model predicted 25.3% of the post-course score variance. Here again O-COURSE students had higher post-course scores. Unlike for the SS factor (Model SS3), for the PV factor gender was also a statistically significant variable (Model PV3). In Figure 17 I show pre-course and post-course factor scores for both SS and PV factors along with their corresponding simultaneous linear regression models.

Table 7: Simultaneous linear regression models for predicting the post-course SS factor scores (on the top) and PV factor scores (on the bottom) of the whole cohort. The reference groups for the categorical variables gender (female or male) and program type (I-COURSE or O-COURSE) were female and I-COURSE. Listed are standardized coefficients (i.e. continuous variables were scaled and centered prior to the regression). Statistical significance (i.e. $p \leq 0.05$) indicated with highlighting. The Studentized Breusch-Pagan test was used to test for heteroscedasticity.

Model SS2		
Variable	Coefficient	p-value
(Intercept)	-0.14577	0.0113
SS Factor (pre-course)	0.45689	< 0.001
Program type	0.30019	< 0.001
Adjusted $R^2 = 0.2645$ F-statistic = 81.91 on 2 and 448 DF with $p < 0.001$ BP = 1.2279, df = 2, p-value = 0.541		
Model PV2		
Variable	Coefficient	p-value
(Intercept)	-0.13607	0.0171
PV Factor (pre-course)	0.47356	< 0.001
Program type	0.28022	< 0.001
Adjusted $R^2 = 0.2533$ F-statistic = 77.31 on 2 and 448 DF with $p < 0.001$ BP = 5.7897, df = 2, p-value = 0.0553		

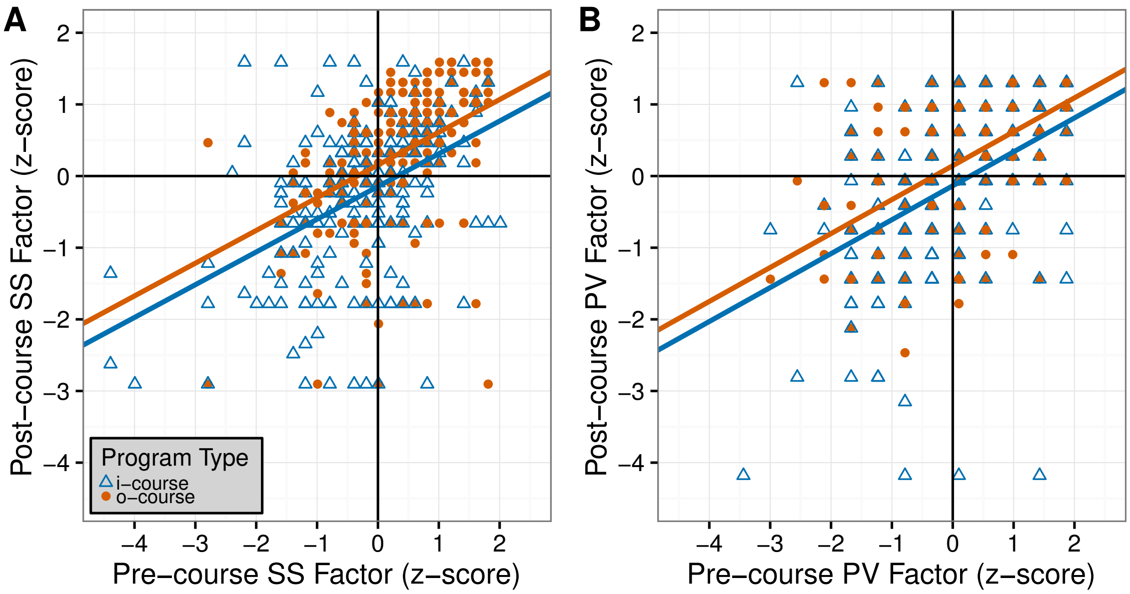

Figure 17: Pre- and post-course Science Attitudes factor scores by program type (I-COURSE in blue and O-COURSE in orange). Shown on the left (A) are the SS factor scores and on the right (B) are the PV factor scores. Lines are simultaneous linear regression fits (see Tables 5 Models SS2 and PV2). All factor scores have been converted to z-scores.

Additionally, to test the significance of differences in pre-course factor scores between I-COURSE and O-COURSE students I used the non-parametric Wilcoxon test. The test was chosen since quantile-quantile (Q-Q) plots showed the factor scores were not normally distributed. For both SS and PV factors, the pre-course score differences between I-COURSE and O-COURSE students were statistically significant (p-values <0.001 and <0.02 respectively). For the linear models, I also considered an interaction term between pre-course scores and program type (Models SS4 and PV4) but those terms were not statistically significant for either SS or PV factors (i.e. linear regression slopes are not significantly different). This further demonstrates that the difference between I-COURSE and O-COURSE students is largely due to their pre-course factor scores.

4.3.4 Relationships between factor scores and final course grade

The SS (r = 0.27), PV (r = 0.17), and Benefits (r = 0.16) factors all displayed some significant positive correlations with final course grades for the whole cohort. However, the pre-course Science Attitudes factor score correlations differed between the O-COURSE and I-COURSE students. Among the O-COURSE students, pre-course factor scores showed significant correlations with final course grade for both the SS factor (r = 0.19, p = 0.004) and the PV factor (r = 0.16, p = 0.02), which was not the case with the I-COURSE students. Benefits factor scores were positively correlated with course grade for students in both groups (r = 0.15, p = 0.03 for the O-COURSE group and r = 0.17, p = 0.01 for the I-COURSE group).

I conducted regressions to further explore the relationships with course grade. I used logistic regressions, over linear regressions, since the course grades were not normally distributed. First I modeled the odds of receiving an A grade in the course (see Tables 21 to 32 in the Appendix). Following from the correlations shown previously, I found higher pre-course SS factor scores predicted greater chances of earning an A grade, but only for O-COURSE students (Models GA1 and GA2). When those models were expanded to include university cumulative grade-point average (GPA) and students' gender, I found the predictive power of SS factor scores to be dramatically lower (Models GA7–9), though the pre-course SS factor remained significant among O-COURSE students (Model GA10). Next, I modeled the odds of a student failing the course (see Tables 33 to 44 in the Appendix). Here I found only a weak predictive relationship for odds of failure as a result of pre-course SS factor scores (see Models GF1 and GF2). GPA remained a strong predictor of failure, as it was of A grades.

Along with GPA and gender, the logistic regressions showed that the SS factor, which quantified the pre- to post-course change, to be a statistically significant positive predictor in predicting A grades. The SS factor had the reverse effect on course failure since it was a negative predictor.

However, the PV factor was not statically significant in predicting either A grades or course failure. Program type was not a significant predictor in these models, in contrast to the findings above for the pre-course factor scores.

4.4 Discussion

4.4.1 What do the factors represent?

4.4.1.1 Science Attitudes factors

Each of the two Science Attitudes factors represents a facet of students' attitudes toward science and learning science. The Science Attitudes section of the CURE survey is intended to measure, through both positive and negative attitudes, how a student views the institution of science, how accurately they conceive of the process of science, and how much value they see in learning science. The high internal consistency from the CURE benchmark dataset (shown in Tables 45 and 46 of the Appendix) indicates that respondents generally respond similarly to these items. However, the correlational differences between the two factors identified in this study show that there is valuable information hidden within the omnibus Science Attitudes section.

Interpreting and naming the two factors was not straightforward. The items are intuitively opposite, yet the results of the factor analysis indicate largely uncorrelated factors (see Table 6). The factor labeled Personal Value (PV) includes four items. Items in the PV factor assess whether students value leaning science. The factor labeled Scientific Sophistication (SS) includes eight items. A high SS factor score would indicate that the student likely has a more advanced understanding of how science works and what it means to do science while a low SS factor score would indicate a more rudimentary understanding.

Overall, I interpret a high SS and PV factor score to indicate the strongest "pro-science" attitude and the reverse as indicating a combination of low value of learning science, dislike of science, and/or disinterest in science. Changes in these scores pre- to post-course reflect shifts in attitudes as a result of the course experience or outside factors.

Though these factors are not exactly the same as factors identified in previous works, there are comparisons that can be made. Previous works, such as Germann (1988), have argued for dividing attitudes pertaining to science into two factors such as "attitudes toward science" and "beliefs about science" as in the case of Walker *et al.* (2013). Such a division is consistent with the Science Attitudes factors in this work, with the PV factor being similar to "attitudes towards science" and the SS factor being similar to "beliefs about science." Additionally, though their surveys were specific to either physics or biology, the "Personal Interest" factors of Adams *et al.* (2006) and Semsar *et al.* (2011) contain items that are similar to the items in the PV factor. This is perhaps an indication that personal value/interest is in fact a stable latent variable. In considering the SS factor, as noted by Deng *et al.* (2011), I heed that since items in the SS factor are declarative statements, a high SS factor score does not necessarily mean that a student has a procedural knowledge of the practice of science. Furthermore, as mentioned by Allchin (2011), agreement or disagreement to declarative statements does not demonstrate a "functional understanding of scientific practice and its relevance to decision making." Thus, I do not suggest that a high SS factor score implies a strong understanding of the Nature of Science (NOS); however, it may be the case that a low SS factor score implies a weaker understanding of the NOS. Deng *et al.* (2011) listed 10 key aspects to the NOS. Of that list, two aspects are not contained in the SS factor: "nature of and distinction between observation and inference" and "nature of and relationships between theories and laws." Overall, both Science Attitudes factors have similarities with previous work, which bolsters their validity as measures.

4.4.1.2 Benefits factor

The 11 items that formed the Benefits factor represent skills and learning outcomes that are consistent with the learning objectives of the course. This factor includes items that ask students if they gained skills in interpreting results and working independently as well as improving their understanding of the role of evidence in science. I expect high scores on this factor to indicate that course learning objectives were met. It is interesting to note that in Table 6 there is a strong, positive correlation between the Benefits factor and the PV factor ($r = 0.52$). This indicates that there is a strong positive correlation between students' change in perceived value of learning science and their perceived benefits of taking the course.

4.4.2 Comparisons between O-COURSE and I-COURSE students

4.4.2.1 Factor scores

The linear regression models show that the primary difference between the Science Attitudes of I-COURSE and O-COURSE students is their pre-course factor scores. This is important since the regression models also show that a large part of the post-course factor score variance is predicted by pre-course factor scores. I find that O-COURSE students appear to be aided in achieving a better course grade by their positive pre-course Science Attitudes. I also find that pre-course SS factor scores were a predictor of course grades for O-COURSE students, which was not the case for their I-COURSE counterparts.

The differences in Science Attitudes factor scores between O-COURSE and I-COURSE students indicate that the O-COURSE students increased their perception of personal value in learning science, while the I-COURSE students did not change their views on personal value in learning science. In that sense, I-COURSE students are similar to the CURE benchmark (shown in Table 47 of the Appendix), which also shows little change in the PV factor from pre- to post-course.

For the pre-course PV factor scores, both the O-COURSE and I-COURSE students have a lower perception of personal value than the CURE benchmark. As mentioned earlier, the CURE survey is nominally administered to science majors, thus it is expected that the pre-course perception of personal value in science should be higher for science majors. For the post-course PV factor scores, the O-COURSE students are higher than the CURE benchmark, while the I-COURSE students are lower. For the SS factor, the I-COURSE students lowered their factor scores from pre- to post-course (i.e., they decreased in their understanding of how science works and what it means to do science), while O-COURSE students showed no change. In that sense, O-COURSE students are similar to the CURE benchmark, which also shows little change in the SS factor from pre- to post-course. For the pre-course SS factor scores, the I-COURSE students are similar to the CURE benchmark, while the O-COURSE students have a higher scientific sophistication than the CURE benchmark. It is surprising that the pre-course CURE benchmark for the SS factor was not higher than both the O-COURSE and I-COURSE students—something that was true for the PV factor. I would have expected science majors to show a higher scientific sophistication than non-science majors regardless of their degree program type (i.e. O-COURSE or I-COURSE). Overall, the O-COURSE students entered the course with both a higher scientific sophistication and a higher personal value in learning science as compared to their I-COURSE counterparts. The O-COURSE students even compare favorably to the CURE benchmark data, which primarily measures science majors' attitudes.

There are also significant differences between I-COURSE and O-COURSE students in their responses to the Benefits items. On average, the O-COURSE students had higher self-reported gains on the items surveyed than their I-COURSE counterparts, though I-COURSE students were closer to the CURE benchmark. Course grades, as well as GPA, were not significantly different between the two groups (see Table 8), so this finding reflects a difference in perceived learning rather than an actual gap in learning outcomes between the two groups.

Though these changes in perceptions did not seem to affect their course grades overall, the differences in perception may affect their future science course performance as well as their likelihood of continuing to be engaged with science in the future.

Table 8: Academic performance for Habitable Worlds students

Academic Performance		I-COURSE students ($n_i = 232$)	O-COURSE students ($n_o = 219$)
Habitable Worlds Grade	Mean	3.34	3.39
	Median	4.00	4.00
College GPA	Mean	3.31	3.32
	Median	3.30	3.46

Why do O-COURSE and I-COURSE students differ in these ways? One possibility is the demographic differences between these two groups, which may lead to certain perceptions about science. The O-COURSE students are on average older than the I-COURSE students, which is typical of students in non-traditional degree programs (Clinefelter and Aslanian, 2016). One prior study presented evidence that online learners' preferences with regard to simulations or games-based learning varied by age (Hampton *et al.*, 2016). However, none of my linear models found age to be a statistically significant variable for predicting post-course Science Attitudes factor scores when controlling for GPA, gender, and program type. From this, I suggest that the distinctive characteristics and life circumstances that lead students to enroll in fully-online degree programs also make them more likely to have more positive attitudes toward science as well as to perceive greater benefits from the learning experience as compared to I-COURSE students.

A second possibility is that the differences between I-COURSE and O-COURSE students' attitudes reflect a difference in why students from each group decided to enroll in the course. As part of the pre-course survey, students were asked to rate the importance of 10 items pertaining to the reasons why they chose to take this course. For these items, the options were "not applicable," "not important," "moderately important," and "very important."

For the "interested in the subject matter" reason, the median response of the I-COURSE group was "moderately important," while the median response of the O-COURSE group was "very important." This difference was statistically significant ($p = 0.001$ using the unpaired Wilcoxon test). A regression analysis indicated that this incoming difference of their interest in the subject was a significant predictor of post-course attitudes toward science. However, program type remained significant even accounting for the interest item. Thus, although initial interest in the subject is more relevant than age in explaining the attitudes results, O-COURSE students are still more likely to have more positive attitudes toward science than their I-COURSE counterparts.

This relationship should be examined more directly in follow-up studies. A student's initial disposition towards a course clearly colors their experience in that course, but the ways in which that disposition varies systematically could be useful for instructors or institutions. If, as I find here, O-COURSE students are more likely to enroll based on interest than are I-COURSE students, that tendency could be used to tailor instruction or course offerings. Certainly, other similar relationships exist and would provide their own distinctive benefits towards the goal of delivering more useful and productive learning experiences.

4.4.2.2 Relationships with course grade

The differences in factor score–course grade correlations between the O-COURSE and I-COURSE students suggest an interesting motivational difference between the two groups. The pre-course factor scores are significant predictors of success or failure in the course for the O-COURSE students, but show no predictive value for the I-COURSE students. It has already been observed that the O-COURSE students were more likely to report enrolling because of strong interest in the subject. Though predictive of positive science attitudes, this preexisting interest has only a small, non-significant correlation with course grade.

If this pattern holds in other online courses, it would suggest that success and failure among O-COURSE students is driven more strongly by students' predisposition for the subject than is the case among I-COURSE students. It would also make the CURE survey, or a similar survey, a valuable diagnostic tool for identifying students in danger of failure.

Unlike the pre-course measure, the post-course measures show the same correlations with course grade among the O-COURSE and I-COURSE students. The post-course and the pre- to post-course changes in both PV and SS are positively correlated with grade. The logistic regressions showed that, while a student's university GPA and gender were important in predicting their course grade, their SS factor score was also statistically significant in predicting their course grade. Similarly, although the O-COURSE students report significantly higher learning gains on the Benefits items, the correlations between total Benefits score and course grade are very similar among O-COURSE and I-COURSE students. This indicates that even though the O-COURSE group exhibited more positive attitude shifts than the I-COURSE group, the better performing students in both groups had similar relative differences in attitude change compared to the lower performing students.

The modest positive correlations of all three factors (i.e., PV, SS, and Benefits) with the final course grade is consistent with previous work by Hough and Piper (1982); Steiner and Sullivan (1984); Germann (1988); Singh *et al.* (2002); who found positive correlations between students' attitudes and course grades. However, the findings of this work are not consistent with Rogers and Ford (1997), who found that positive attitudinal changes correlated negatively with course grade. Though they found attitudes towards biology (particularly personal relevance) to be correlated with course performance, the direct correlation was weak, which led Partin and Haney (2012) to drop the term from their model. These results illustrate the complexity of linking students' affect to course performance.

4.4.3 What are the implications of this work?

4.4.3.1 Students' attitudes towards science

The two populations of students (O-COURSE and I-COURSE) began the course with different attitudes towards science, and they changed their views differently after taking the course. In spite of these differences in attitudes, there was not a significant difference in final course grades between the two groups. This may be explained by the short duration of the intervention (the course) in this study—only 7.5 weeks—which is very brief in comparison to a student's entire academic program. Over this period of time, differences in attitudes may not affect course performance or the effect may be too small to be detected. By comparison, in a longitudinal study over a four-year period of students' attitudes toward science, Hansen and Birol (2014) observed a positive relationship between the development of expert attitudes toward science and academic performance. Therefore, although the attitudinal differences that I observed in this work did not have a corresponding difference in final course grades for O-COURSE and I-COURSE students, those attitudinal differences may predict students' future performance in science courses or their future engagement with science.

Given the importance of students' attitudes towards science, it might be suggested that online courses (and perhaps traditional, in-person courses) should try to positively change students' attitudes towards science during the course. However, changing students' attitudes towards science is both complex and difficult. Part of the complexity is illustrated by the example of positive self-statements being helpful to some people but damaging to others (Wood *et al.*, 2009). The difficulty has been noted by a number of previous works that found no changes in students' attitudes towards science. For example, Gabel (1981) found no change in attitudes towards science from pre- to post-course during an in-person, introductory geology course for non-majors. Additionally, Cook and Mulvihill (2008) found no change in students' confidence in doing science or their interest in science from pre- to post-course.

They used a general attitudes survey during an in-person course for non- majors called "Food, Values, Politics and Society." However, for the same course, data from the Biology Attitude Scale showed improved attitudes towards biology from pre- to post-course. There are many complications that hinder an instructor's attempts to improve students' attitudes toward science; for example, it becomes more difficult to change attitudes as students age (e.g. Savelsbergh *et al.*, 2016). In spite of these difficulties, some studies have identified ways by which students' attitudes toward science can be improved. For example, Wheland *et al.* (2013) showed that attitudes of non-STEM majors towards science improved by having them engage in authentic scientific activities during a four-course block of English composition, oral communication, freshman seminar, and a special-topics course (led by a biologist). But not all interventions are effective. A meta-analytic study by Savelsbergh *et al.* (2016) found that certain teaching approaches improved students' attitudes while others improved achievement, but they did not find a correlation between an intervention's success in improving attitudes and success in increasing achievement. Thus, past studies have demonstrated that changing students' attitudes towards science is not straightforward.

Previous works contend that students' attitudes towards science can be improved by implementing certain types of instructional design such as active-learning lectures (Armbruster *et al.*, 2009) and building models during the learning process (Brewe *et al.*, 2009). Though educators should look for opportunities to improve learning outcomes, we should avoid suggesting simplistic universal solutions. It has been shown that both positive and negative affect can be beneficial depending on the individual and on the circumstance. For example, George and Zhou (2002) found that when people were both aware of their moods and they were rewarded for creativity, negative moods correlated with increased creativity while positive moods correlated with decreased creativity. Additionally, Martin *et al.* (1993) found that those with positive moods stopped a task faster than those with negative moods when they were directed to achieve a certain goal.

However, they found that those with positive moods continued with the task longer than those with negative moods when they were directed to continue as long as they enjoyed the task. Thus, the goal of the present work and work that follows should focus on helping students with diverse affect to learn the course material and meet course objectives rather than trying to change particular aspects of their affect. Overall, the implication of prior findings and this work is that improving students' attitudes with the aim of improving learning outcomes is unreliable. Instead, I recommend using pre-course attitude surveys to guide pedagogical decision-making. For example, the results of this work suggest that O-COURSE students, who express higher value in science, will be more willing to engage with learning activities that allow them to explore and discover scientific concepts without regard for their utility in other contexts. In the same way, I-COURSE students may be more interested in learning activities that emphasize the implications to everyday life or the student's own non-science interests. Those suggestions are supported by the work of Berg (2005) who studied attitudes of first-year university chemistry students. They conducted follow-up interviews of students who had the largest changes (positive and negative) in their attitudes as measured by a pre- and post-course attitude questionnaire. They found that students who had large positive changes in attitudes were more motivated and were more persistent. Students who had large positive changes were also more willing to do open ended or exploratory exercises than those who had large negative changes in attitudes. Berg (2005) state that "for tasks requiring more self-regulated learning, such as planning open experiments and tutorials, students with positive attitude shifts reveal greater acceptance, while students with negative attitude shifts are more reluctant to express positive views, even if they expressed an understanding of the relevance of such tasks." Future work should explore how students with different pre-course attitudes towards science respond to different pedagogies.

4.4.3.2 Student motivation

Motivation is sometimes conceived as a mediator between students' attitudes toward science (part of their affect) and their behaviors. Motivation and its role in learning have been conceptualized differently by various authors (cf. Eccles and Wigfield, 2002). However, motivation is commonly divided into intrinsic motivation (i.e., driven by interest or desire to perform a task) and extrinsic motivation (i.e., driven by rewards or external forces to perform a task). The PV factor may be a proxy for students' intrinsic motivation since the factor identifies a certain personal value in learning science. This would be consistent with the findings of Glynn *et al.* (2007) who found that perceived relevance of science to students (who were non-science majors) to their future careers was correlated with their motivation (with the correlation stronger among female students). They also concluded that motivation was correlated with student achievement (i.e., GPA). Similarly, Partin and Haney (2012) also argued that personal relevance contributes to intrinsic goal orientation (i.e. intrinsic motivation). Furthermore, the "Intrinsic Motivation" factor of Glynn *et al.* (2011) is similar to my PV factor when the constituent items are compared and, though they used a semantic differential scale, the "Interest and Utility" factor of Bauer (2008) may also be similar to my PV factor. If the PV factor is in fact a proxy for intrinsic motivation, then the higher pre-course PV factor scores of O-COURSE students and their further increase in post-course PV factor scores could mean that O-COURSE students are more intrinsically motivated than their I-COURSE counterparts. This has implications for their education since those who are intrinsically motivated are more likely to persist when they face obstacles (e.g. Simons *et al.*, 2004; Grant, 2008), which might be particularly important to the long-term success of O-COURSE students. Unlike I-COURSE students, O-COURSE students may have limited access to on-campus support (such as tutoring centers and visiting instructor's office hours).

Future work can further test if in fact the PV factor is a proxy for intrinsic motivation by considering if there are correlations between positive PV factor scores and persistence (e.g., by considering the number of reattempts for questions that a student initially answered incorrectly).

4.4.3.3 Connection to the affect-cognition-behavior framework

Affect, cognition, and behavior interact with each other in complex ways, but all three are important to learning. The results of this work demonstrate that there is a connection between students' affect (specifically attitudes in this work) and both cognition and behavior (as implied by course grade). Though it is reasonable to assume that a student's course grade would measure their cognition and behavior during the course, future work should address this directly. Additional specific measures of cognition (e.g. individual lesson and question scores) and behavior (e.g. time spent on individual lessons or discussion board participation) would allow fine-grained behaviors or learning to be tied to different science attitudes. The significant relationships shown between SS and PV factor scores and course grade, particularly among O-COURSE students shows the potential of this line of research, yet the far greater predictive power of student GPA shows the limits of the current aggregate-level analyses. Overall, this work further demonstrates the fruitfulness of considering student affect in education.

4.4.4 Limitations

4.4.4.1 Changes to the CURE survey and some individual items

As noted above, I excluded 11 items, one Science Attitudes and 10 Benefits items, from the factor analysis. The decision to exclude those items does, in some ways, limit how this work may be compared to previous CURE research.

At the same time, it also represents a need that will be common to other large enrollment courses that also do not include substantial writing or research activities. My CURE subset will likely be more appropriate for those classes to use than the full CURE survey.

Starting in the Fall 2015 semester, the wording of 9 Science Attitudes items were revised, two of which were ultimately included in my identified factors (see Table 4). This revision was informed by results from an expert review wherein a group of faculty, research scientists, postdoctoral researchers, and graduate students within our department at ASU answered the 22 Science Attitudes items and commented on their interpretations of each item. Based on these results, I changed the wording of 9 items to clarify them without changing their initial meanings. To test whether these revisions changed the relationships between the Science Attitudes items and the proposed factors, response data were divided into two groups: original wording (Fall 2014 and Spring 2015) and revised wording (Fall 2015 and Spring 2016). A factor analysis was then conducted for each group using only the 12 Science Attitudes items the initial analysis found to load onto the SS and PV factors. Although the exact factor loadings (i.e., eigenvalues) differed between the two response groups, the same groupings shown in Table 4 held. Thus, I argue the item modifications do not materially alter my findings with respect to the two Science Attitudes factors.

4.4.4.2 Student interpretation of survey items

It is possible that not every student in the cohort interpreted the items of the survey in exactly the same manner. Given individual experiences and viewpoints, students in this cohort may have taken various survey items to mean different things. For example, the item regarding creativity ("Creativity does not play a role in science") might evoke different meanings to different students depending on how they interpret the word "creativity." Some students might associate creativity with the arts (i.e., painting, music, dance, acting, etc.), while others might take it to mean thinking in a creative manner (which is closer to the intended interpretation of the item).

To understand and possibly account for this possible variance, I am in the process of conducting think-aloud interviews with students in the current Habitable Worlds offering.

4.4.4.3 General limitations

The population of students included in my analysis accounts for only about half the total number of students who completed the course during the period of my analysis. There are two major reasons for this difference: non-consent for research participation, and course attrition and non-completion of the post-course survey (typically a consequence of course attrition). Such selection biases are common in survey research, but they raise concerns that the retained students do not represent the overall population. Because substantially more students completed the pre-course survey than the post-course, the average pre-course response for each factor between the included population and those with partial responses were compared. In spite of the large number of students who were excluded due to incomplete post-course responses, there is no evidence that this exclusion has affected the results. Pre-course Science Attitudes factor scores and the Benefits scores for the students who were excluded are statistically indistinguishable from scores for the students used in this study. Thus, although one could speculate that students who failed to complete a course may have different attitudes than those who did, the data show no cause for concern.

The second potential selection effect is that from participant non-consent. I cannot present survey responses from the non-consenting students, but the demographics of those students (working from the class averages and removing the known makeup of the consenting students) can be considered. Non-consenting students are much more likely to be I-COURSE students and more likely to be male. There are no significant differences in overall GPA or course grade.

Given this information, and working under the assumption that the decision to consent to research participation reflects a positive disposition towards the course, I conclude that the study population likely holds more positive attitudes toward science than the course as a whole. However, this strengthens the claim that the O-COURSE students differ from I-COURSE students.

Items using a Likert response format have a relatively constrained range; thus, analysis of pre- to post-course changes could have ceiling (or floor) effects. To account for this, item score changes were recalculated to show only the increase or decrease regardless of magnitude. Scores that began and ended at the highest value were coded as an increase; scores at the lowest value were treated as a decrease. The resultant factors were very similar to the ones shown in Tables S1 and S2. Thus, ceiling and floor effects are not significant.

Finally, some skepticism is always warranted when working with self-reported data. Even though self-assessments are important for learning (Guest *et al.*, 2001) and people believe that they can accurately assess themselves (Pronin *et al.*, 2002), self-assessments are flawed in some regards. Dunning *et al.* (2004) listed two major reasons for this: (1) there are only small correlations between people's perception of how skilled they are at a particular activity and their objective performance, and (2) people are generally too optimistic about their skills and their mastery of those skills. However, given the emphasis in the items used here on attitudes and opinions over skills and proficiency, I argue that self-reported data are meaningful for this work.

4.5 Conclusions

I have administered the CURE survey to three semesters of the online, introductory astrobiology course Habitable Worlds. Additionally, data from the Spring 2016 offering were used for the confirmatory factor analysis. I find that the items with relevance to the experience of non-science majors in an online general education undergraduate course can be described by three factors.

The Scientific Sophistication (SS) factor characterizes a general understanding of science and the process of doing science. The Personal Value (PV) factor characterizes a general perception of personal value in learning science. The Benefits factor characterizes the perceived skills and knowledge gained by taking this course.

The results indicate that there are significant differences between students enrolled in traditional, in-person degree programs (I-COURSE) and students enrolled in fully-online degree programs (O-COURSE). Overall, students in the fully-online program have more positive views about science coming into the course and they shift further towards more favorable views of science after taking the course. They also report greater benefits from taking the course than their I-COURSE counterparts.

I find that the pre-course CURE survey can be used as a predictor of success for the O-COURSE students. Interestingly, this predictive power does not hold for the I-COURSE students. It is expected that students in fully-online degree programs have different life experiences, priorities, and outlooks than the traditional, in-person degree student. In particular, there is evidence that fully-online degree program students consider interest in the subject to be a more important factor in choosing to enroll in Habitable Worlds than do traditional, in-person degree program students. The finding that science attitudes predict outcomes only for O-COURSE students should not be taken to mean that attitudes are only useful predictors among non-traditional students. Instead, it argues for a richer consideration of the circumstances that may change the salience of specific attitudes to the success of specific students.

Online education has proliferated and research into its effectiveness is still being developed. Given the steady rise in the number of fully-online degree seekers, there are clear benefits to further research in this area. Previous works have demonstrated that students' attitudes towards the subject are important to their learning. In this study, I have shown differences in attitudes towards science between traditional, in-person degree seeking students and fully-online degree seeking students.

These findings can now be used to better serve these different populations of students and to compare these results with other online, introductory science courses.

Chapter 5

SUMMARY

...and the end of all our exploring
will be to arrive where we started
and know the place for the first
time.

T. S. Eliot

I introduced affect as a theme in Chapter 1 to connect three seemly incongruent topics: asteroid interiors (Chapter 2), the Moon's thermal evolution (Chapter 3), and students' attitudes towards science (Chapter 4). Below, I briefly state the main conclusions of those three chapters.

In Chapter 2, I used a Discrete Element Modeling code to model size sorting of constituent particles for a simulated asteroid. While previous preparatory works conducted experiments and computer simulations to demonstrate the Brazil Nut Effect (BNE) in vertical containers, this work is the first demonstration of the BNE in a three-dimensional self-gravitating configuration of particles. I have argued that this type of simulation is more relevant to asteroids. Like previous work, this work showed that the BNE is plausible on asteroids. Yet, unlike previous work, this work showed that friction is not essential to this process. I also showed that while the BNE is plausible, only the outer layers of asteroids are likely to undergo size sorting. Lastly, though I did not definitively state that the driving mechanism of the BNE is percolation (i.e. smaller particles filling into void spaces), I showed evidence for percolation being more dominant to that of granular convection.

In Chapter 3, I used a thermal model to calculate a range of solidification times for the Lunar Magma Ocean (LMO) while including the effect of impacts. I found that when impacts only punctured holes into the lunar crust, the LMO solidification time was reduced to ~ 5 Myr for the most intense bombardment case.

However, for a more realistic and moderate impact intensity, the solidification time was $\sim$ 21 Myr. Both solidification times were lower compared to the $\sim$ 32 Myr it would have taken without impacts. When the thermal energy imparted by impacts was also considered, the solidification time was dependent on both the intensity of the bombardment and the efficiency by which impacts converted their kinetic energy to thermal energy. For the lowest impact intensities, even the most inefficient kinetic energy imparting caused LMO solidification time to be greater than the $\sim$ 32 Myr it would have taken without impacts. For the highest impact intensities, regardless of the efficiency of kinetic energy conversion, LMO solidification time was less than the no impacts time (i.e. $\sim$ 32 Myr) by a factor of 5 to 6. Thus, when impacts punctured holes into the lunar crust and imparted thermal energy, LMO solidification could have taken as little as $\sim$ 5 Myr or as long as $\sim$ 53 Myr with the more likely case being 21 Myr. Even when the most reliable crust sample ages are considered, this would require an additional heat source such as tidal heating to have prolonged LMO solidification. On the other hand, if the age range of the lunar crust spans $\sim$ 200 Myr as some studies have suggested, that requires a source that could have provided about 4 TW of additional heating (or greater for more intense bombardments) throughout the LMO solidification process.

In Chapter 4, I used a survey to characterize changes in students' attitudes towards science as they completed an online astrobiology course. I studied two groups of students: those enrolled in fully-online degree programs and those enrolled in traditional, in-person degree programs. The online program students started the course with better attitudes towards science than their traditional program counterparts. Online program students also improved their attitudes towards science more than their counterparts during the course. My factor analysis identified two latent variables, which were named Scientific Sophistication and Personal Value. Though a student's university GPA and gender were highly predictive of getting an A grade in the course, I found that, to a lesser degree, their Scientific Sophistication score was also predictive of getting an A grade in the course. That demonstrated the link between a student's affect, cognition, and behavior.

While the survey characterized their affect, I was limited to the final course grade as a metric for both their cognition and behavior during the course. The other latent variable, Personal Value, may be used as a proxy for intrinsic motivation. This can be tested in the future by identifying if higher Personal Value scores correlate with persistence in the course (e.g. a student reattempting to answer a question that they initially got incorrect), which is an indication of intrinsic motivation.

My scientific research has its origins in my own interests in asteroid interiors and the Moon's thermal evolution. Additionally, my science education research shows how affect can influence students' performance in the course. Taken together, this work demonstrates the importance of affect in both scientific research and science education. Affect is a common link that can either attract or repel both researchers and students from science. As such, I hope that this work encourages a closer partnership between researchers and educators to enhance both scientific research and science education.

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APPENDIX A

SUPPLEMENTAL MATERIAL FOR CHAPTER 2

A.1 Considering the Effects of Particle Sizes, Shapes, and Densities on Sorting

A.1.1 Particle Sizes

In Chapter 2, I simulated a simplified asteroid composed of particles of two sizes. While that assumption helped isolate and demonstrate the Brazil Nut Effect (BNE), asteroids are clearly not composed of particles of only two sizes. Experimental and simulation work have shown that having more diversity in particle sizes results in a reduced BNE (Metzger *et al.*, 2011). As such, for an asteroid of similar mass and size as my simulated asteroid and that happened to experience a similar vigorous shaking due to impacts, the BNE is expected to be less on the asteroid due to its distribution of particle sizes. Since seismic data of asteroids are not available and will be limited going into the future, the dependence of the BNE on the particle size distribution may provide an important means of estimating the internal size distribution of asteroids by imaging their surfaces. Again for a given asteroid with a certain impact history, a more binomial distribution of particles will make the BNE more pronounced. As such, larger boulders should be seen on the surface. On the other hand, for that same example asteroid, a wider distribution of particles would lead to a reduced BNE meaning perhaps that fewer large boulders should be seen on the surface. Adding to the complexity is the fact that even though the BNE is expected to occur to a lesser degree on bodies with a wider distribution of particle sizes, as compared to the idealized binomial size distribution, a single large particle (discussed further in Appendix A.2) may rise faster in the case of the wider distribution of particle sizes (Liao, 2016). Thus, future work on the BNE, should further study the effect of various particle sizes.

A.1.2 Particle Shapes

For simplicity, for isolating parameters, and due to computational limitations, most works so far have used spherical particles in both experimental and computer simulation work. Nevertheless, as noted in Chapter 2, asteroids are not made of perfectly spherical particles. Thus, the effect of particle shapes on the BNE should also be considered. While Ahmad and Smalley (1973) found particle shape to be inconsequential, Rippie *et al.* (1967) found particle shape to have a substantial effect on size sorting. Rippie *et al.* (1967) noted that in mixtures with small spherical particles and large particles made of paired-spheres, size sorting occurred with less vibrational energy than in the case with spherical small and large particles. That result can be taken to mean that it is easier to size sort non-spherical large particles. However, they also found that when both constituent particles were particles made of paired-spheres, size sorting seemed to be hindered. Thus, since asteroids are composed of non-spherical particles, this may mean that the BNE will be hindered. As computer modeling of non-spherical particles becomes more available, it would be valuable to further explore the effect of particle shape on size sorting.

A.1.3 Particle Densities

In Chapter 2, I made the simplifying assumption that particles of both sizes had the same density. That assumption helped isolate the geometric effect of particle sorting (i.e. the Brazil Nut Effect). However, it could be argued that while constituent particles of asteroids will have different sizes, they will also likely have different densities. In the simple case of equally sized particles of different densities, it would be intuitively expected that there would be sorting with denser particles moving parallel to the local gravity vector. However, experiments by Rippie *et al.* (1964) found no tendency for the denser lead and steel balls to collect at the bottom of the container when they were embedded in a collection of glass balls. They note that particles' coefficient of restitution (the ratio of relative velocities prior to and after a collision) and/or the specific mode of vibration used for their work might have caused the unexpected result. Experimental work has shown that large particles with a certain range of densities ($\geq 50\%$ to about 120% or 170% of the surrounding material density) will rise to the top while low-density large particles ($< 50\%$ of the surrounding material density) will move towards the bottom (Shinbrot and Muzzio, 1998). Overall, as noted by Rippie *et al.* (1964) the BNE has a non-linear dependence on both particle size and density when both are considered together. As such this is another interesting direction for future research.

A.2 The Intruder Model

A.2.1 Motivation

Most works on the BNE have used one large particle embedded in a collection of smaller particles (e.g. Matsumura *et al.*, 2014). This Intruder Model is convenient for tracking the larger particle; however, it may not be the typical scenario for asteroids. To further understand this Intruder Model and to explore the driving mechanism of the BNE, I made a number of aggregates with one or a few large particles embedded within a collection of smaller particles as an extension of my work discussed in Chapter 2.

A.2.2 Methods

I created 30 aggregates (10 aggregates each with one large intruder, two intruders, and three intruders). The total number of particles in each case was 1,000. While all particles had a density of 3 g/cm^3, the smaller and larger particles had radii of 40 m and 80 m respectively, similar to the work in Chapter 2. To properly resolve the collisions in these simulations, I used the smaller particle radius and mass to calculate a spring constant of $k_n = 2.827 \times 10^9$ kg/s^2 and a time step of 3.949×10^{-2} s. The tangential spring constant, k_t, was taken to be equal to $\frac{2}{7} \times k_n$. Table 9 shows the aggregates' masses, bulk radii, and bulk densities depending on the number of large intruder particles that were in the aggregates. These masses, radii, and densities are typical values for asteroids.

Table 9: Simulation Aggregate Properties

Intruders	Mass (kg)	Bulk Radius (m)	Bulk Density (g/cm^3)
1	8.10×10^{11}	525	1.65
2	8.16×10^{11}	538	1.71
3	8.21×10^{11}	521	1.70

Similar to the process described in Chapter 2, I put the 1,000 particles into a simulated rectangular box of 2 km per side and let the particles gravitationally settle. For the masses involved and the size of the box, I calculated the free-fall time to be about 3 hours (about 276,000 time steps). I therefore let the particles settle for a total of 700,000 time steps to ensure that the aggregates had reached an equilibrium state before continuing with the simulations. For the aggregate formation process, I set the coefficients of friction to zero since I wanted to create spherical aggregates to make the analysis easier. After the aggregates formed, friction was turned on. I used a static friction coefficient of 0.7 and a rolling friction coefficient of 0.1 similar to nominal values used in Chapter 2 and by Matsumura *et al.* (2014).

Like in Chapter 2, I did not directly simulate impacts since I was again interested in the overall effect of impacts over time. I assigned to each particle a random velocity (i.e. with a random direction and a magnitude that was chosen between 0 and 50% the escape velocity of the aggregate). The maximum magnitude was chosen as to not disrupt the aggregate but rather to vigorously shake it. Simulations ran for about 104 simulation days.

A.2.3 Results

Tables 10, 11, and 12 show the initial and final radial positions (with respect to the center of mass) of intruders for the one, two, and three intruder aggregates respectively. Intruders that made it to the surface (as defined by having a radial position beyond the bulk radius of the aggregate minus the radius of the intruder) are marked in blue.

Table 10: Initial and final radial positions (with respect to the center of mass) of intruders for the ten one-intruder simulations. Intruders that made it to the surface (defined to be beyond a radial position of the bulk radius of the aggregate minus the intruder radius) are highlighted with blue text.

	Intruder 1	
Run	Initial (m)	Final (m)
1	252	238
2	169	174
3	284	252
4	**421**	**496**
5	330	317
6	289	326
7	**392**	**538**
8	292	288
9	341	355
10	352	334

Except for one case (i.e. Run 2 in Table 11), intruders that made it to the surface all started near the surfaces of the aggregates (as defined by the radial position of the intruder being between the aggregate's bulk radius and 110% of the aggregate's bulk radius minus the intruder diameter).

While Tables 10, 11, and 12 show the initial and final intruder radial positions, Figure 18 shows intruder radial positions over time for the one, two, and three intruder cases. It should be noted that while all 10 one intruder aggregates are shown in Figure 18, only one case is shown for the two and three intruder cases for clarity. As was the case with Tables 10, 11, and 12, for the most part, unless the intruders start near the outer regions of the aggregates they do not rise to the surface.

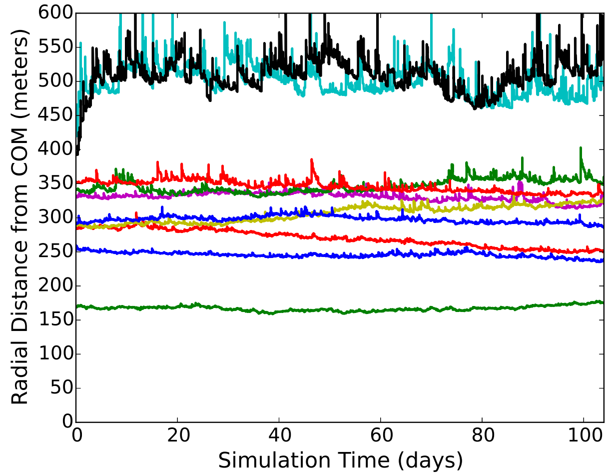
Figure 19 shows the intruder initial and final positions as a percentage of the aggregate bulk radius for all three aggregate types (i.e. one, two, and three intruder cases). While intruders starting with a position that is less than 60% of the bulk radius have limited movement, all intruders starting with a position that is greater than 70% of the bulk radius were able to rise to the surface.

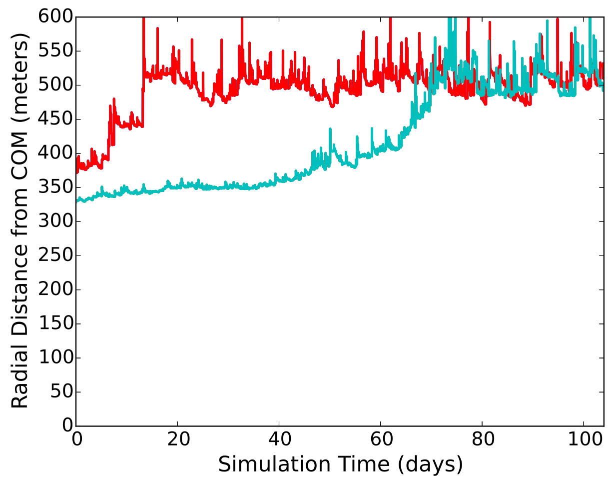
Table 11: Initial and final radial positions (with respect to the center of mass) of intruders for the ten two-intruder simulations. Intruders that made it to the surface (defined to be beyond a radial position of the bulk radius of the aggregate minus the intruder radius) are highlighted with blue text. Note that the numbering of the intruders is arbitrary. Yellow highlighting indicates a starting intruder position more than 10% deeper from the bulk radius minus the intruder diameter distance.

	Intruder 1		Intruder 2	
Run	Initial (m)	Final (m)	Initial (m)	Final (m)
1	239	246	311	278
2	**372**	**515**	**329**	**523**
3	**409**	**484**	**368**	**488**
4	**395**	**492**	109	114
5	349	331	168	188
6	**396**	**503**	**355**	**514**
7	320	327	288	301
8	**382**	**495**	**415**	**540**
9	**388**	**523**	**420**	**493**
10	281	271	**398**	**525**

Table 12: Initial and final radial positions (with respect to the center of mass) of intruders for the ten three-intruder simulations. Intruders that made it to the surface (defined to be beyond a radial position of the bulk radius of the aggregate minus the intruder radius) are highlighted with blue text. Note that the numbering of the intruders is arbitrary.

	Intruder 1		Intruder 2		Intruder 3	
Run	Initial (m)	Final (m)	Initial (m)	Final (m)	Initial (m)	Final (m)
1	199	221	**374**	**522**	**401**	**459**
2	**398**	**470**	309	318	274	312
3	317	324	306	314	286	254
4	215	198	363	376	**435**	**511**
5	315	321	**390**	**488**	**431**	**511**
6	**400**	**501**	243	257	**419**	**488**
7	325	342	**413**	**502**	344	321
8	356	396	**374**	**495**	311	322
9	178	196	253	254	290	317
10	**408**	**530**	**398**	**523**	180	174





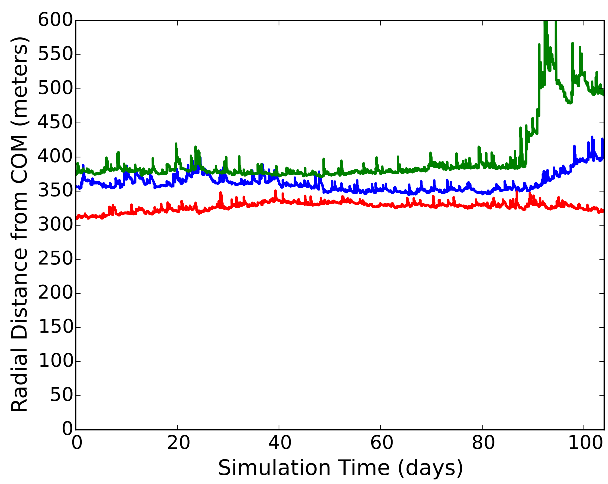


Figure 18: Intruder particles tracked over time as a function of their radial positions from the center of mass (COM). Top: 10 simulations of aggregates that each had one intruder. Middle: One simulation of an aggregate with two intruders. Bottom: One simulation of an aggregate with three intruders. Colors distinguish the different intruders for each case. Only one simulation from each of the two and three-intruder simulations are shown here for clarity.

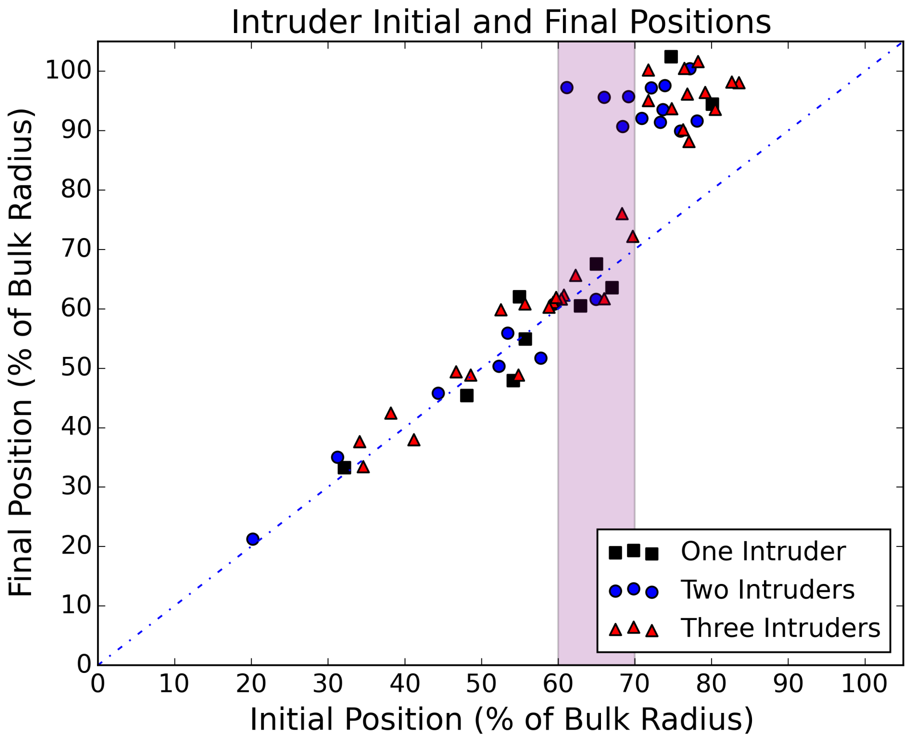


Figure 19: Intruders' initial and final positions with respect to the aggregates' centers of mass. The positions are shown as percentages of the aggregates' bulk radii. The various marker shapes and colors identify from which set of simulations (i.e. one intruder, two intruders, or three intruders) the data are from. Initial positions of 60% to 70% of the bulk radius is highlighted to mark the transition of size sorting of the intruders.

Some intruders whose starting position were between 60% and 70% of the bulk radius were able to rise to the surface, while the movement of others were limited. This may imply that between 60% and 70% of the bulk radius is a transition point.

Lastly, to further examine the driving mechanism for the BNE, Figure 20 shows the initial and final position of the 1,000 particles of two sizes from Chapter 2 (Run 12). Going radially outwards from the interior of the aggregate, the distribution of large particles spreads (meaning that while some larger particles are moving upward, some are moving downward). However, it is clear that smaller particles that started in the outer regions of the aggregate have fallen inward at the end of the simulation. This may be evidence of percolation taking place.

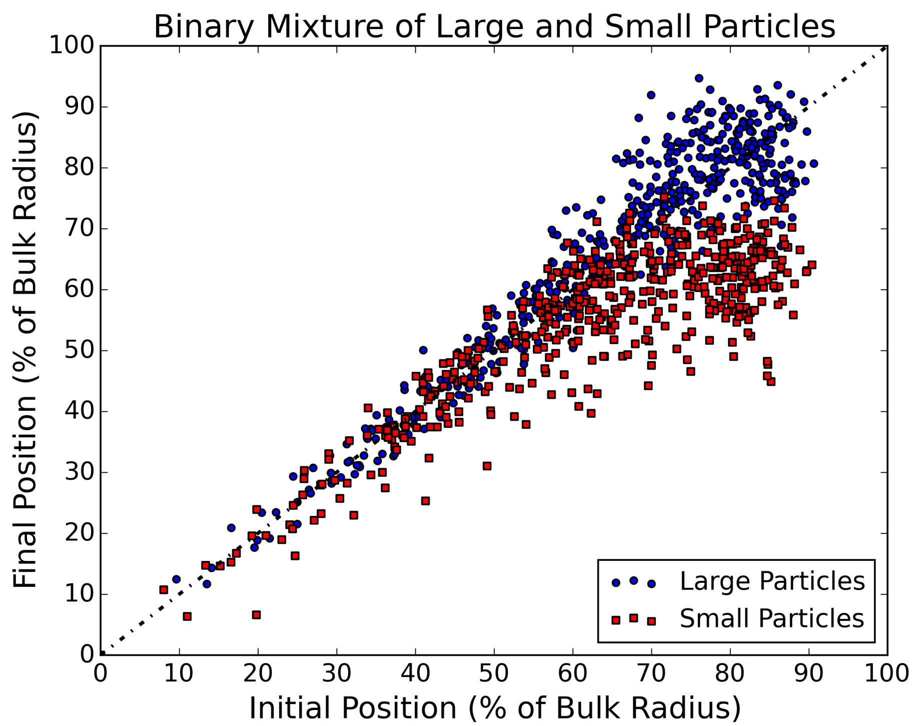


Figure 20: Initial and final positions (in percentages of the bulk radius) of constituent particles of an aggregate composed of 500 large and 500 small particles (Run 12 in Chapter 2)

A.2.4 Conclusions

Chapter 2 hinted that percolation might be the more prominent driving mechanism of the BNE in asteroids. The Intruder Models shown here concur since aggregates made of one, two, and three intruders only show a BNE when the intruders start near the surface of the aggregates. Percolation explains this by noting that when the number of intruders are limited, there are limited void space created. Void spaces are necessary for the small particles to percolate. Since these aggregates should follow the large-scale kinetics of asteroids shaken by impacts, I further propose that for asteroids, the important driving mechanism of the BNE may be percolation.

APPENDIX B

SUPPLEMENTAL MATERIAL FOR CHAPTER 3

B.1 Calculating the LMO Convective Flux

For this work I used the Nusselt number (Nu) to calculate the convective flux of the LMO (Equation 3.4). Breuer and Moore (2015) suggest that depending on the convecting layer's geometry, mode of heating, and boundary conditions, a may range from 0.195 to 0.339 and β may range from 1/4 to 1/3. They also note that Equation 3.4 is only valid if the change in viscosity in the convecting layer is small. I use $a = 0.124$ and $\beta = 0.309$ from experimental work by Niemela *et al.* (2000). It is worth noting that Ra is typically $\sim 10^{22}$ for the LMO, which is considerably higher that what is achievable by experiments. The highest Ra experiments are also conducted with liquid helium (Niemela *et al.*, 2000), which is a rather different environment to the LMO. There is an alternative method of calculating the convective heat flux. Neumann *et al.* (2014) and Monteux *et al.* (2016) used an effective thermal conductivity for convection so that they could use the Fourier law formulation. Nevertheless, I use the Nu procedure stated above for this work.

B.2 Stefan Problem

The Stefan problem was originally used to calculate ice thickness as a function of time as a body of water freezes while it is cooled from the surface. However, the formulation can be used generally for a liquid, such as magma, that is undergoing solidification. There are two key assumptions: (1) The thickness of the solidifying layer is a function of the thermal diffusion length as given by

$$y_m = 2\lambda_1\sqrt{\kappa t}, \tag{B.1}$$

where y_m is the thickness of the solidifying layer as a function of time t, λ_1 is a constant, and κ is the thermal diffusivity. (2) The upper and lower boundaries of the solidifying layer have fixed temperatures.

For an infinitesimal time period, the crux of the Stefan problem is balancing the solidification energy and energy released conductively through the solidified layer as shown by

$$\rho L \frac{dy_m}{dt} = k \left(\frac{\partial T}{\partial y} \right)_{y=y_m}, \tag{B.2}$$

where ρ is the density of the liquid, L is the heat of fusion of the liquid, k is the thermal conductivity of the solid, and T is temperature. By making substitutions to Equation B.2 and assuming that the density and thermal diffusivity of the liquid and the solid are the same, gives the following transcendental equation

$$\frac{L\sqrt{\pi}}{c\left(T_m - T_0\right)} = \frac{e^{-\lambda_1^2}}{\lambda_1 erf \lambda_1}, \tag{B.3}$$

which can be utilized to calculate λ_1. Once λ_1 is know, Equation B.1 can be used to find the thickness of the solid layer as a function of time.

APPENDIX C

SUPPLEMENTAL MATERIAL FOR CHAPTER 4

Table 13: Factor analysis of the difference between the pre- and post-course responses to the 21 Science Attitudes items with corresponding eigenvalues shown (loadings of 0.5 or greater are highlighted in orange).

Science Attitudes Item	Factor 1	Factor 2
All valid	0.24	0.20
Creativity	0.77	-0.16
Experience	0.30	0.16
Just tell	0.68	-0.10
Missing facts	0.11	0.24
No major	0.66	-0.11
Not connected	0.76	-0.16
Satisfaction	-0.18	0.60
Think skills	-0.22	0.64
True	0.09	0.43
Do well	-0.17	0.64
Experiment fail	0.27	0.10
Explain	-0.20	0.62
Facts	0.27	0.21
Figure out	0.60	-0.09
Know before	0.66	-0.01
Lab confirm	0.20	0.42
Only experts	0.62	-0.08
Statistics	0.53	0.08
Straight line	0.37	0.16
Work ourselves	0.03	0.39

Table 14: Factor analysis of the post-course responses to the 11 Benefits items with corresponding eigenvalues shown.

Benefits Item	Factor Loading
Analyze	0.91
Demanding	0.88
Evidence	0.88
Integrate	0.90
Interpret	0.83
Knowledge construction	0.91
Obstacle tolerance	0.87
Real scientists	0.88
Independence	0.74
Science	0.83
Scientists think	0.85

Simultaneous linear regression models for predicting the post-course SS factor scores (SS models) and PV factor scores (PV models) of the whole cohort. The reference groups for the categorical variables gender (female or male) and program type (I-COURSE or O-COURSE) were female and I-COURSE. Listed are standardized coefficients (i.e. continuous variables were scaled and centered prior to the regression). Statistical significance (i.e. $p < 0.05$) is indicated with highlighting. The Studentized Breusch-Pagan test was used to test for heteroscedasticity (when heteroscedasticity is present the p-values are marked with red text).

Table 15: Model SS1

Variable	Coefficient	p-value
(Intercept)	2.783×10^{-16}	1
SS Factor (pre-course)	4.968×10^{-1}	< 0.001
Adjusted $R^2 = 0.2451$		
F-statistic = 147.1 on 1 and 449 DF with $p < 0.001$		
BP = 0.3275, df = 1, p-value = 0.57		

Table 16: Model SS3

Variable	Coefficient	p-value
(Intercept)	-0.16026	0.024
SS Factor (pre-course)	0.45629	< 0.001
Program type	0.30210	< 0.001
Gender	0.02819	0.73
Adjusted $R^2 = 0.263$		
F-statistic = 54.54 on 3 and 447 DF with $p < 0.001$		
BP = 1.4596, df = 3, p-value = 0.69		

Table 17: Model SS4

Variable	Coefficient	p-value
(Intercept)	-0.15245	< 0.01
SS Factor (pre-course)	0.43097	< 0.001
Program type	0.29665	< 0.001
SS Factor (pre-course) X Program type	0.06335	0.46
Adjusted $R^2 = 0.264$		
F-statistic = 54.74 on 3 and 447 DF with $p < 0.001$		
BP = 1.6136, df = 3, p-value = 0.66		

Table 18: Model PV1

Variable	Coefficient	p-value
(Intercept)	5.154×10^{-16}	1
PV Factor (pre-course)	4.869×10^{-1}	< 0.001
Adjusted $R^2 = 0.2354$		
F-statistic = 139.5 on 1 and 449 DF with $p < 0.001$		
BP = 3.9901, df = 1, p-value = 0.0458		

Table 19: Model PV3

Variable	Coefficient	p-value
(Intercept)	-0.22015	0.00205
PV Factor (pre-course)	0.45890	< 0.001
Program type	0.29221	< 0.001
Gender	0.16264	0.0497
Adjusted $R^2 = 0.258$		
F-statistic = 53.16 on 3 and 447 DF with $p < 0.001$		
BP = 9.8755, df = 3, p-value = 0.0197		

Table 20: Model PV4

Variable	Coefficient	p-value
(Intercept)	-0.13164	0.0212
PV Factor (pre-course)	0.52146	< 0.001
Program type	0.28161	< 0.001
PV Factor (pre-course) X Program type	-0.10730	0.19
Adjusted $R^2 = 0.254$		
F-statistic = 52.19 on 3 and 447 DF with $p < 0.001$		
BP = 5.3961, df = 3, p-value = 0.145		

Logistic regression models for predicting course grade of the whole cohort. Binary dependent variable was whether (1) or not (0) a student received an A for their course grade. The reference groups for the categorical variables gender (female or male) and program type (I-COURSE or O-COURSE) were female and I-COURSE. Listed are standardized coefficients (i.e. continuous variables were scaled and centered prior to the regression). Statistical significance (i.e. $p < 0.05$) is indicated with highlighting.

Table 21: Model GA1

Variable	Coefficient	p-value
(Intercept)	0.58702	< 0.001
SS Factor (pre-course)	0.00738	0.96
Program Type	-0.01455	0.94
SS Factor (pre) X Program Type	0.44155	0.038

Table 22: Model GA2

Variable	Coefficient	p-value
(Intercept)	0.580112	< 0.001
SS Factor (pre) X I-COURSE	0.005799	0.96
SS Factor (pre) X O-COURSE	0.447192	< 0.01

Table 23: Model GA3

Variable	Coefficient	p-value
(Intercept)	0.7926	< 0.001
University GPA	1.4777	< 0.001

Table 24: Model GA4

Variable	Coefficient	p-value
(Intercept)	0.3102	0.019
Gender	0.6983	< 0.001

Table 25: Model GA5

Variable	Coefficient	p-value
(Intercept)	0.3712	0.0196
University GPA	1.5372	< 0.001
Gender	0.9493	< 0.001

Table 26: Model GA6

Variable	Coefficient	p-value
(Intercept)	0.2519	0.203
University GPA	1.5409	< 0.001
Gender	0.9839	< 0.001
Program Type	0.2469	0.32

Table 27: Model GA7

Variable	Coefficient	p-value
(Intercept)	0.4136	0.0111
University GPA	1.5396	< 0.001
Gender	0.9125	< 0.001
SS Factor (pre-course)	0.1403	0.26
PV Factor (pre-course)	0.1072	0.42

Table 28: Model GA8

Variable	Coefficient	p-value
(Intercept)	0.3302	0.11
University GPA	1.5422	< 0.001
Gender	0.9358	< 0.001
SS Factor (pre-course)	0.1193	0.35
PV Factor (pre-course)	0.1091	0.41
Program Type	0.1690	0.51

Table 29: Model GA9

Variable	Coefficient	p-value
(Intercept)	0.27948	0.17
University GPA	1.54627	< 0.001
Gender	0.95390	< 0.001
SS Factor (pre-course)	0.03826	0.80
Program Type	0.16083	0.53
SS Factor (pre) X Program Type	0.36639	0.16

Table 30: Model GA10

Variable	Coefficient	p-value
(Intercept)	0.35852	0.0276
University GPA	1.54377	< 0.001
Gender	0.93084	< 0.001
SS Factor (pre) X I-COURSE	0.05588	0.70
SS Factor (pre) X O-COURSE	0.42294	0.0491

Table 31: Model GA11

Variable	Coefficient	p-value
(Intercept)	0.4002	0.0161
University GPA	1.5045	< 0.001
Gender	1.0478	< 0.001
SS Factor	0.5452	< 0.001
PV Factor	0.2505	0.09
Benefits Factor	0.1510	0.29

Table 32: Model GA12

Variable	Coefficient	p-value
(Intercept)	0.3682	0.0245
University GPA	1.4836	< 0.001
Gender	1.0346	< 0.001
SS Factor	0.5576	< 0.001

Logistic regression models for predicting course grade of the whole cohort. Binary dependent variable was whether (1) or not (0) a student received a failing course grade. The reference groups for the categorical variables gender (female or male) and program type (I-COURSE or O-COURSE) were female and I-COURSE. Listed are standardized coefficients (i.e. continuous variables were scaled and centered prior to the regression). Statistical significance (i.e. $p < 0.05$) is indicated with highlighting.

Table 33: Model GF1

Variable	Coefficient	p-value
(Intercept)	-3.3892	< 0.001
SS Factor (pre-course)	0.7794	0.0689
Program Type	0.2831	0.5884
SS Factor (pre) X Program Type	-1.2514	0.0230

Table 34: Model GF2

Variable	Coefficient	p-value
(Intercept)	-3.2382	< 0.001
SS Factor (pre-course) X I-COURSE	0.7189	0.0633
SS Factor (pre-course) X O-COURSE	-0.4860	0.1813

Table 35: Model GF3

Variable	Coefficient	p-value
(Intercept)	-4.2338	< 0.001
University GPA	-1.3875	< 0.001

Table 36: Model GF4

Variable	Coefficient	p-value
(Intercept)	-2.9178	< 0.001
Gender	-0.8294	0.125

Table 37: Model GF5

Variable	Coefficient	p-value
(Intercept)	-3.8872	< 0.001
University GPA	-1.4027	< 0.001
Gender	-0.9662	0.11

Table 38: Model GF6

Variable	Coefficient	p-value
(Intercept)	-3.6419	< 0.001
University GPA	-1.5391	< 0.001
Gender	-1.0267	0.0915
Program Type	-0.7672	0.22

Table 39: Model GF7

Variable	Coefficient	p-value
(Intercept)	-4.24157	< 0.001
University GPA	-1.39034	< 0.001
SS Factor (pre-course)	0.08498	0.78
PV Factor (pre-course)	-0.11029	0.73

Table 40: Model GF8

Variable	Coefficient	p-value
(Intercept)	-4.0454	< 0.001
University GPA	-1.5084	< 0.001
SS Factor (pre-course)	0.1179	0.70
PV Factor (pre-course)	-0.1117	0.73
Program Type	-0.6838	0.27

Table 41: Model GF9

Variable	Coefficient	p-value
(Intercept)	-4.0926	< 0.001
University GPA	-1.4799	< 0.001
SS Factor (pre-course)	0.6573	0.15
Program Type	-0.5613	0.38
SS Factor (pre-course) X Program Type	-1.0669	0.0684

Table 42: Model GF10

Variable	Coefficient	p-value
(Intercept)	-4.2725	< 0.001
University GPA	-1.3833	< 0.001
SS Factor (pre-course) X I-COURSE	0.7760	0.10
SS Factor (pre-course) X O-COURSE	-0.3866	0.27

Table 43: Model GF11

Variable	Coefficient	p-value
(Intercept)	-4.5833	< 0.001
University GPA	-1.4074	< 0.001
SS Factor	-0.5402	0.012
PV Factor	-0.4041	0.18
Benefits Factor	0.2256	0.57

Table 44: Model GF12

Variable	Coefficient	p-value
(Intercept)	-4.5184	< 0.001
University GPA	-1.4315	< 0.001
SS Factor	-0.5105	0.0148

Table 45: Unpaired and unpublished CURE benchmark data for the Science Attitudes items (aggregate of over 5,000 students from the 2014-2015 academic year).

	Pre-course		Post-course		Change	
Item Label	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Factor
No major[3]	3.74	1.03	3.54	1.19	-0.20	Scientific Sophistication (SS)[4]
Figure out	3.32	0.91	3.23	1.02	-0.09	
Just tell	3.14	1.09	3.15	1.15	0.01	
Creativity	4.11	0.90	3.97	1.04	-0.14	
Not connected	4.00	0.94	3.85	1.07	-0.15	
Only experts	3.59	0.89	3.49	0.99	-0.10	
Know before	4.02	0.87	3.90	1.02	-0.12	
Statistics	3.16	1.01	3.21	1.10	0.05	
Thinking skills	4.10	0.74	4.07	0.92	-0.03	Personal Value (PV)
Satisfaction	4.23	0.77	4.12	0.95	-0.11	
Do well	4.01	0.75	3.90	0.92	-0.11	
Explain	4.09	0.81	4.01	0.92	-0.08	
True	3.35	0.87	3.28	0.98	-0.07	
Experience	2.99	0.89	3.08	1.03	0.09	

Continued on next page

[3] This benchmark data does not include the results of this work. Benchmark Cronbach Alpha values for the 22 Science Attitudes items: Pre-course = 0.72 & Post-course = 0.87

[4] Items in this factor were reverse scored

Table 45 – Continued from previous page

	Pre-course		Post-course		Change	
Item Label	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Factor
Missing facts	2.95	0.97	3.00	1.04	0.05	None
All valid	2.60	1.01	2.68	1.09	0.08	
Facts	3.11	0.97	3.10	1.04	-0.01	
Experiment fail	1.86	0.86	1.92	1.02	0.06	
Straight line	3.05	0.90	3.22	0.98	0.17	
Work ourselves	3.26	0.95	3.35	1.00	0.09	
Lab confirm	3.72	0.81	3.59	0.98	-0.13	
Write	3.94	0.73	3.86	0.90	-0.08	Excluded

Table 46: Unpaired and unpublished CURE benchmark data for the Benefits items (aggregate of over 5,000 students from the 2014-2015 academic year)

Item Label	Mean	Std. Dev.	Factor
Interpret	3.52	1.04	Benefits
Obstacle tolerance	3.49	1.05	
Demanding	3.40	1.09	
Knowledge construction	3.41	1.06	
Integrate	3.44	1.05	
Real scientists	3.57	1.08	
Evidence	3.62	1.07	
Analyze	3.72	1.02	
Science	3.57	1.07	
Scientists think	3.39	1.10	
Independence	3.33	1.16	
Career	2.94	1.24	Excluded
Your field	3.44	1.12	
Ethical	3.11	1.22	
Lab techniques	3.73	1.10	
Self confidence	3.18	1.23	
Learning community	3.44	1.14	
Teacher	2.90	1.27	
Primary literature	3.32	1.17	
Oral	3.10	1.25	
Writing	3.29	1.18	

Table 47: Science Attitudes and Benefits factor scores by degree program type along with CURE benchmark data.

		Mean Values[a]		
	Factor	Pre-course	Post-course	Change[b]
Full cohort (n = 451)	SS	3.74	3.59	-0.16**
	PV	3.94	4.05	0.11***
	Benefits	–	3.69	–
O-COURSE students (n_o = 219)	SS	3.91	3.83	-0.08
	PV	4.00	4.19	0.19***
	Benefits	–	3.92	–
I-COURSE students (n_i = 232)	SS	3.58	3.35	-0.23***
	PV	3.89	3.92	0.03
	Benefits	–	3.48	–
CURE benchmark data[c]	SS	3.64	3.54	-0.10
	PV	4.11	4.02	-0.09
	Benefits	–	3.50	–

[a] Significance indicators: $p < 0.05$ (*), $p < 0.01$ (**), $p < 0.001$ (***)

[b] Change calculated from paired pre- and post-course responses

[c] Unpaired pre- and post-course numbers (see Tables 45 & 46 above for the complete CURE benchmark dataset)

APPENDIX D

INSTITUTIONAL REVIEW BOARD APPROVAL FOR HUMAN SUBJECTS RESEARCH

EXEMPTION GRANTED

Chris Mead
Earth and Space Exploration, School of (SESE)
-
Chris.Mead@asu.edu

Dear Chris Mead:

On 1/5/2016 the ASU IRB reviewed the following protocol:

Type of Review:	Initial Study
Title:	Ongoing Habitable Worlds Research
Investigator:	Chris Mead
IRB ID:	STUDY00003679
Funding:	Name: National Science Foundation (NSF), Funding Source ID: NSF-National Science Foundation
Grant Title:	
Grant ID:	
Documents Reviewed:	• Individual Investigator Agreement for Sanlyn Buxner, Category: Other (to reflect anything not captured above); • additional survey questions.pdf, Category: Measures (Survey questions/Interview questions /interview guides/focus group questions); • CURE Pre-Survey, Category: Measures (Survey questions/Interview questions /interview guides/focus group questions); • NSF Grant Document, Category: Grant application; • CITI certification for Sanlyn Buxner, Category: Non-ASU human subjects training (if taken within last 3 years to grandfather in); • CURE Post Survey, Category: Measures (Survey questions/Interview questions /interview guides/focus group questions); • Generic_Course_Information Letter, Category: Consent Form; • Letter from Smart Sparrow, Category: Off-site

	authorizations (school permission, other IRB approvals, Tribal permission etc); • CV for Lev Horodyskyj, Category: Vitaes/resumes of study team; • Ongoing Habitable Worlds.docx, Category: IRB Protocol; • Buxner_CV.pdf, Category: Other (to reflect anything not captured above); • CITI certification for Lev Horodyskyj, Category: Non-ASU human subjects training (if taken within last 3 years to grandfather in);

The IRB determined that the protocol is considered exempt pursuant to Federal Regulations 45CFR46 (1) Educational settings, (2) Tests, surveys, interviews, or observation on 1/5/2016.

In conducting this protocol you are required to follow the requirements listed in the INVESTIGATOR MANUAL (HRP-103).

Sincerely,

IRB Administrator

cc:

Ariel Anbar
Lev Horodyskyj
Steven Semken
Jude Viranga Dingatantrige Perera

APPENDIX E

STATEMENT OF PERMISSION FROM CO-AUTHORS

The previously published article titled "The spherical Brazil Nut Effect and its significance to asteroids" had the following list of co-authors: Alan P. Jackson, Erik Asphaug, and Ronald-Louis Ballouz. The article in press titled "Students in fully-online programs report more positive attitudes toward science than students in traditional, in-person programs" had the following list of co-authors: Chris Mead, Sanlyn Buxner, David Lopatto, Lev Horodyskyj, Steven Semken, and Ariel D. Anbar. The article titled "Effect of Re-impacting Debris on the Solidification of the Lunar Magma Ocean" is in the submission process and had the following list of co-authors: Alan P. Jackson, Linda T. Elkins-Tanton, and Erik Asphaug. All co-authors have granted their permission for use of these articles in this dissertation.