Civil Engineering Undergraduate Honors Theses   Civil Engineering

5-2015

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Citation

An Undergraduate Honors College Thesis

in the

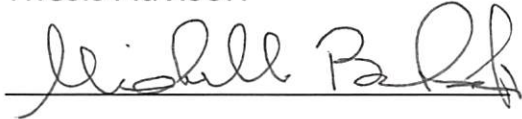College of Engineering
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April 24, 2015

This thesis is approved.

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Interpore 2015: Padova, Italy
Minisymposium MS3.4

A Study of the Influence of Particle Gradation in Bonded Assemblies

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Keywords: Discrete element method; bonded assembly; particle gradation

Abstract

The discrete element method (DEM) has been used extensively to study soil, rock, and masonry behavior because of its ability to model the materials as individual particles or bonded clumps of particles. DEM allows for examination of the macro- and micro-scale response and provides a means to study the fundamental material behavior, but it is still considered computationally expensive in relation to other methods. To lower computational costs, the smallest particle sizes are often considered negligible and are left out of the model. Additionally, rock or intact materials are often modeled as a bonded assembly of uniform spheres. To date, few research studies have considered the influence of particle size and gradation on the strength and fracture behavior of bonded assemblies. This research aims to examine the influence of particle gradation in bonded assemblies through laboratory calibrated DEM simulations. Additionally, the role of the cement-sized particles will also be investigated. While the overall motivation for this study is related to the behavior of mortar in historic preservation applications, the preliminary studies can be directly applied to other geo-related materials such as cemented sands and rock specimens.

This study addresses two critical questions associated with the computational efficiency of bonded assembly models (1) Does particle gradation influence the overall strength and fracture behavior, and (2) Do the smallest size particles influence the overall results enough to justify the additional computational cost? In this study two mortar materials, varying only in sand particle gradation, are subjected to physical laboratory compression strength tests to assess whether or not the influence is observed in physical experiments. Additionally, the compression test results act as a means of calibrating the simulations in DEM. These simulations will examine the macro- and micro-scale influence of particle gradation on the strength of bonded assemblies. Additional simulations are used to examine the effects of modeling the cement-sized particles in the bonded assembly. The results of the physical experiments and the development of the DEM simulations are discussed herein.

Introduction

Mortar has been used for centuries as a civil engineering building material and continues to be used regularly in today's construction. Mortar is a paste material used to bind layers of stone, brick, or other masonry blocks. With a basic composition of sand, cement, and water, mortar is easily manufactured and performs well as a workable material to fill the gaps between masonry units. While the overall use of mortar has not changed through the centuries, the chemical makeup and mixture proportions have changed significantly. The original historic mortars consisted of lime cement rather than the portland cement more commonly used today. Lime, similar to portland cement, is created from the pulverization of limestone rock (calcium carbonate); however, unlike portland cement, lime does not contain any siliceous or aluminous additions. Since the patenting of portland cement in 1824, the use of portland cement has surpassed the use of lime cement in today's society because of portland cement's precedence in the concrete industry (Mitchell, 2007). Portland cement is advantageous for its higher strength, faster setting time, and its ability to harden underwater (hydraulic). These factors have assisted in the ease of masonry constructability and therefore created limitations in the production and availability of lime cement in today's masonry construction.

This study's initial objective was to understand the micro-mechanical behaviors of lime cement mortar versus portland cement mortar to be used in historic masonry preservation. As the initial investigation began on the material properties of typical portland cement mortars, the variations in sand particle gradation became of particular interest and resulted in a shift in the focus of the study. The goal of the current study is to investigate whether or not particle size and gradation affect the physical response of mortar and determine the most efficient and accurate modeling scheme to capture these differences. Discrete element method (DEM) simulations provide a useful platform to study the behavior of bonded assemblies; however, they become very inefficient and impractical if the entire range of particle sizes must be modeled. The simulations developed in this study are aimed at addressing whether or not the smallest size particles influence the overall results enough to justify the additional computational cost, or whether the presence of a cementitious material can be simulated more efficiently by using parallel bonds.

Background

Mortars used in typical construction practices today contain varying amounts of both portland cement and lime. In the construction industry, mortar is classified on the respective proportion of portland cement to lime used in the mortar mix. Mortar is classified into one of five categories as listed: Type M, Type S, Type N, Type O, Type K, with Type M containing the highest proportion of portland cement to lime and Type K containing the lowest proportion of portland cement to lime. Average compressive strength ranges from 17.2 MPa (2500 psi) in Type M mortar to 2.4 MPa (350 psi) in Type O (ASTM C270, 2014). Because of its low strength and minimal usage, ASTM C270 (2014) no longer includes Type K mortar and its respective average compressive strengths. ASTM C270 (2014) also provides a guide for selecting the proper mortar type based upon the construction purpose as well as recommended mix proportions to obtain such a mortar. Typically Type S and Type N are the most common mortar types used in today's construction practices and are widely available for purchase.

This study conducted material properties on Type S mortar because it is commonly used in construction practices and is readily available. Table 1 provides gradation limits for natural sand to be used as aggregate in masonry mortar as specified in ASTM C144 (2011). Figure 1 depicts the particle size gradation limits for natural sand as listed in Table 1. Note that ASTM C144 (2011) also includes gradation limits for manufactured sand; however, this study only considers natural sand. It shall be noted that within ASTM C144 (2011) Section 4.4, it is stated that the aggregate may fail the gradation limits and still be permitted for use as long as the mortar complies with the aggregate ratio, water retention, air content, and compressive strength requirements of ASTM C270 (2014). The lack to enforce gradation limits for aggregate used in mortar raises the question of the importance of particle gradation on mortar properties, specifically compressive strength.

Table 1: Percent passing limits for aggregate in masonry mortar (ASTM C144, 2011).

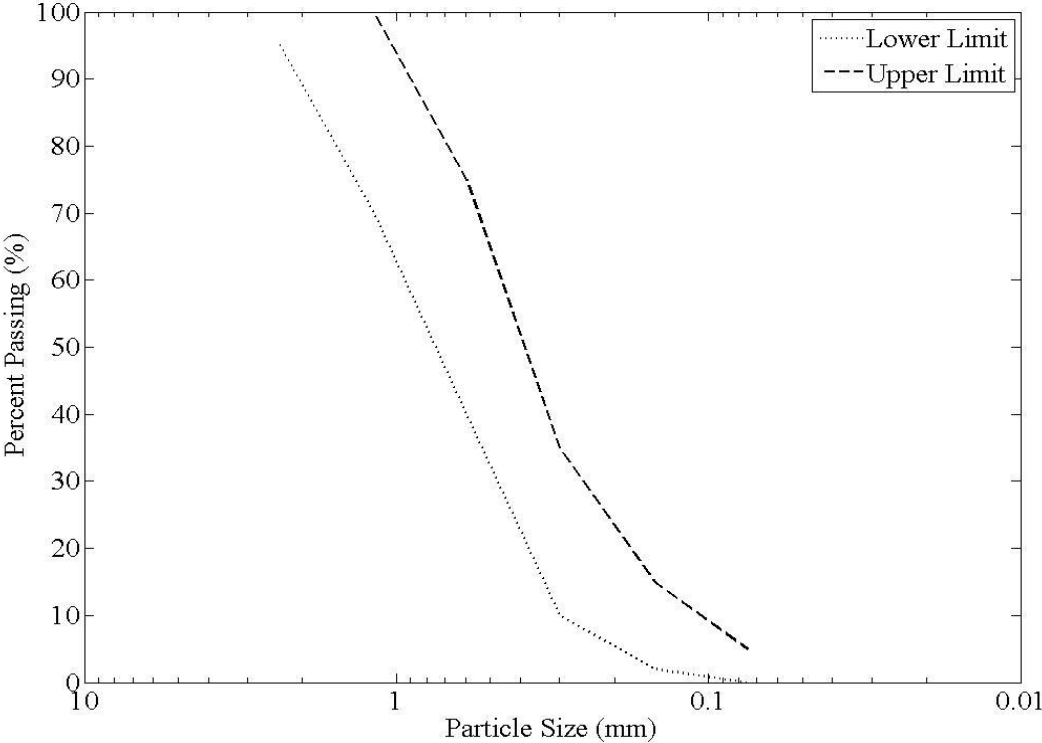| Sieve Size		Percent Passing
4.75-mm	No. 4	100
2.36-mm	No. 8	95 to 100
1.18-mm	No. 16	70 to 100
600-μm	No. 30	40 to 75
300-μm	No. 50	10 to 35
150-μm	No. 100	2 to 15
75-μm	No. 200	0 to 5

Figure 1: Particle size distribution for natural sand aggregate used in masonry mortar.

Limited research exists on the influence of sand gradation on the compressive strength of mortar. (Venkatarama Reddy and Gupta, 2008). Research conducted by McIntosh (1970) has shown significant differences in compressive strength from the effects of grading alone. Instead, research has been primarily focused on the effects of sand gradation on mortar properties such as workability, consistency, and flowability with significant results indicating that sand particle size does have an effect on these given properties. Workability is a property of mortar that is often considered of high importance in characterizing a fresh mortar; however, the property cannot be easily quantitatively measured and instead is highly dependent on the response of the individual mason to the mortar. With no direct measurement, workability is measured using standard flow tests which measure the flowability of mortar. However, flowability does not address all factors influencing the workability property such as ease of placement, consolidation efforts, and setting time. Neville (1996) notes that many aggregate factors influence the behavior of mortars in the fresh and hardened state including: mineralogical composition, particles size distribution, and shape and surface texture of aggregates.

Many studies have concluded that the water to cement ratio is the most important factor in the compressive strength of mortar (Haach et al., 2011; Venkatarama Reddy and Gupta, 2008). In addition, the water to cement ratio is often the easiest property to change in a mortar mix design to gain a desired workability and setting time. In fact, ASTM C270 (2014) notes in section X1.5.1 that workability is largely determined by aggregate grading however the final adjustment is dependent on water content.

It has been suggested by many that well graded sands require a higher water content than poorly graded sands per unit volume to reach the same consistency of mortar. This is due to the fact that well graded sands have better particle packing tendencies as compared to poorly graded sands. This packing tendency observed in well graded sands increases the specific surface area of sand per volume of mortar; thereby, requiring a higher water content to coat each individual sand grain. This principle also applies to fine sands, which exhibit the need for a higher water content than coarse sands because of the higher specific surface area per unit volume. This indirect correlation of mortar properties, specifically compressive strength, to aggregate gradation brings about the concern for the importance of particle size gradation in mortar mixes not only in the physical sense, but also from a numerical simulation point of view.

Discrete element method (DEM) is a numerical modeling technique that has been used extensively in soil mechanics to simulate granular material behavior. In most cases DEM models consist of an assembly of spherical particles that simulate the behavior of a given material to stress responses, although clumps of spheres can also be used. Simulations are often either calibrated or validated with physical laboratory tests on the material being studied. The use of DEM has been limited in the studies of cemented matrices because of the excessive computational cost required to model the large number of cement sized particles in an actual sample. As the number of cement and fine sand (particle size below 150-μm) sized particles increases, the computational speeds become very slow. Few studies have considered the impact of particle gradation on bonded assemblies and whether or not an influence of particle gradation is seen in the numerical results. In addition, past studies often do not include the smallest particles within the simulations and negate their effect in bonded assemblies. Instead, most studies have simulated cement bonds between particles with parallel bonds.

One recent study conducted by Evans et al. (2014) has included cement sized particles in the simulation of bio-cemented sands. This study modeled the cement bond in the form of a cement chain which surrounded the bond of two aggregate particles. Physical laboratory compression tests served as a validation of the simulation to the bio-cemented sands. Evans et al. (2014) suggests that parallel bonds are incapable of simulating the interaction that was noted between cement particle chains with partially-debonded particle assemblies. The study also noted that an increase in cement particles within a single cement chain would lead to an increase in the overall system stiffness and an increase in the strength of the cement chain; thus further highlighting the importance of including small sized particles in simulations.

This study attempts to address the importance of particle size gradation in mortar and the most appropriate modeling scheme for replicating the physical behavior. Physical laboratory tests will be conducted using two different sand gradations in hopes of distinguishing a difference in mortar compressive strength. With recent advances in DEM, it is our hope to better simulate mortars and other cemented arrays.

Experimental Overview

For the first portion of this study, a typical Type S mortar was purchased from a local hardware store. The Type S mortar was a pre-blended mix, which included Type I portland cement, hydrated lime, and a natural river sand. The proportion of portland cement to lime by volume in the Type S mixture is approximately 2:1. In an attempt to study the influence of particle size gradation, a second sand was retrieved which was substituted for the pre-blended sand. The sand used for substitution of the pre-blended sand is a natural, river sand dredged from the Arkansas River and packaged in Van Buren, Arkansas. The substituted sand will be identified as Van Buren sand throughout this study.

The first test conducted on the Type S pre-blended mortar was a dry sieve analysis. Most mortar mixes contain very little, if any, amounts of silt and clay particles passing the 75-μm (No. 200) sieve. Because of their small particle size, clay and silt particles can cause for an increase in water content to reach a given consistency and are therefore often minimal, if not completely absent, in mortar mixes. In addition, cement particle size ranges from 10-50 μm. From this, it was assumed that all material passing the 75-μm (No. 200) sieve was either portland cement or lime (cementitious material). Because of the tendency for the cementitious material particles to adhere to the sand grains, following the dry sieve a wet sieve was conducted on the sand portion.

A dry sieve analysis was also conducted on the Van Buren sand. No wet sieve analysis was necessary for the Van Buren sand for it was delivered before pre-blending operations with cementitious material. The sieve analysis results for the pre-blended sand and Van Buren sand are reported in Table 2 and the particle size distributions are displayed in Figure 2. Note that Figure 2 also includes the upper and lower limits for the gradation requirements of aggregate as previously mentioned in ASTM C144 (2011).

The results of the sieving process indicate that neither the pre-blended sand nor the Van Buren sand met the requirements as specified in ASTM C144 (2011). The pre-blended sand was well outside the gradation limits; however, the Van Buren sand closer resembled the requirements.

As stated previously, ASTM C144 (2011) does not require the aggregate to meet the gradation specifications. The fact that sand in pre-blended mortar mixes sold locally and sand retrieved from a processing plant do not meet gradation requirements brings up to question the importance of the gradation limits outlined in ASTM C144 (2011) relative to strength.

Table 2: Sieve analysis results for pre-blended and Van Buren sands.

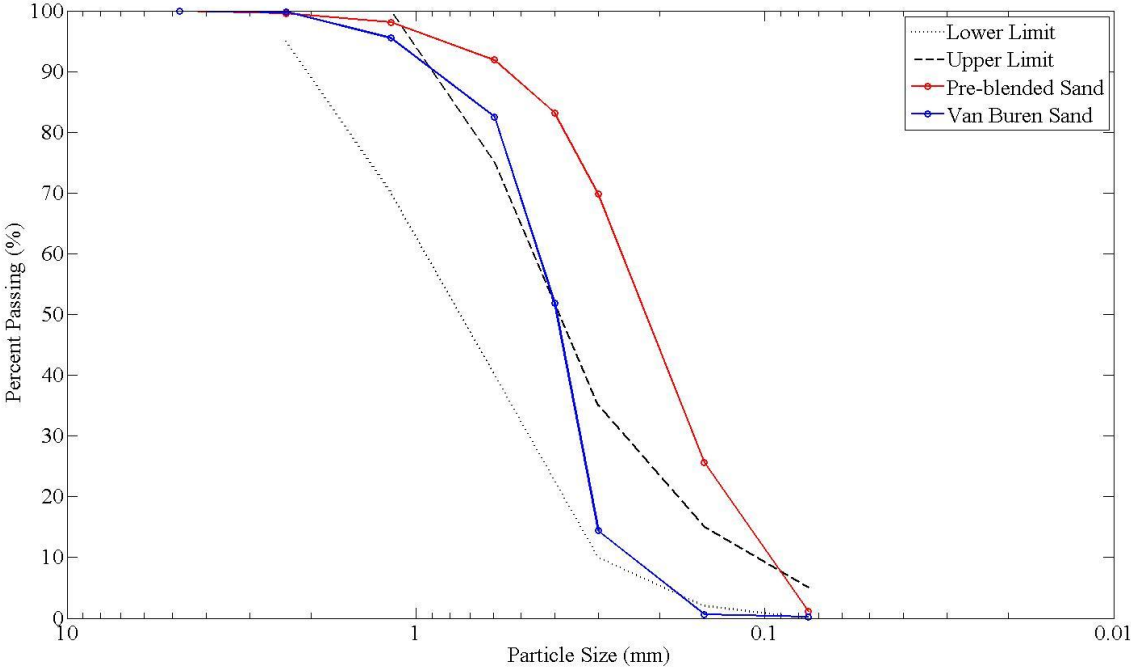| Sieve Size	Particle Size (mm)	Percent Passing (%) Pre-blended	Percent Passing (%) Van Buren
#4	4.75	100.0	100.0
#8	2.36	99.6	99.8
#16	1.18	98.1	95.5
#30	0.595	91.9	82.5
#40	0.4	83.2	51.9
#50	0.3	69.9	14.4
#100	0.149	25.6	0.6
#200	0.075	0.0	0.0

Figure 2: Particle size distribution for pre-blended and Van Buren sand.

Using the particle size distribution curves in Figure 2, the C_c and C_u values were calculated for each sand type and used in classifying the sands. Based on the Unified Soil Classification System, both the pre-blended sand and Van Buren sand are classified as poorly graded sands (SP). It was observed in the laboratory that the pre-blended sand was a finer sand when compared to the Van Buren sand. It was presumed prior to batching that the mortar with the pre-

blended sand would have a lower workability because of the larger specific surface area as compared to the mortar with the Van Buren sand.

Using procedures outlined in ASTM C128 (2015), the specific gravity was determined for both the pre-blended sand and Van Buren as 2.64. The specific gravity was used as a method to determine a density value for the DEM simulations. Additionally from the sieve analysis, the cementitious material content was determined as approximately 30% of the total mass of the pre-blended mortar mixture. From this determination, an approximate water to cement ratio was determined for the mix design.

The next portion of the study consisted of batching mortar mixes using both types of sand to create 50-mm (2-in) cubes to be used in the determination of compressive strength. Table 2 in ASTM C270 (2014) recommends a volume proportion of cementitious materials to sand for Type S mortar of 1:2.25–3. The mix design in this study used an approximate volume ratio of 1:2.6. Having determined the approximate mass percent of cementitious materials in the pre-blended mortar mix, a predetermined water to cement ratio of 0.53 was used. A portion of the cementitious material that was dry sieved from the pre-blended mortar mix was collected and blended with the Van Buren sand to create a separate batch of cubes. It is important to note that the only difference in the batching procedures was the type of sand used. All material quantities remained constant for the purpose of this study. Table 3 provides the mix design used to batch each set of cubes.

Table 3: Mixture proportions for 50-mm (2-in) cubes.

Material	Mass (g)
Cementitious Material	1290
Sand (Pre-blended or Van Buren)	3010
Water	680
w/c ratio = 0.53 cementitious material to sand volume ratio = 1:2.6	

The cubes were batched and molded in accordance to ASTM C109 (2013). Each batch created 9 cubes. During batching, it was observed that the consistencies in the two mortar types differed. The mortar with the pre-blended sand was observed to be a much stiffer mortar; whereas, the mortar with the Van Buren sand had a much better workability and ease in molding the cubes. As mentioned previously, this enhanced workability is most likely due to the reduced specific surface area of sand particles within the coarser Van Buren sand.

After curing for 24 hours, the cubes were de-molded and submerged in water saturated with calcium hydroxide (lime). All cubes were allowed to cure for a minimum of 28-days before compressive strength tests began. A total of 27 cubes were created using the pre-blended sand and a total of 12 cubes were created using the Van Buren sand.

Compressive strength tests were conducted in accordance to ASTM C109 (2013) with the use of an MTS machine. Each cube was placed on the machine so that the finished face was not in

contact with the loading platens. The two faces in contact with the platens were lightly sanded with sandpaper to reduce any irregularities or surface defects, which might cause for an uneven loading surface with the platens. Compression tests were stroke controlled at a rate of 0.008 which resulted in an equivalent loading rate between 900 – 1800 N/s (200 – 400 lb/s) as specified by ASTM C109 (2013) for allowable loading. An extensometer was placed on the central portion of each cube to more accurately measure stiffness, which will be used in calibrating the bond strengths in the DEM simulations. Figure 3 depicts a mortar cube during compression testing.

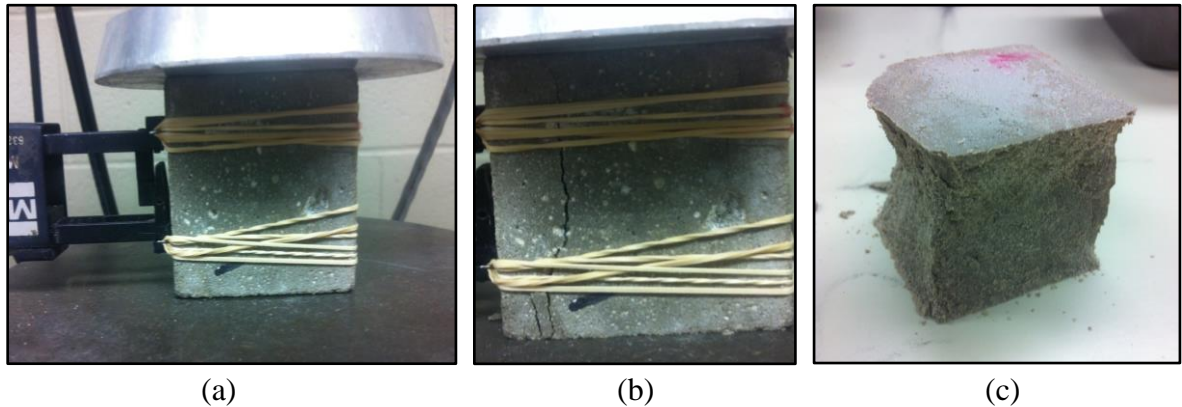| (a) | (b) | (c) |

Figure 3: Mortar cube in compression (a) before compression test, (b) showing initial signs of fracture, and (c) complete fracture.

The stress-strain data for the two types of mortar cubes are presented in Figure 4. It can be suggested that the mortar cubes with pre-blended sand have a noticeably higher compressive strength than the mortar cubes with Van Buren sand. Table 4 reports the maximum peak strength, minimum peak strength, average peak strength, and standard deviation results for mortar cubes with the pre-blended sand and mortar cubes with the Van Buren Sand. It was also observed that the mortar cubes with pre-blended sand reached a peak strength at lower strains than the mortar cubes with Van Buren sand. This observation may suggest that the particle gradation can have an impact on the strain rate at which peak strength is reached. It should also be noted that a large variation in strength is not uncommon for mortar mixes and a significant difference in the types and gradations of sands sourced for this purpose is common.

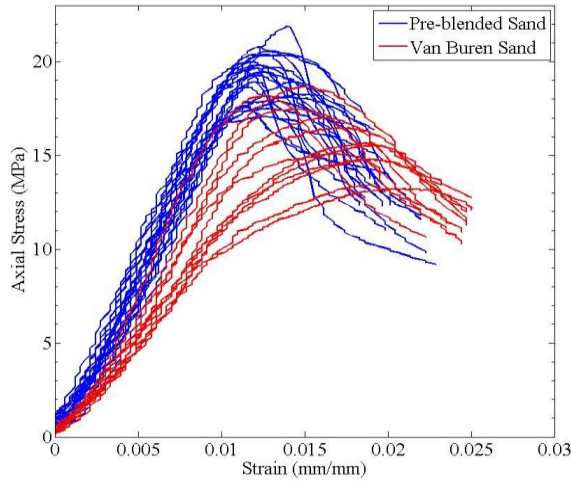Table 4: Compressive strength properties.

	Pre-blended Sand	Van Buren Sand
Maximum peak strength, MPa (psi)	21.87 (3,172)	18.65 (2,705)
Minimum peak strength, MPa (psi)	17.07 (2,476)	13.21 (1,916)
Average peak strength, MPa (psi)	19.25 (2,792)	15.86 (2,300)
Standard deviation, MPa (psi)	1.23 (178)	1.75 (254)
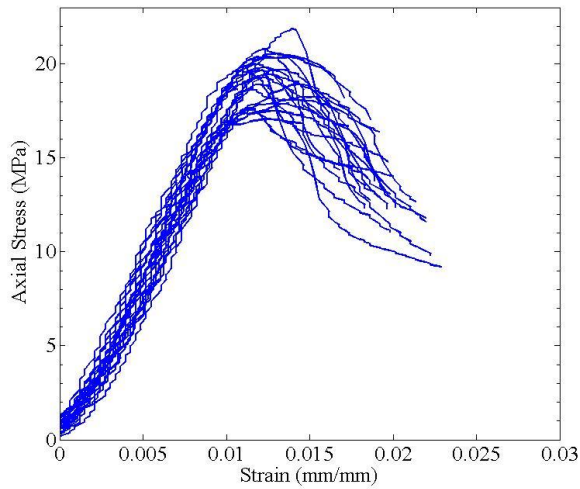
(a)
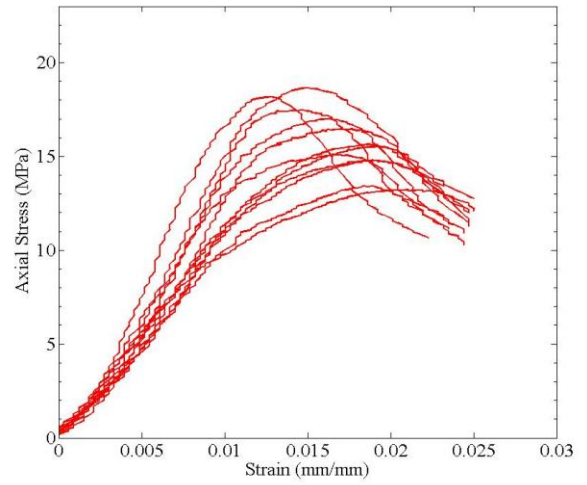
(b)

(c)

Figure 4: Stress-strain curves (a) pre-blended sand, (b) Van Buren sand, and (c) Pre-blended and Van Buren sand.

Although these data indicate differences in the strength, it is difficult to determine the significance of this difference based solely on the physical experiments conducted. The tests do, however, serve as a means to determine the expected range of strength variation in the numerical results. The data retrieved from the extensometer will be used to more accurately determine the modulus of elasticity of the two sets of mortar cubes, so that a comparison can be made between the two mixes and the simulation results.

For purposes of DEM simulations, the parallel bond must be properly calibrated to replicate the fracture of an intact specimen under compression tests. This is usually carried out in a trial-and-error type procedure and is considered almost in some cases as an inverse problem. Based on additional experimental tests on the cement used and examination of the fracture surfaces using a

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microscope (Figure 5), it was confirmed that fracture occurred at the cement-sand bond and not through the cement matrix itself. This observation was expected based on the fact that the strength of cement is much stronger than the cement-to-sand bond strength. Additionally, from Figure 5, it is observed that the actual aggregate particles are not crushing and instead their exposed intact surface protrudes outward on the fracture surface where the cement bond has broken from the aggregate edge. Previous studies on concrete and mortar further suggest the concept that failure tends to occur at the cement-sand interface. Moavenzadeh and Kuegal (1969) provide results indicating that during fracture in concrete and mortar, the cracks follow a meandering path and will tend to follow a path around the aggregate rather than cracking through the aggregate. Strange and Bryant (1979) also provide evidence that as a crack migrates through a mortar, it tends to pass along the matrix-aggregate interface and then re-enter the matrix. Further evidence suggests that the weakest link occurs at the matrix aggregate interface and progressive microcracking bridges a path between nearby bond cracks (Carrasquillo et al., 1981). This observation is useful for the numerical portion of the study because the particles in the DEM simulations are modeled as rigid particles and particle crushing or deformation is not considered.
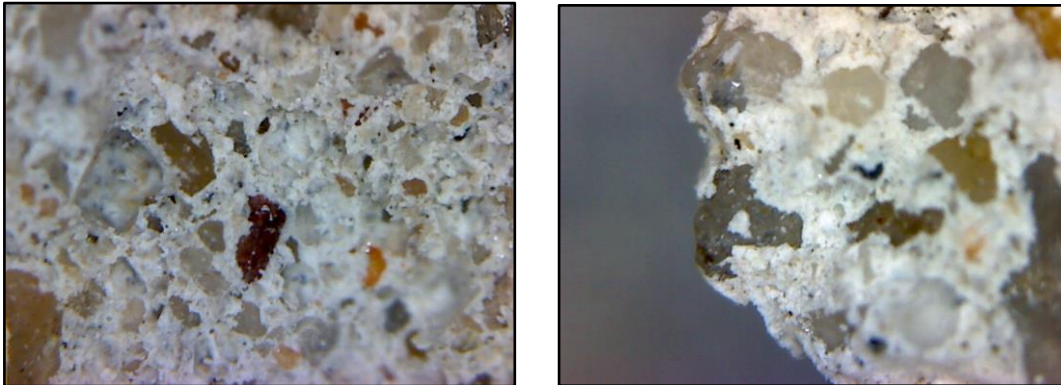

Figure 5: Fracture surface at cement-sand interface (magnification 200x) (a) Pre-blended sand, (b) Van Buren sand showing protruding, unbroken aggregate.

Simulation Overview

The numerical models in this study were created using the PFC^{3D} platform by Itasca Consulting Group, Inc. (Itasca, 2015). Several inputs are required in order to realistically model a granular material. These inputs can either be determined based on similar studies or they can be determined experimentally in some cases. Inputs used in this study including the particle size distribution and density of the sand were directly measured, whereas the linear contact stiffness and parallel bond strength were calibrated using the laboratory data through a trial-and-error procedure. The DEM simulations are systematically altered until the compressive strength values are similar to the reported compressive strengths obtained in the physical laboratory. It should be noted that the simulations used perfectly spherical particles; however, natural sand grains are not perfectly spherical in nature and instead contain surface irregularities. The use of spheres in modeling simulations is computationally much more efficient and quite common in

DEM studies. A 50-mm (2-in) cube in the simulation contains approximately 1,218,000 spherical particles (Figure 6). With such a large quantity of particles within the simulation, using perfect spheres was an assumption that allowed for reduced computational cost. The authors suggest that while these simulations were calibrated based on the laboratory data so that similar strengths were obtained, it is likely that the interlocking mechanisms which may add to the strength in the physical cube are not replicated in the simulations. The assumption of spherical particles allowed for simplification of the model and the authors warrant use of extrapolating the findings to describe the behavior of non-spherical particles. The DEM simulations are intended to be compared only with the DEM simulations to determine the effects of particle gradation and the role of parallel bonds in bonded assembly models.

The simulations are currently being conducted to increase understanding of the role the cement particles play in the overall response. In the initial simulations the pre-blended sand gradation was used to represent the particles. In these simulations the cement particles were not included and instead a parallel bond was created between particles. The virtual cubes will be subjected to the same compression testing conditions used in the laboratory and the parallel bonds will be calibrated. This parallel bond strength will be used for the remainder of the simulations where the Van Buren sand gradation is considered. Comparisons of the simulation results for the two sand types will be used to determine the influence sand gradation has on the overall behavior.
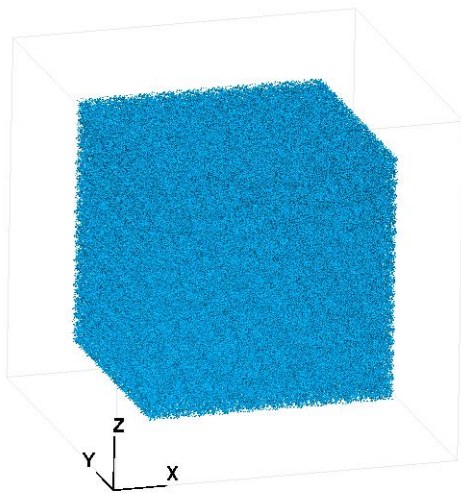

Figure 6: DEM simulation of 50-mm (2-in) mortar cube.

Conclusions and Future Work

In conclusion, DEM simulations can allow great advancements and understandings in the macro- and micro-mechanical behavior of bonded assemblies, but they are computationally expensive in some cases. This study addressed the influence of particle gradation on the effect of bonded assemblies for physical experiments while the equivalent study using DEM simulations is currently ongoing. Within the physical laboratory testing of mortars, it was observed that a

change in particle gradation of sand with all other factors remaining constant can indeed influence the compressive strength. It was also observed that changing the sand gradation can influence fresh mortar properties such as workability and consistency. Continuance of DEM simulations will be used to better understand the influence of particle gradation on mortar properties. Additionally, continued research will identify whether or not including the cement sized particles within DEM simulations is necessary or if the behavior can be accurately modeled using parallel bonds. As a part of the future work, it is proposed that simulations with and without the cement particles will be compared to address the importance of including cement sized particles and the relationship between computational time and accuracy.

It is also proposed that the reasoning for not requiring the limitations of aggregate gradations for mortar in ASTM C144 (2011), is the over-arching concern for compressive strength alone. Even though both sand types used in this study failed the gradation limits, they both reported compressive strength values well above the required standard compressive strength of 12.4 MPa (1800 psi) for Type S mortar as identified in ASTM C270 (2014). Variations in aggregate gradation may not be drastic enough to reflect compressive strengths below standard requirements because the effect of aggregate gradation is minimal in relative comparison to the water to cement ratio; however, this does not negate the importance of aggregate gradation in mortar and the questions which arise in the proper modeling of bonded assemblies. Even though both sand types used in the mortar provided allowable compressive strengths, differences were noted in comparing the relative strengths as well as the strain at which the peak strengths occurred.

Because mortar has traditionally been viewed by many as a highly variable material to research, additional mortar cubes should be batched and tested to better understand the material and its variance under differing environmental conditions. Continued physical testing will entail more accurate simulations for further comparisons in hopes of better understanding the importance of modeling cement sized particles within bonded assemblies.

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