Mars Global Simulant MGS-1: A Rocknest-based open standard for basaltic martian regolith simulants

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Abstract

The composition and physical properties of martian regolith are dramatically better understood compared to just a decade ago, particularly through the use of X-ray diffraction by the Curiosity rover. Because there are no samples of this material on Earth, researchers and engineers rely on terrestrial simulants to test future hardware and address fundamental science and engineering questions. Even with eventual sample return, the amount of material brought back would not be enough for bulk studies. However, many of the existing regolith simulants were designed 10 or 20 years ago based on a more rudimentary understanding of martian surface materials. Here, we describe the Mars Global Simulant (MGS-1), a new open standard designed as a high fidelity mineralogical analog to global basaltic regolith on Mars, as represented by the Rocknest windblown deposit at Gale crater. We developed prototype simulants using the MGS-1 standard and characterized them with imaging techniques, bulk chemistry, spectroscopy, and thermogravimetric analysis. We found the characteristics of the MGS-1 based simulant compare favorably to rover- and remote sensing-based observations from Mars, and offer dramatic improvements over past simulants in many areas. Modest amounts of simulant will be produced at the University of Central Florida. By publishing the mineral recipe and production methods, we anticipate that other groups can re-create the simulant and modify it as they see fit, leading to region-specific and application-specific versions based on a common standard.

1.0 Introduction

Planetary materials available for laboratory study come from a handful of sample return missions, as well as a large meteorite collection dominated by ordinary chondrites. Because actual planetary samples tend to be rare and often expensive, various groups have produced simulated planetary materials, or "simulants", that aim to replicate one or more features of a reference sample. These features commonly include the chemistry, mineralogy, spectral properties, and geotechnical characteristics of rocks, regolith or fine dust. Simulants have been used to test engineering hardware (e.g., Bernold, 1991), for astrobiology studies (e.g., de Vera et al., 2004), and plant growth experiments (e.g., Wamelink et al., 2014), among other applications. However, past simulants (particularly lunar ones) have been plagued by a lack of quality control (Taylor et al., 2016). Previous simulants often sacrificed accuracy for convenience, had poor documentation, and the resulting products have been assumed to be appropriate for all types of research. Perhaps more problematic is that simulants have usually been produced in large batches, and when the initial batch runs out it can be difficult to re-create the original material.

Simulants for martian regolith (informally, soil) are prone to these same issues, and the most cited martian simulants have seen their supplies exhausted. The most prominent Mars simulant is Johnson Space Center JSC Mars-1 (Allen et al., 1998), which was later reproduced as JSC Mars-1A by Orbitec when the original supply ran out. However, the Orbitec simulant website was taken down sometime in 2017 and it appears that JSC Mars-1A is no longer available. The other notable Mars simulant is Mojave Mars (MMS) (Peters et al., 2008), that is not currently available outside of NASA. An education company called The Martian Garden sells two simulants that are reported to be derived from the same source material as MMS, but in fact they have mined a highly altered red cinder material instead of the original Saddleback Basalt (see below). The utility of these simulants (JSC Mars-1, MMS, and their updated versions) comes mostly from the fact that they are fine-grained, roughly basaltic composition materials: this may be appropriate for certain uses that do not require high fidelity simulants, but inappropriate for others.

The goal of this work is to develop an open standard for a martian regolith simulant (Mars Global Simulant, MGS-1) with high fidelity in mineralogy, chemistry, physical properties, and spectral properties compared to an appropriate reference material, in this case the windblown soil Rocknest at Gale crater (Fig. 1a) (Bish et al., 2013; Blake et al., 2013; Leshin et al., 2013; Minitti et al., 2013; Archer et al., 2014; Sutter et al., 2017). We produced and analyzed prototype simulants (Fig. 1b) using this standard, some of which are being used in soil remediation and plant growth studies for future human exploration of Mars. Our group at UCF is building the capacity to produce modest quantities of MGS-1 based simulant (tens to hundreds of kilograms) available to the community at cost. However, as an open standard the same mineral recipe and methods described below can be used to re-produce MGS-1 and modify it as desired (§4.2).

1.1 Previous Mars simulants

JSC Mars-1 and MMS have been used in a variety of laboratory studies as "soil simulants" (e.g., Shkuratov et al., 2002; de Vera et al., 2004; Arvidson et al., 2009; Zacny et al., 2013), but these simulants are based on early studies of martian regolith. JSC Mars-

1 (Fig. 1c) was sourced from an altered palagonitic tephra from the Pu'u Nene cinder cone between Mona Loa and Mona Kea in Hawaii (Allen et al., 1998). It consists almost entirely of amorphous palagonitic material, with minor crystallites of plagioclase and magnetite. JSC Mars-1 was designed as a spectral simulant, in that the nanophase iron oxides (npOx) present in the altered Hawaiian tephra produced a good match to the visible/near-infrared (VNIR) spectra from dusty deposits on Mars, particularly at shorter wavelengths (Evans and Adams, 1979; Bell et al., 1993; Morris et al., 1993; Allen et al., 1998; Morris et al., 2001).

MMS was designed as a geotechnical simulant and was sourced from the Saddleback Basalt near the NASA Jet Propulsion Laboratory: it consists of crystalline plagioclase, pyroxene, magnetite, and hematite, with trace ilmenite and olivine (Peters et al., 2008). Although the original MMS is not available outside of NASA, The Martian Garden company sells a product marketed as Mojave Mars Simulant, renamed MMS-1, and an "enhanced" version, MMS-2 (Fig. 1d). MMS-2 is described as being spiked with hematite, magnesium oxide, and unnamed sulfates and silicates. However, The Martian Garden company had no contact with the creators of MMS, and their simulants do not resemble the original version (compare Fig. 1d with Fig. 2 in Peters et al. (2008)). The company is instead mining the highly altered red cinder material described by Beegle et al. (2007) instead of the original Saddleback Basalt. Quantitative mineralogical analysis is not available for either JSC Mars-1, MMS, MMS-1, or MMS-2, although this is not really feasible for JSC Mars-1 due to its mostly amorphous character.

There are a number of important differences between these older Mars simulants and new *in-situ* measurements of martian regolith. In terms of crystallinity, JSC Mars-1 is almost completely amorphous, while MMS, MMS-1 and MMS-2 are nearly 100% crystalline. In contrast, martian soils are a subequal mixture of crystalline and amorphous phases, as revealed by the CheMin instrument on the Mars Science Laboratory (MSL) (Bish et al., 2013; Dehouck et al., 2014). JSC Mars-1 is extremely hygroscopic, contains >20 wt.% H_2O at ambient conditions, and is known to contain significant amounts of organic matter as well. Most of the older simulant varieties contain almost no sulfur, whereas martian regolith contains up to 6 wt.% SO_3 (assuming all S is in the form of sulfate; Yen et al., 2005; Ming and Morris, 2017). As noted above, the MMS-2 simulant is spiked with sulfates and other phases to resolve discrepancies in bulk chemistry, but the composition on the package confusingly lists both mineral percentages and wt.% oxides in the same table, summing them to 100%.

Other Mars simulants have also been developed based on terrestrial basalts, natural weathering profiles, and commercial sand products. Nørnberg et al. (2009) described Salten Skov 1, a magnetic dust analog mostly composed of crystalline iron oxides. Schuerger et al. (2012) created a series of analog soils by spiking a terrestrial basalt with various salts and carbonates; they used them to test the survival of microbial colonies in martian conditions. Other countries have developed Mars simulants, including a series of nepheline and quartz sands as geotechnical simulants for the European Space Agency (Gouache et al., 2011), terrestrial basalt spiked with magnetite and hematite for China's Mars exploration program (Zeng et al., 2015), and basalt mixed with volcanic glass in New Zealand (Scott et al., 2017). These simulants have not yet been widely distributed or adopted.

1.2 New insights on martian regolith

The surface of Mars is covered by an unconsolidated regolith produced by the combined action of impact comminution, physical erosion by wind, water, and lava, and chemical weathering by fluids and oxidants (mostly early in the history of Mars) (McCauley, 1973; Malin and Edgett, 2000; Golombek and Bridges, 2000; Goetz et al., 2005; Yen et al., 2005; Murchie et al., 2009). The finest particle size fraction, known as dust, is lofted high into the atmosphere by winds and is implicated in global storm patterns (Toon et al., 1977). Martian dust is somewhat chemically distinct from the underlying soil, with a larger component of npOx responsible for its ochre hue (Morris et al., 2001; Berger et al., 2016). Presumably the dust was or still is derived from regolith-forming processes, such that martian dust is a more "processed" and oxidized version of the underlying coarser soil. The soil itself has a basaltic composition (Yen et al., 2005; Ming and Morris, 2017), derived from a globally basaltic crust (McSween et al., 2009).

Martian soils have been examined *in-situ* at seven locations by landers and rovers, with supplemental information from orbital remote sensing. Soil major element chemistry and mineralogy are quite similar at the Spirit, Opportunity, and Curiosity landing sites (Yen et al., 2013; Ming and Morris, 2017), supporting the presence of a global basaltic soil that may be locally to regionally enriched in rarer evolved volcanic compositions (e.g., Christensen et al., 2005) or alteration phases (e.g., Squyres et al., 2008). However, we note that the three landing sites compared in Yen et al. (2013) are all from sulfur-rich terrains (Karunatillake et al., 2014), and a true global average may have less sulfur-bearing minerals consistent with this bulk chemistry constraint. Regardless, the MGS-1 standard is modeled on the Rocknest windblown soil at Gale crater, with supplemental information from measurements by other landed and orbital assets. Rocknest is the best-characterized martian soil to date (Bish et al., 2013; Blake et al., 2013; Leshin et al., 2013; Minitti et al., 2013; Archer et al., 2014; Sutter et al., 2017), and based on currently available data its chemical similarity to soils at disparate landing sites makes it an appropriate reference material from which to develop a new simulant standard.

2.0 The MGS-1 standard

2.1 Design philosophy

Our general approach to designing asteroid and planetary simulants is to start from the mineralogy, because minerals are the basic building blocks of planetary materials. Simulants designed to match bulk chemistry might provide a close match to more readily available measurements (from Alpha Particle X-ray Spectrometer instruments, for example), but a simulant could be designed from infinite combinations of random compounds to reproduce the bulk chemistry of a reference material without having any of the right minerals inside of it. By starting with the correct mineral constituents, the derived properties (geotechnical, spectral, chemical, etc.) should fall out of the final product, with adjustments made where necessary based on analyzing initial prototypes. We applied this mineral-based design philosophy for the MGS-1 standard, based on X-ray Diffraction (XRD) analyses for the crystalline portion of the Rocknest soil (Bish et al., 2013), and inferences for the amorphous component (Bish et al., 2013; Dehouck et al., 2014; Achilles et al. 2018).

2.2 Mineral recipe and calculated bulk chemistry

2.2.1 Crystalline fraction

The crystalline fraction of Rocknest is well constrained by XRD (Bish et al., 2013). These measurements provide quantitative mass fractions of all minerals present at ~1 wt.% or greater, and crystal chemistry constraints from unit cell parameters and/or site occupancy. We adopt most of the same mineral proportions reported by Bish et al. (2013) (Table 1), re-normalized for a 30% amorphous content that is intermediate between low and high estimates of how much amorphous material is present (Bish et al., 2013; Dehouck et al., 2014). The detected crystalline phases in Rocknest include plagioclase, pyroxene, olivine, magnetite, anhydrite, hematite, ilmenite, sanidine, and quartz (Bish et al., 2013). For simplicity and sourcing concerns we do not include ilmenite, sanidine or quartz in the MGS-1 standard, which were near the detection limits of CheMin. Magnetite, anhydrite and hematite were also near the detection limit, but magnetite is important for magnetic properties, anhydrite for sulfur contents, and hematite for pigmenting properties.

2.2.2 Amorphous fraction

Poorly crystalline and/or X-ray amorphous material makes up at least 21-22% of the Rocknest soil sample by weight (Dehouck et al., 2014), and it is still not entirely clear what this material is. Dehouck et al. (2014) and Morris et al. (2015) isolated the elemental chemistry of the amorphous component using a mass balance approach (Table 2), showing that it is deficient in SiO_2, Al_2O_3, and CaO, and enriched in SO_3 and H_2O compared to the bulk soil. The amorphous component likely cannot be explained by a single phase, and is likely a mixture of npOx phases like ferrihydrite (Dehouck et al., 2014; Dehouck et al., 2017), silica-bearing phases such as basaltic glass or opal, and one or more sulfate species like ferric sulfate (Sklute et al., 2015) or sulfate anions adsorbed onto other phases (McAdam et al., 2014; Rampe et al., 2016). Crystalline carbonates were not detected in Rocknest, but evolved gas analysis suggests that one or more carbonate-bearing phases is present (Sutter et al., 2017), such that a mixture could be present, or the carbonates could be poorly crystalline. Other components not uniquely detectable by XRD could include allophane, hisingerite, and gels/protoclays.

Despite this inherent uncertainty, we chose to represent the amorphous component in the MGS-1 standard with materials for which there is independent evidence, and/or whose combination approximates the derived chemistry (Dehouck et al., 2014; Morris et al., 2015) of the Rocknest amorphous material. For MGS-1 this includes basaltic glass, ferric sulfate, ferrihydrite, and iron carbonate. A least squares approach was used to find the relative proportion of these phases that best reproduces the estimated chemistry of the CheMin amorphous component. The goal was to include a parsimonious and easy-to-source selection of phases that covered the major anion groups, instead of including every possible amorphous material listed above. In terms of the silica-bearing portion of the amorphous component, we note that glass on Mars has been severely underappreciated in the past, and for some reason all but dismissed by some authors interpreting the CheMin results. But glassy spherules are clearly observed in soils at both the Phoenix and Curiosity landing sites (Goetz et al., 2010; Minitti et al., 2013), and the widespread presence of glass is supported by recent orbital investigations (Horgan and Bell, 2012; Cannon and Mustard, 2015; Cannon et al., 2017; Horgan et al., 2017). Indeed, more recent detailed analysis of CheMin data suggest that basaltic glass makes up ~68%

of the amorphous material in Rocknest (Achilles et al. 2018), exactly in line with the standard (Table 1). Ferric sulfate and iron carbonate, two of the four “amorphous” species in MGS-1, are added to the prototype simulants in the crystalline state as iron (III) sulfate pentahydrate and siderite, respectively. These species can be synthesized in amorphous form by evaporating appropriate solutions in vacuum, but they are prone to recrystallize in normal laboratory conditions.

2.2.3 Oxychlorines and nitrates

Oxychlorine species are also present in martian soil and could include (per)chlorate salts (Hecht et al., 2009; Sutter et al., 2017) and/or peroxide species (Clancy et al., 2004; Crandall et al., 2017). Nitrates are also present (Stern et al., 2015). Perchlorates in particular have received significant attention because of their possible toxicity, and they will present a challenge and opportunity for human exploration in the future (Davila et al., 2013). No crystalline (per)chlorate salts were detected in Rocknest above the ~1 wt.% detection limit, but evolved ClO_4 was detected (Archer et al., 2014). This suggests that a mixture of such salts is likely present, or they are present as amorphous/adsorbed species. We included crystalline nitrate and perchlorate salts in some of our initial prototypes designed for agricultural studies, but do not include them in the root MGS-1 standard.

2.2.4 Elemental chemistry

Because MGS-1 is a mineralogical standard, the bulk chemistry of simulants created from the standard will change based on the crystal chemistry of the minerals used. Table 2 lists the elemental chemistry of the bulk Rocknest soil and the isolated amorphous component (Morris et al., 2015). In developing the mineral recipe, we calculated an estimated chemical composition for MGS-1 simulants using the mineral fractions in Table 1 and idealized chemical formulas for the constituent minerals, including the actual Mars crystal chemistries for plagioclase, pyroxene and olivine from Bish et al. (2013) and Morris et al. (2015). Average martian crust was used for the basaltic glass composition (Taylor and McLennan, 2009). This results in an elemental chemistry within ~2 wt.% of bulk Rocknest for all major oxide species. It can be difficult to find large quantities of terrestrial minerals with crystal chemistries appropriate for Mars, such that actual MGS-1 based simulants will deviate from the calculated chemistry depending on the specific silicates used. More effort put into sourcing accurate mineral chemistries (or combinations of endmembers) will result in a more accurate elemental chemistry for the final product.

2.2.5 Additional considerations

Mars Global is not meant to be a perfect standard for simulants (if such a thing exists), and there are almost certainly trace mineral species present in martian soil that aren't represented in MGS-1: these could include phosphates, sulfides, chromates, oxalates, and other rare species. Additional phases may be present in an amorphous or poorly-crystalline state, as discussed above. As well, silicate minerals are likely shocked to various degrees on Mars, whereas the basic MGS-1 standard does not account for this. Some phases are detected in localized regions on Mars like opaline silica (Squyres et al., 2008; Milliken et al., 2008), clays (Poulet et al., 2005), halide salts (Osterloo et al., 2008), and potassic feldspar (Le Deit et al., 2016), and would be expected to be mixed into regional soils, but likely not on a global scale at detectable (>1 wt.%) amounts. In §4.2 we discuss how different versions of MGS-1 could be created to simulate these regional soils.

3.0 Prototype simulant production

Using the MGS-1 mineral standard, we created prototype regolith simulants and analyzed them using a variety of instrumental techniques. The production methods and results are described below.

3.1 Source materials

We have built up a large library of source minerals as part of ongoing work developing high-fidelity asteroid simulants. These minerals have been crushed into powders and analyzed by XRD, VNIR spectroscopy, and X-ray Fluorescence (XRF) to verify their identity and detect any contaminants present. The source materials for the MGS-1 prototypes come from a combination of these existing mineral stocks, newly acquired stocks, and synthesized materials (ferrihydrite, and re-melted basaltic glass fibers).

The crystal chemistry of the major silicates (plagioclase, pyroxene and olivine) differs between the prototype simulants and actual Rocknest measurements. Unit cell parameters for Rocknest minerals indicate ~An_{57} plagioclase (Bish et al., 2013), a mixture of augite and pigeonite (Bish et al., 2013), and ~Fo_{40} olivine (Morris et al., 2015). In the prototype simulants we used a sodic plagioclase from North Carolina, a single bronzite-variety pyroxene from Brazil, and a highly forsteritic olivine from Arizona. Natural, high-purity sources of fayalitic olivine, pigeonite, and unweathered calcic plagioclase are rare on Earth, but efforts to source them in the future will greatly improve the bulk chemistry of the simulants.

3.2 Simulant preparation

To create simulants using the MGS-1 standard, we mixed mineral components in the proportions listed in Table 1. If the mineral powders are simply mixed together dry, the resulting material will not accurately represent the properties of true martian regolith, which consists of polymineralic grains of eroded basalt mixed with secondary minerals. To address this, we used some of the same techniques for our asteroid simulants, where polymineralic fused solid “cobbles” are created and then mechanically ground to achieve a power law particle size distribution. To create these cobbles, the plagioclase, pyroxene, olivine, basaltic glass, magnetite and hematite were combined (Fig. 2a) and mixed with water and sodium metasilicate pentahydrate in a 100:20:2 ratio by weight. This mixture was mechanically combined and kneaded to form a thick mud (Fig. 2b) that was then placed in a microwave oven to fully remove the water (time and power settings depend on the dimensions of the mud disk). Upon heating and drying, the sodium metasilicate forms a polymer network that acts as a binder, such that the resulting cobbles are solid and quite hard (Fig. 2c). These cobbles were then ground and mechanically mixed with the remaining water-soluble phases (iron (III) sulfate, ferrihydrite, anhydrite, siderite) to create the final simulant (Fig. 1b).

An alternative approach to create an MGS-1 based simulant would be to add the mafic silicates as a pre-existing, unweathered olivine-rich basalt, or a combination of unweathered ultramafic rocks that achieves roughly the correct combination of minerals. However, sourcing this kind of material presents its own set of challenges, and usually requires a large capital investment if the right material is not already being mined. The other phases in the MGS-1 standard are available in relatively pure forms from either natural sources or as synthetic chemical supplies.

3.3 Analyses

The prototype simulants were analyzed using a variety of imaging techniques and bulk analyses. Results from these analyses were compared to relevant datasets from various orbital and *in-situ* spacecraft measurements as appropriate.

The simulants were imaged using a JEOL JSM 6480 scanning electron microscope (SEM) at the Materials Characterization Facility AMPAC at UCF to characterize particle textures, and to assess the distribution of the re-mixed soluble phases like ferrihydrite amongst the larger mostly silicate grains. The grain density of the simulant was calculated by measuring the volume of a cold-pressed pellet using displacement in acetone, and the bulk density was calculated by gently pouring loose simulant into a graduated cylinder to measure its volume.

Bulk elemental chemistry of the simulant prototypes was measured at the AMPAC using a PANalytical Epsilion XRF operating in oxides mode. Unpressed powders were used, and the average of 5 analyses was taken. XRF has some difficulty measuring Na and S; ideally, fused bead analysis on a microprobe or mass spectrometer could be used in the future to more accurately measure bulk chemistry, but XRF measurements are sufficient for the prototypes because the chemistry will change based on the specific minerals used.

Spectral properties of the simulants were measured using an Analytical Spectrum Devices FieldSpec spectroradiometer from 320 to 2550 nm. This range covers typical measurements made by rovers and orbital remote sensing platforms at Mars. The JSC Mars-1, MMS-1 and MMS-2 simulants were measured at the same time for comparison. All the simulants were ground and dry-sieved to the same 45-75 μm size fraction.

Thermogravimetric analyses for the simulants were conducted with a TA Instruments SDT Q600 instrument at the Kennedy Space Center. Approximately 8.5 mg of simulant was heated to 1000 °C using a ramp rate of 30 °C/min, with the mass and heat flow measured as a function of time. Historical TGA and/or evolved gas analysis data are available for both JSC Mars-1 and MMS, and for Mars soils from the Phoenix Thermal and Evolved Gas Analyzer (TEGA) instrument (Smith et al., 2009) and the MSL Sample Analysis at Mars (SAM) instrument (Archer et al., 2014; Sutter et al., 2017). However, these Mars data were acquired under lower pressures with different atmospheric compositions and different ramp rates, such that care must be taken in drawing direct comparisons. The Dynamic Albedo of Neutron (DAN) instrument on Curiosity also provided information on near-surface hydrogen contents in Rocknest materials (Jun et al., 2013).

4.0 Results

A photograph of the MGS-1 based simulant is shown in Fig. 1b, compared with an approximately true color image of the Rocknest windblown soil (Fig. 1a) taken by the MSL Mars Hand Lens Imager (Minitti et al., 2013). MGS-1 has a similar burnt umber color to Rocknest, mostly caused by the mixture of gray to black silicates and the ferrihydrite and hematite, which act as strong pigments. Fig. 3a shows a scanning electron micrograph of the simulant grains, where the polymineralic nature is clearly visible. Fig. 3b shows a closer view of the surface, where ~μm-sized flecks of ferrihydrite and/or ferric sulfate are adsorbed onto the surface of a larger silicate grain.

4.1 Physical properties

The grain (or particle) density of the prototype simulant is 2.72 g/cm^3, and the bulk density for loosely deposited material is 1.23 g/cm^3, which gives a porosity of 55%. Using more accurate Fe- and Ca-rich silicate compositions would result in higher densities. By comparison, soils at the Pathfinder landing site had an estimated bulk density of 1.07-1.64/cm^3 (Moore et al., 1999), and drift material at the Viking 1 landing site had an estimated bulk density of 1.15±0.15 g/cm^3 (Moore and Jakosky, 1989), although the lower gravity may affect bulk density somewhat. We could not find a published estimate of density or porosity for the Rocknest windblown soil. Pristine martian basalts have much higher grain densities (>3 g/cm^3), but this density would be lowered through physical and chemical weathering processes during regolith formation.

The particle size distribution of simulants is highly adjustable through crushing and sieving. For most of the prototypes we ground the material to a <6.3 mm grain size, with a natural power-law size distribution created by crushing. The particle size distribution for martian regolith is not well constrained, mostly due to camera resolution limits. Pike et al. (2011) reported that ~1 vol. % of the Phoenix surface materials were <4 μm, but Ming and Morris (2017) estimate that due to chemical alteration, 15-25 wt.% of typical soils should consist of clay-sized grains. However, these alteration phases may be adsorbed onto larger grains, and it is not clear whether they should count as discrete "particles" in the context of geotechnical properties. In the past, highly detailed sieving, separation and recombination methods have been used to generate simulants that match the geotechnical properties of lunar regolith (e.g., Jiang et al., 2011). This may become possible in the future for Mars with more detailed analysis of natural martian regolith.

4.2 Bulk chemistry

Table 2 lists the measured bulk chemistry of the prototype simulants as measured by XRF (rightmost column), in addition to the forward-calculated estimates for the MGS-1 standard described above. As expected, there are deviations from the Rocknest measurements due to the crystal chemistry of the silicate minerals used in the prototypes. CaO, FeO and MgO are most affected. Other elements such as SiO_2, Al_2O_3, and SO_3 are much closer to the measured values from Rocknest, and compare favorably to older martian simulants. For future versions of MGS-1 simulants, the best way to achieve a more accurate bulk chemistry will be to use a more calcic plagioclase and a more fayalitic olivine, or to physically combine endmember phases in appropriate proportions.

4.3 Spectral properties

Fig. 4 shows the reflectance spectrum of the MGS-1 prototype simulant compared to previous simulants, and to telescopic and orbital data from Mars. At shorter wavelengths, the MGS-1 based simulant is similar in shape and albedo to the Rocknest spectra acquired by Mastcam (Wellington et al., 2017). In particular, the absorptions and shoulders are consistent between 400 and 1100 nm, associated with (1) Fe^{2+}-Fe^{3+} and Fe-O charge transfer, and (2) Fe^{2+} crystal field splitting. At longer wavelengths, the simulant spectrum is similar to low albedo regions on Mars imaged by the Observatoire pour la Minéralogie, l'Eau, les Glaces, et l'Activité (OMEGA) orbital spectrometer (Milliken et al. 2007). However, the negative spectral slope at wavelengths >1000 nm in the remote data is not as strong in the simulant, and the simulant is brighter. These observed differences may be caused by a combination of differences in crystal chemistry, the specific amorphous compounds present on Mars, shock darkening, as well as the fact that the simulant spectra were measured at ambient laboratory conditions.

The other Mars simulants measured, JSC Mars-1, MMS-1 and MMS-2, are not close matches to Rocknest or low albedo terrains measured by OMEGA. JSC Mars-1 has a significantly higher albedo than the remote measurements, with strong H_2O- and OH-related absorptions at 1400 and 1900 nm. The MMS-1 and MMS-2 simulants from The Martian Garden company have even higher albedos than JSC-Mars 1, and at shorter wavelengths are dominated by the signature of hematite. All three of the other simulants have significant structure from 1900-2500 nm indicative of multiple different alteration phases present in significant amounts. We did not measure the original MMS simulant described by Peters et al. (2008), but the spectra shown in their Fig. 4 (no absolute reflectance scale) and in Beegle et al. (2007) do not resemble the MMS-1 or MMS-2 simulants, and are more representative of actual Mars materials.

4.4 Thermogravimetric analysis

Fig. 5 shows the TGA data for the prototype simulant. The simulant lost 3.4% relative mass at low temperatures (<300 °C), likely from physisorbed or weakly bound H_2O. An additional 4.5% mass is lost between 300 and 1000 °C, which could include additional H_2O, but is likely dominated by SO_2 and CO_2 from the breakdown of carbonates and sulfates in the simulant. In comparison, Allen et al. (1998) reported that JSC Mars-1 lost 21.1 wt.% (mostly water) when heated to 600 °C, while Peters et al. (2008) report that MMS lost 1.7 wt.% by 100 °C and 7.2 wt.% by 500 °C. The significant and unrealistic water contents of JSC Mars-1 were cited as a motivating factor in developing the original MMS simulant (Peters et al., 2008), and MMS has recently been augmented further to achieve even more realistic volatile release patterns (Archer et al., 2018).

The TEGA instrument did not a detect low temperature water release in soil samples at the Phoenix landing site (Smith et al., 2009), but did detect a minor H_2O release starting at 295 °C and a major release starting at 735 °C. In contrast, the SAM instrument detected a broad H_2O release in Rocknest starting at low temperatures, finding 2.0 ± 1.3 wt.% total evolved water averaged over four runs (Archer et al., 2014). This is consistent with the 1.5 wt.% water equivalent hydrogen in the upper layer of Rocknest materials measured by DAN (Jun et al., 2013). Overall, these data show that the MGS-1 and MMS simulants are both more hydrated than martian soils, but are much closer in hydration to reality than is JSC Mars-1. The differences between the MGS-1 based simulant and Rocknest could be due to hygroscopicity in a humid terrestrial atmosphere, and the exact nature of the amorphous component in Rocknest is probably key to understanding the unique water release patterns measured by SAM (Archer et al., 2018). TGA data are not available for MMS-1 or MMS-2, but judging from their spectral properties (Fig. 4) these simulants have significant water contents, possibly on par with JSC Mars-1.

5.0 Discussion

Simulants created using the MGS-1 standard are superior to previous martian simulants, and accurately capture advances in the understanding of real martian regolith in the 10 years since MMS was described (Peters et al., 2008) and the 20 years since JSC Mars-1 debuted (Allen et al., 1998). The high fidelity of MGS-1 simulants is made possible by the mineralogy-based synthesis, where mostly pure, individual components are mixed together from scratch. This is in contrast to previous simulants, where a natural, roughly basaltic terrestrial material was found that superficially matched Mars in terms of spectral or geotechnical properties. That is not to say these previous simulants have no value, especially where applications only require a bulk granular material that behaves somewhat similarly to actual regolith on Mars.

5.1 Applications

Simulants based on MGS-1 are appropriate to use for a variety of scientific and engineering-based investigations, as well as for testing flight hardware and developing *in-*

situ resource utilization (ISRU) technology. For lunar simulants, NASA developed the concept of a fit-to-use matrix (Schrader et al., 2010), where various simulants are compared by describing applications for which they are or are not recommended. For example, the highlands simulant NU-LHT-1D was not recommended for drilling studies because of its fine particle size distribution, but was deemed appropriate for oxygen production studies. A simulant fit-to-use matrix is more relevant for the Moon because of the vast proliferation of different lunar simulants, at least 28 by our count (not including later derivatives). The situation for Mars is different, with only a handful of formally described simulants so far (http://sciences.ucf.edu/class/planetary-simulant-database/): the most prominent of these (MMS and JSC Mars-1) are no longer available, and the others have not yet been widely adopted. Nevertheless, without a formal fit to use table we can still list the various strengths and weaknesses of the MGS-1 standard in terms of different use cases.

MGS-1 simulants are most recommended in applications where mineralogy and volatile contents are important controlling factors. These include ISRU technology development, plant growth and astrobiology studies, human health assessments, and recurring slope lineae experiments, among others. JSC Mars-1 is not recommended for these applications because it has virtually none of the same minerals as actual Mars soil, and its volatile content (>20 wt.% H_2O) is highly unrealistic. The original MMS simulant, and some of the newer simulants (JMSS-1, UC Mars1) may be appropriate for some of these cases where accurate mineralogy is not critical. However, we caution against using MMS-1 or MMS-2 due to their lack of rigorous documentation and the discrepancies between these and the original MMS, as described above.

MGS-1 simulants are also recommended in applications for testing flight hardware such as drilling, where geotechnical properties are important. MGS-1 is appropriate for these cases because the synthesis method produces a “regolith” of polymineralic grains with an adjustable particle size distribution, instead of simply mixing dry powders together. However, the geotechnical properties of actual martian regolith are poorly constrained compared to returned lunar regolith that has been studied extensively on Earth. As well, in the prototypes we did not control for detailed aspects like particle shape that can be important in influencing geotechnical properties, and our initial physical properties measurements in this study are limited. Thus, at this time we can only say that MGS-1 based simulants can likely be made to be as appropriate or more so for hardware testing compared to previous Mars simulants. Mojave Mars Simulant was developed specifically for geotechnical applications (Peters et al. 2008), and if the original version can be obtained it is recommended for these uses. Again, due to apparent changes between MMS and MMS-1/2, we do not recommend these simulants. Newer Mars simulants (JMSS-1, UC Mars1, ES-X) may also be appropriate for geotechnical applications. In order to improve the usefulness of Mars simulants for flight hardware tests, more detailed study of martian regolith physical properties are needed. Some of this may come from the InSight and ExoMars missions, which will hammer and drill deep into surface materials. In addition, it would be useful to conduct a rigorous testing and inter-comparison of martian simulants for physical properties (including thermophysical properties).

We do not recommend using MGS-1 simulants for detailed geochemical studies such as aqueous alteration experiments. This is due to the uncertainty in the exact amount and nature of the amorphous component in martian soils, and the difficulty in sourcing silicates on Earth with crystal chemistries appropriate for Mars. For these types of studies, it may be better to use pure minerals in experiments, and/or to rely on geochemical modeling based on primary volcanic compositions from martian meteorites or rover measurements. In theory it is possible to create a small amount of extremely high fidelity regolith simulant that satisfies both mineral and chemical constraints simultaneously, but as described above it is cost-prohibitive to make this kind of simulant in large quantities accessible to the community.

4.2 Availability and future development of MGS-1

In the past, simulant production has followed a now predictable lifecycle: the need for a specific simulant arose, a NASA center or private company produced an initial large batch of the simulant, then eventually the batch ran out, or national interest in a given planetary body faded and the simulant was discarded. Efforts may be made to re-create the original material under a different name, but this can often be difficult if the source material is no longer accessible.

With MGS-1, we hope to avoid some of these pitfalls and move toward a more open and sustainable model for simulant development. This starts with the general philosophy of the standard: MGS-1 essentially means any simulant created based on the mineralogy of average basaltic regolith on Mars, as captured by the mineral recipe in Table 1. While we have chosen to add the plagioclase, pyroxene and olivine separately in our prototypes, they could also be added in the form of basalt or ultramafic rocks provided the mineral proportions are accurate. The MGS-1 recipe can be updated in the future based on new analyses (for example, refining the amorphous component; Achilles et al., 2018) and exploration of new landing sites. In this way, there is no batch of MGS-1 to run out, but a general standard to follow. We intend to produce modest quantities of MGS-1 based simulant and distribute it to the community at cost, but we also encourage others to re-create the same types of simulant using a similar standard. Indeed, a group at the Johnson Space Center is also developing a Rocknest-based version of the MMS simulant to be used for ISRU development (Archer et al., 2018).

NASA developed the concept of "root" and "branch" simulants for the Moon, where the root is a basic, well-characterized version of the simulant. Specialized branch versions can be derived from the root, either by the manufacturer or by end users. MGS-1 will benefit from the same scheme, where the recipe in Table 1 forms the basic root, and various branches can be created either by us or others. For example, clay-rich Noachian regolith, or perchlorate and nitrate-bearing agricultural soils can be created by adding the desired additional components to the root simulant. These may evolve into standardized simulants with version numbers to achieve better consistency, instead of each individual lab developing their own simulant recipe. We encourage others to develop branched versions of MGS-1 and add modifiers to the name as they see fit.

6.0 Conclusions

We developed a new standard for a Mars simulant, MGS-1 Mars Global Simulant, based on the Rocknest soil examined by the Curiosity rover. Unlike previous simulants sourced from landscaping material, Mars Global is meant to be assembled *ab initio* from pure components to provide an accurate match to the mineralogy of martian regolith. The spectral properties, water content, and physical properties of prototype simulants based on MGS-1 are similar to measurements of Rocknest and other soils on Mars, and are an improvement over previous simulants. MGS-1 based simulants are recommended for a variety of applications including ISRU development, agriculture/astrobiology studies, and testing flight hardware. Modest amounts of simulant will be produced and made available to the community at cost, but through an open source philosophy we encourage end users to freely replicate and modify the MGS-1 standard using the recipe and procedure described here.

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Table 1. Mineral recipe for the MGS-1 standard.

Component	**Proportion (wt. %)**
Crystalline phases	
Plagioclase	29.4
Pyroxene	20.5
Olivine	16.2
Magnetite	1.5
Anhydrite	1.1
Hematite	0.8
Amorphous phases	
Basaltic Glass	20.0
Fe-sulfate[1]	6.0
Ferrihydrite	2.7
Fe-carbonate[2]	1.9
Sum	100

[1]In the prototype simulants we added crystalline iron (III) sulfate pentahydrate.
[2]In the prototype simulants we added crystalline siderite.

Table 2. Elemental chemistry.

Oxide	RN bulk[a]	Calc. MGS-1[b]	RN amorph.[a]	Calc. MGS-1 amorph.[c]	Prototype MGS-1[d]
SiO_2	41.2	42.5	35.9	33.4	41.4
TiO_2	1.1	–	1.4	–	0.2
Al_2O_3	9.0	10.8	5.52	7.1	11.2
Cr_2O_3	0.5	–	0.8	–	0.1
FeO_T	19.3	21.4	19.9	29.5	13.3
MnO	0.4	–	0.5	–	.1
MgO	8.3	10.2	8.6	6.1	14.2
CaO	7.0	6.2	4.6	4.7	2.2
Na_2O	2.6	2.0	3.0	2.0	4.3
K_2O	0.5	0.1	0.7	0.3	2.3
P_2O_5	0.9	–	1.9	–	0.3
SO_3	5.2	3.6	9.9	10.0	8.9[e]
H_2O	2.0	1.3	4.1	4.5	-
CO_2	1.0	0.7	2.1	2.4	-
SUM	99.0	98.8	98.9	100.0	98.5

[a]From Morris et al. (2015). RN = Rocknest.
[b]Calculated bulk chemistry of MGS-1 using idealized mineral chemical formulas weighted by the proportions in Table 1, with the actual crystal chemistries of martian silicates from Bish et al. (2013) and Morris et al. (2015).
[c]Here, "amorphous" includes the basaltic glass, ferrihydrite, Fe-sulfate, and Fe-carbonate.
[d]Average of 5 measurements.
[e]XRF has difficulty measuring sulfur accurately.

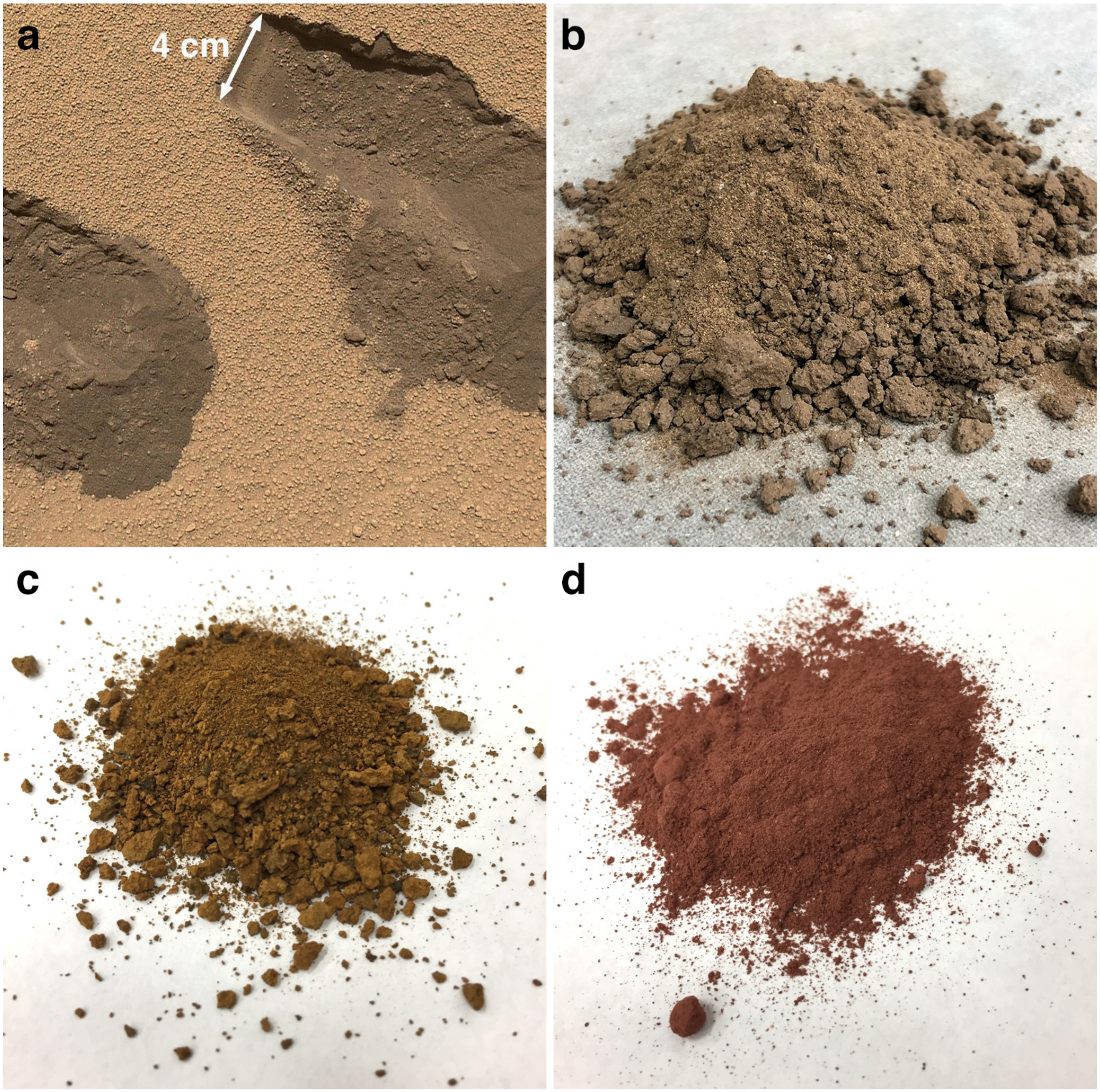

Figure 1. Comparison of martian simulants. a) MAHLI image of the scooped Rocknest soil; image credit NASA/JPL/Malin. b) Photograph of MGS-1 prototype simulant produced for this work. c) Photograph of JSC Mars-1. d) Photograph of MMS-2 sold by the Martian Garden company.

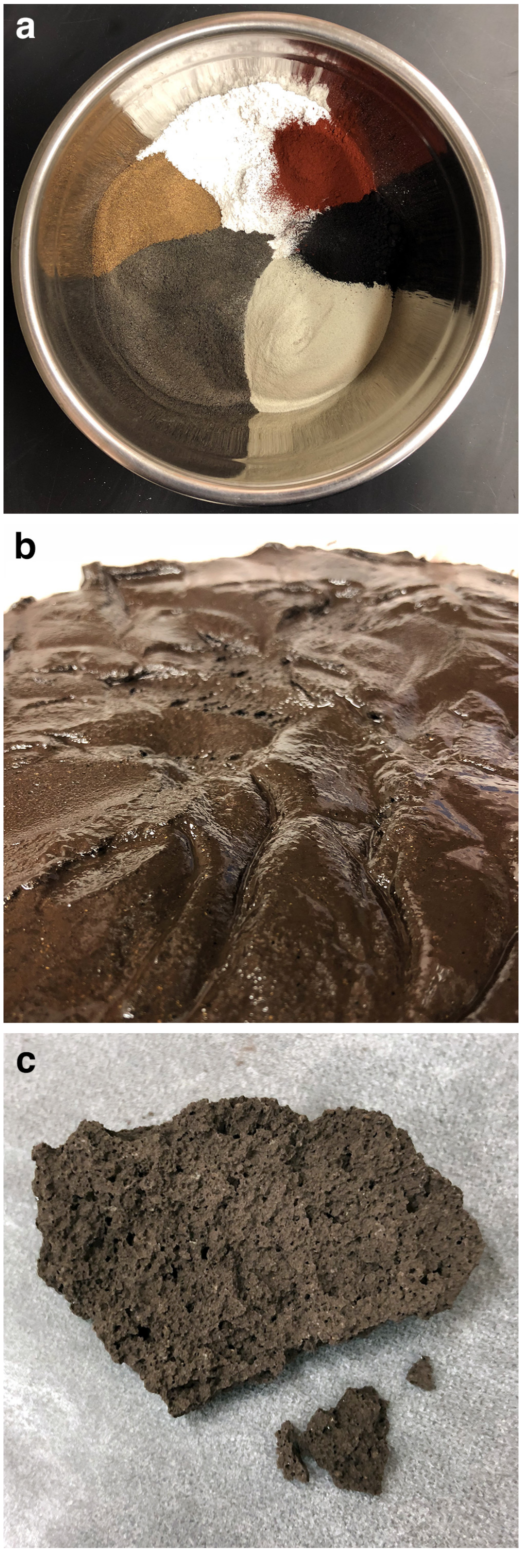

Figure 2. Production process for MGS-1 simulants. a) Insoluble ingredients before mixing. b) Thick mud paste formed from insoluble components, water, and sodium metasilicate. c) Resulting solid cobble formed after microwaving the mud.

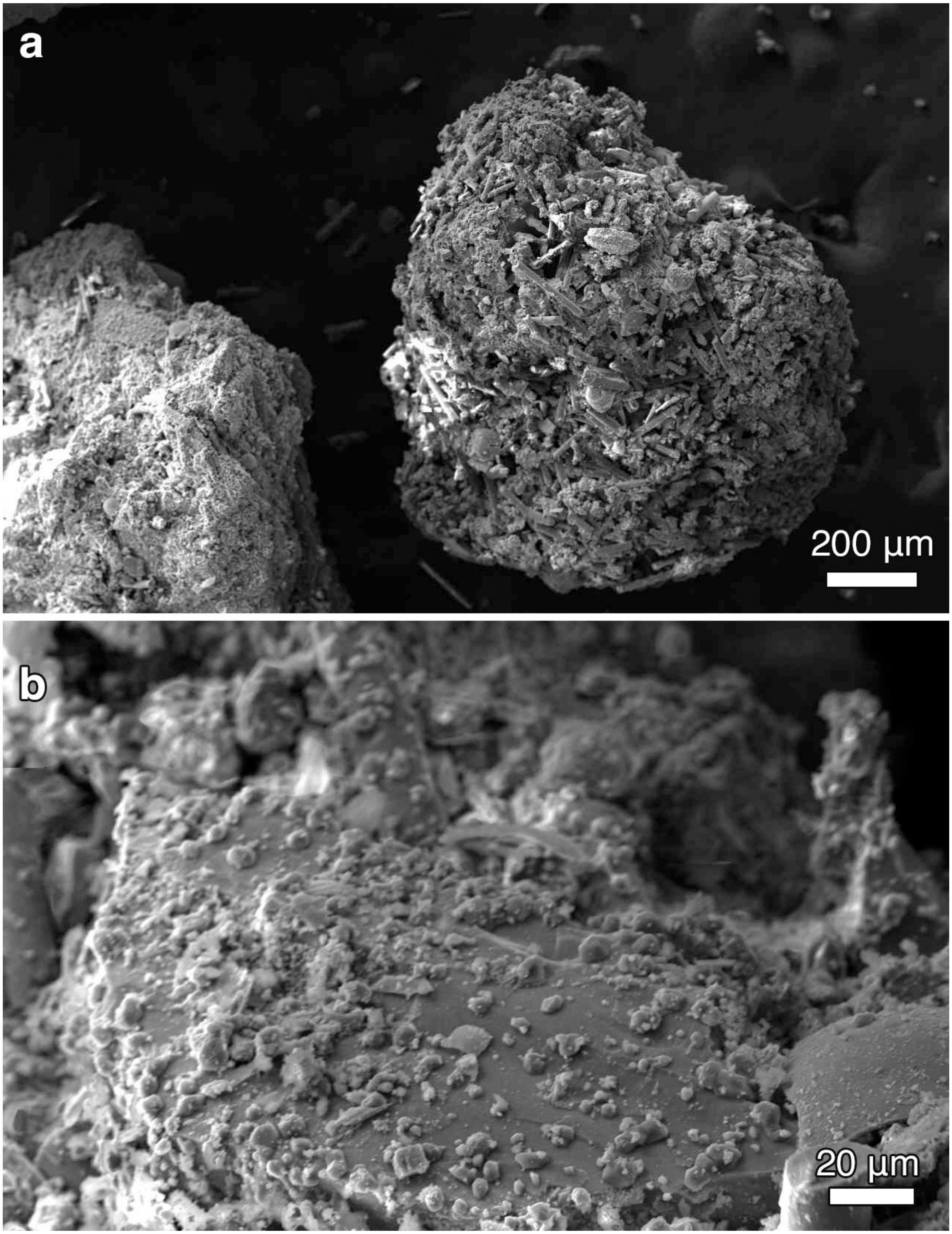

Figure 3. Scanning electron micrographs of MGS-1 prototype simulant grains. a) Zoomed out view showing polymineralic particles made up of multiple mineral constituents. b) Zoomed in view of the surface of a silicate grain covered with adsorbed ferrihydrite and/or ferric sulfate.

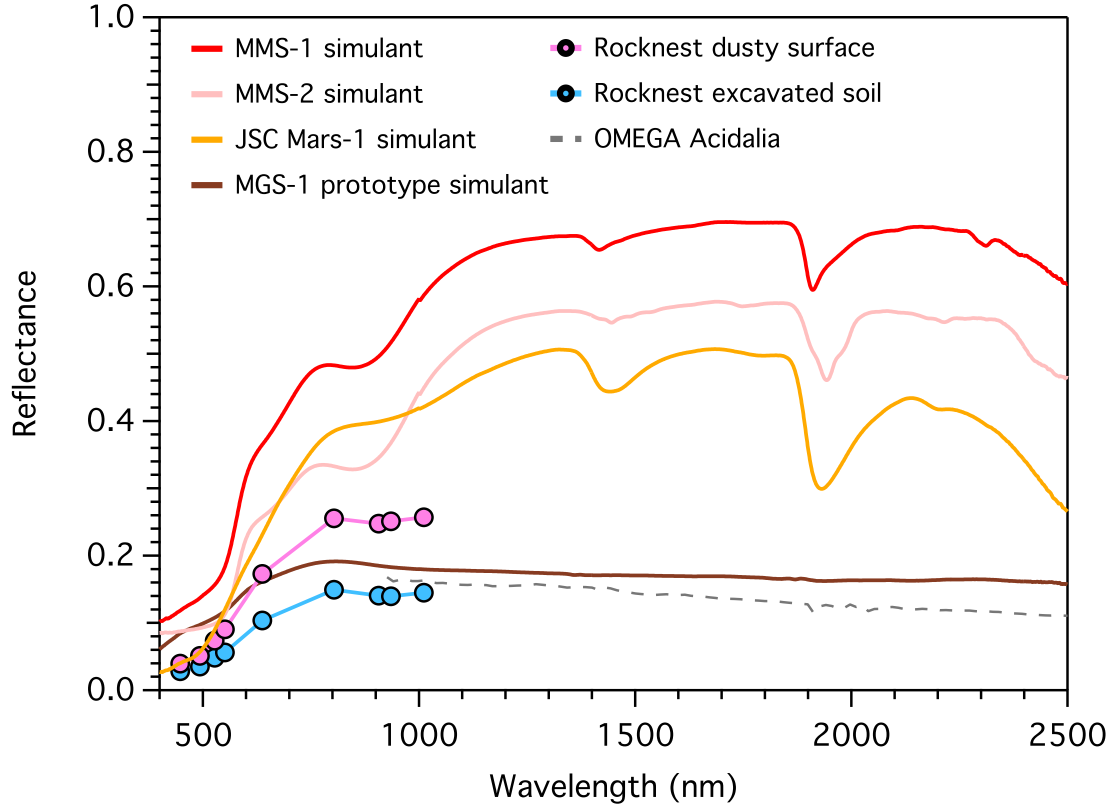

Figure 4. Spectral comparison of the MGS-1 simulant prototype, previous Mars simulants, and remotely sensed data from Curiosity and OMEGA. Mastcam data (filled circles) were reproduced from Fig. 5 in Wellington et al. (2017), and OMEGA data courtesy of R. Milliken. None of the spectra have been offset or scaled.

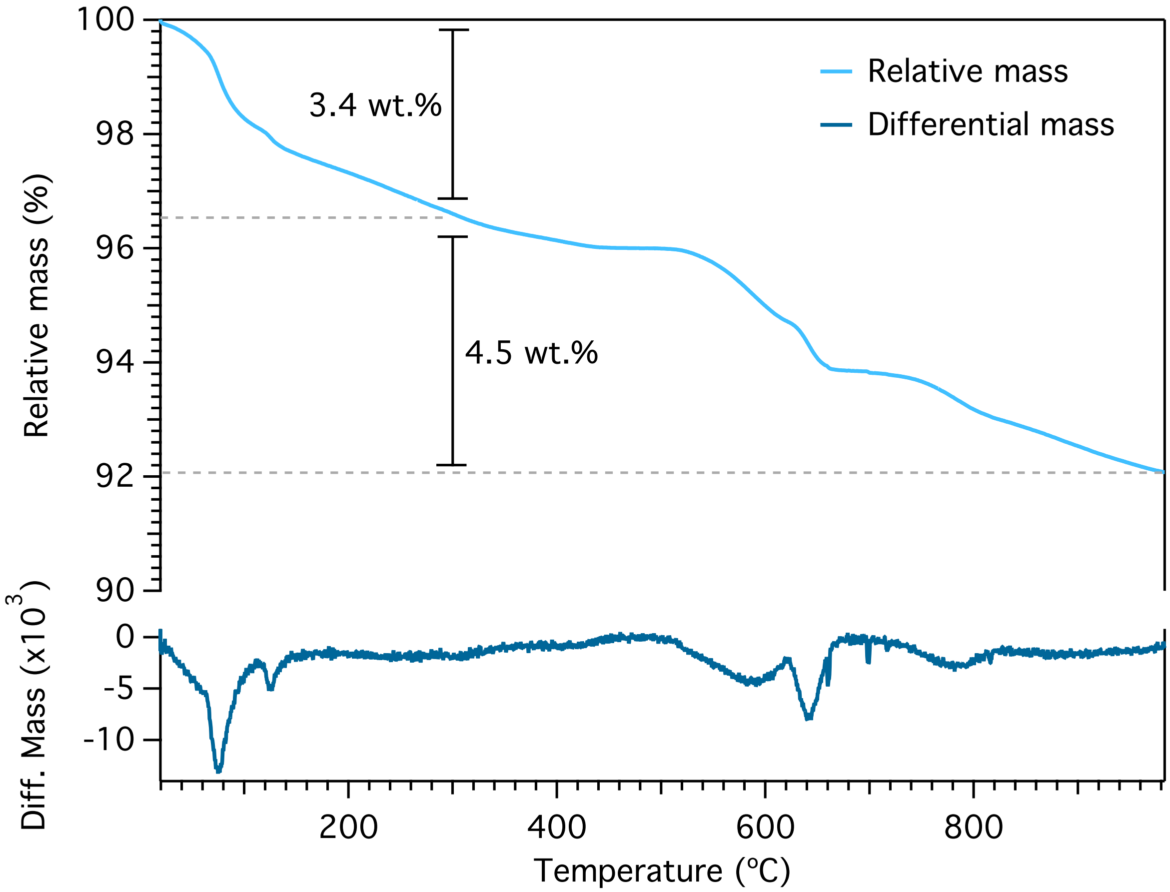

Figure 5. Thermogravimetric analysis of the MGS-1 prototype simulant.