The Art of Simplification:
Making the choices that allow simulants to be made and used

A paper read before the Lunar System Innovation Consortium - Lunar Surface Working Group
June 15, 2023.

by Doug Rickman
Jacobs Space Exploration Group

1. Foreword

1. I am deeply honored that Karen thinks I have enough of value to say, that I should be invited as the first speaker of this series. I hope that judgment is not misplaced.
2. Any speaker should respect the honor that listeners are paying him. Thank you for that honor.
3. I hope that when I have finished, you will think that everything I said was obvious. If that happens, it means you have absorbed all that I have tried to communicate.
4. I have purposely not provided a lot of literature citations. My library has almost 2,000 relevant citations, but such details for this purpose detract from hearing the main points.
5. The interested listener will realize that I present multiple places where work might be done to advance the arts of simulants.

2. Introduction

Most of what I will say are simplifications. Sometimes fairly substantial simplifications. When experts get together, the fine details and exceptions are fair game. But not here.

Some of the major points that will be covered:
- We cannot reproduce the many diagnostic features of the lunar regolith.
- The simulants inherit various non-lunar characteristics from the source feedstocks used to make the simulants.
- We frequently do not know the sensitivity of a test to features in the regolith or the simulants, and the two sensitivities can be different.
- There are far too many variables, both in using and fabricating simulants, to understand, let alone control.
- Users and simulant producers must use numerous simplifications. The question becomes what simplifications, when, and at what risk?

Much of the following will use the terminology of “geology.” It is how we understand the lunar material, and the geology is in turn ultimately driven by the chemistry and physics of the genetic processes that made the regolith. There is no other applicable, common or universal language. I will attempt to define terms that might not be familiar to you as I proceed.

3. Engineering Complexities

Begin with the complexities in the interactions of engineering systems with the lunar "*regolith*" (broken rock). There are few, if any, engineering tests that are solely dependent on a single characteristic of the tested material. To quantitatively understand the relative significance of each parameter to a specific test is largely beyond our knowledge. In many cases, those involved in using simulants may not even know a characteristic of the regolith/simulant exists. Usually, the best we can hope for is a judgment about the relative importance of the parameters.

To add yet more complications, the engineering problem actually has three different, and frequently significant, parts.

(1) There are the expected interactions with the actual lunar material.
(2) There are the observed interactions with the simulant.
(3) There are the differences between the simulant and the lunar regolith.

All three of these have to be wrestled with when trying to evaluate a test using terrestrial simulants compared to expected performance on the Moon.

For the lunar material, it is common for the parameters of interest to a specific engineering problem, to not be fully known. An official view of known lunar parameters, and it is a well informed, careful, consensus document, is captured in the DSNE (SLS-SPEC-159 Cross-Program Design Specification for Natural Environments (DSNE); Revision G available at https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20200000867.pdf). While this document is a first reference for anyone trying to do lunar oriented engineering, it has significant limitations. In some cases, more specific or specialized information should be harvested from literature, if one understands the literature. Neither the DSNE nor the literature provides answers for many questions. Not enough is known about the lunar material to do that. To add yet more complexity, the lunar regolith also has significant variation over a wide range of spatial scales.

Frequently the simulants are also not as well characterized as a user desires. In fact, most simulants have very minimal characterization. The forthcoming simulant NUW-LHT-5M will have at least 30 discrete parameters measured and reported. Only JSC-1A has been measured for a comparable number of parameters. And even those substantial numbers of measurements do not cover all of the parameters of interest.

There is also a glaring hole in our knowledge about how any simulant differs from any given lunar material. Very few people ever deal with this topic in a quantitative sense. Generally, at most there are qualitative opinions. Which is minimally useful for engineering. A quantitative, engineering approach is addressed below.

The final point under the topic of complexities related to engineering is the problem of how to measure the simulant for parameters of interest to a specific application. One tabulation of potential desired simulant properties was attempted in 2005 and resulted in 36 parameters (Table 2, Sibille et al., 2006). A more complete list would likely be many times larger. Though engineers may want these measurements, even the short list of 36 is far beyond what any simulant producer can deal with. The 36 parameters are also not relevant to the practical design of a simulant. In other words, there is no way to take most desired engineering parameters and deduce what a simulant should look like.

The problem of numerous, design-irrelevant parameters can be simplified by rethinking the problem and using a simpler, more robust approach. To start, answer a basic question – if we duplicate a sample of the lunar regolith to the smallest detail, will the reproduction perform exactly like the original? Very simple. And extremely important! Everything else flows from this as logical necessity. It means that even if an engineering property has not been measured on lunar material, it can still be obtained by measuring a perfect simulant. However, if you understand both the making of simulants and the lunar regolith, you know perfect reproduction of a lunar sample is in fact impossible. Therefore, some measure of how close a simulant matches the lunar regolith is needed. This is the Figure of Merit (FoM), which is not an ISO standard. The FoM quantifies the differences between a lunar regolith and a simulant in terms of four basic measures: composition, shape distribution, size distribution, and bulk density. Values in the standard are between 0 and 1. The closer each parameter is to 1, the more similar the two materials are. This gives users, buyers, and manufacturers a common, defined, measurable, standard way to do what they each need to do. It is argued that almost all of the values measured as engineering parameters are controlled by the FoM parameters, plus the state variables, such as temperature and pressure.

A caveat -- the existing 4 parameter FoM is not sufficient to perfectly characterize all of the differences between a simulant and a lunar sample. The missing parameter is *texture* (spatial relationships within particles). More on texture later. However, it is known that for many, probably most, applications the four enumerated FoM measures are sufficient to give a user a very good idea about how similar a simulant is to a given lunar sample.

In review, engineers have to make many simplifications. This is certainly true when our target is to do something on the Moon that has never been done before.

4. Geologic Complexities

Much of the following will hinge on the characteristics of the lunar regolith. When seen in petrographic thin sections (27 mm X 46 mm X 30 μm thick), the lunar regolith is easily distinguished from anything naturally occurring on Earth. For example thin section images of the lunar material, see https://www.virtualmicroscope.org/collections/apollo . While there are definitely non-terrestrial composition, size, and shape features of the lunar material, the really obvious, and diagnostic, difference is texture. Indeed, some of the lunar regolith textures are beyond our technical ability to synthesize at functionally useful scales. Textures include not just the well-known agglutinates, but also the intense, internal shattering of particles, the common existence of 20 μm rocks, spherical glass beads, randomness of shapes, sizes, and composition, and features like maskelynite. On the flip side, to a great extent, lunar composition, size, shape, and density are within terrestrial norms. Again, the question becomes what level of accuracy is acceptable? This is a real problem as engineers can't tell simulant manufacturers what they need in quantitative, meaningful terms. None of us are there. Yet!

Of the four FoM metrics, bulk density is effectively within user control, so here we will focus on the other three parameters.

Composition

To a geologist "*composition*" is the makeup of a material in terms of its *minerals* (crystals of uniform and consistent composition), and includes components that are usually labeled as *mineraloids* (not strictly minerals), such as glass.

Major compositional elements

By terrestrial standards the lunar mineralogy is quite simple at the 95% level. The dominant single mineral is from the *plagioclase* family of minerals, specifically the mineral *anorthite* (~ $Ca_{0.90-1.00}\ Na_{0-0.10}\ Al_2Si_2O_8$). Unfortunately for simulant users, there may be no natural source on Earth of anorthite in both large quantities and high purity. Simulant producers must therefore substitute other members of the plagioclase family, usually *labradorite* (~ $Ca_{0.50-0.70}\ Na_{0.30-0.50}\ Al_2Si_2O_8$) or the preferred *bytownite* (~ $Ca_{0.70-0.90}\ Na_{0.1-0.30}\ Al_2Si_2O_8$). There is a penalty for doing this for some applications, but not for most mechanical tests, which is the interest of a majority of users. For applications where the chemistry matters, users need to find a simulant with as high a Ca/(Ca+Na) ratio, called the "*An*" number, as practical. Maximum, practical values using natural sources are generally in the An70 to An80 range. I emphasize natural sources here because anorthite has been produced synthetically.

There is a cost for using these natural plagioclases. On Earth they are always accompanied by minerals that are not found on the Moon. These non-lunar minerals also enter into any test, and can affect mechanical and chemical properties. Therefore, they must be considered in some tests. How does a user know if the test is sensitive? To do that you have to understand the physics and chemistry of the test, the nature of the simulant, and the actual lunar regolith. A very tall order. Such knowledge usually requires multiple, specialized knowledge-bases, and usually is beyond the reach of any one person. The NASA Lunar Regolith Simulant Advisory Team (john.e.gruener@nasa.gov) can often help with this.

After the plagioclase problem, the manufacturer generally needs to include minerals from three additional families: *ortho-pyroxenes* (e.g. *enstatite*), *clino-pyroxenes* (e.g. *diopside* and/or *augite*), and an *olivine*, such as *forsterite*. All three of these mineral families, as is plagioclase, are *silicates* (dominated by silicon-oxygen tetrahedra), and to a large extent are characterized by their Mg to Fe ratio. These minerals are harder, break into sharper pieces, melt at higher temperatures than plagioclase, and are important sources of Mg and Fe in the simulants. Unfortunately, if the feedstock(s) used to make a simulant does not contain a desired pyroxene, there are very limited sources for these minerals in useful quantities. Also, when using what is available, there are always other minerals that get dragged along, which of course is likely to "contaminate" the simulant. This is the same problem that occurs with the plagioclase sources. Always, there is other, undesired, stuff in the feedstocks. While rather pure olivine can be purchased commercially, the sources are very few, so there is very little choice in the available Mg to Fe ratio. Given there is interest in the iron content of the simulants, this is a notable limitation for simulant producers and users.

Please note, chemical oxides are a very minor part of the lunar regolith. The few oxides that do exist are largely compounds of chromium, iron, and titanium.

Glass makes up ~20 – 60% of the lunar regolith. And the properties of glass are very different from the properties of the minerals we have been talking about. The lunar glasses come from three geologically discrete sources, though there is a tendency for the glass to be similar to the average mineralogy it is with. So rather than try to add multiple glasses to their simulants, an average target is aimed for. In fact, this is the standard in the Figure of Merit. While there are many sources for natural glass on Earth, high calcium glasses do not naturally occur. Therefore, either glass is not part of the simulant, or an available, natural glass is used. Again, doing the latter introduces something desirable, but carries with it non-desirable tag-alongs. As a rule, the best natural glass sources are rocks called *basalts*, or preferably *basaltic volcanic ash*. One commonly used basaltic volcanic ash is from the Merriam Crater near Flagstaff, Arizona. As with all of the choices so far, this comes with its own problems. Such sources work reasonably well for mare-type simulants, but are generally too high in Mg and Fe for highland compositions.

In two cases to make highland simulants, NASA has resorted to having glass synthesized in substantial quantities. The first production was done by Zybek of Boulder, Colorado in collaborations with Steve Wilson and Doug Stoeser of the USGS. They made glass from the waste sand produced by the Stillwater platinum mine near Nye, Montana. The composition of the glass was close to the average composition of the feedstock rocks used to make NU-LHT-series simulants. The Ca to Na ratio for the glass is ~ An92. Zybek no longer makes this glass. The second glass production is now being done by Matt Creedon of Washington Mills, Niagara Falls, New York. This is done starting with commercially available oxides. Therefore, the composition is close to the design target: average Apollo 16 highland material. The Ca to Na value for this glass is ~ An95. The down sides to synthesizing glass are the expense and the limited number of facilities that are willing to make a custom glass in ton-load quantities.

Minor parameters – Trace Minerals - Lunar

Commonly ignored in the discussion of lunar simulants are the minor and trace phases both in the lunar regolith and in terrestrial feedstocks. The terms minor and trace are not rigorously defined. Minor minerals are roughly those with abundance less than 10% but greater than 1.0%. A trace mineral has an abundance less than approximately 1.0%. On the Moon there are slightly more than 100 minerals. In contrast, there are considerably more than 4,000 terrestrial minerals.

Other than the major lunar minerals listed above, the remaining 100+ lunar minerals are commonly trace phases. To a large extent the only trace to minor phase in the lunar regolith commonly discussed is ilmenite. This is because Apollo returned some materials with unusually high ilmenite concentrations. These samples were the exception, but for oxygen extraction purposes a lot of attention has been paid to these unusual samples, and specialized simulants have been made for this one purpose.

Otherwise, the three most commonly discussed trace lunar phases are nano-phase iron, nFe^0, He^{3+}, and sulfur-bearing minerals as a group. Simulants are only rarely designed with any of these three in mind. An exception is the NU-LHT-series, in which sulfur was specifically included in the design. Another exception is some materials made by Orbitec under an SBIR contract which created verified, physically appropriate nFe^0. The latter simulants, in limited quantities (a few kilograms) are held at MSFC under the control of Jennifer Edmunson. He3+ has never been introduced into a simulant, so far as I am aware.

There are multiple reasons why simulant makers do not pay much attention to the lunar minor and trace minerals. First, the manufacturers have little or no practical capability to detect these phases in their feedstocks, let alone control the abundance of such phases. Second, the practical significance of these phases is largely unknown, but probably quite small. Third, the cost of dealing with such things would have to be added to the cost of the simulant. Again, simplification is needed.

Minor Minerals - Simulants

Compared to the lunar regolith, the situation with respect to minor phases in the terrestrial feedstocks is very different, and commonly of practical importance. This exists because the number of geologic environments and the history of the terrestrial materials are much more complicated than for the lunar material. In "geology-speak" the lunar materials have a limited range of *igneous* (fire formed) origins followed by a long history of monotonous, hypervelocity impacts, and some space weathering. The terrestrial material, although lacking the hypervelocity and space weathering, can come from a wider range of igneous origins, and almost always have been subsequently altered by some combination of *metamorphism* (changed by temperature and pressure), *hydrothermal alteration* (added high temperature water), and/or surficial *weathering* (exposure at the Earth's surface) in an environment extremely rich in oxygen and H_2O. All of these terrestrial processes imprint feedstocks with mineralogy that is characteristic of the rock's history, and those minerals are definitely not found on the Moon. Simulant producers cannot avoid these non-lunar phases.

The common simplification by the producer is to ignore the signature minerals generated by these various terrestrial processes. Frequently this is well justified. But -- sometimes it is not. It depends on both the engineering test and the specific simulant. Unfortunately, given our knowledge levels both in engineering and production, it can take unusual expertise to recognize when a problem may exist. It should be noted that so far, problems have been observed more with the highland simulants than for mare simulants. Again, this is due to the geologic history of the rocks that must be used to make such simulants.

Following are examples of non-lunar minerals in simulants and some of their impacts.

Quartz, SiO_2, another silicate, has been measured at varying levels in all of the simulants tested, except those made exclusively from Merriam Crater ash. Quartz can cause silicosis, a lethal condition that cannot be cured. When the feedstock is milled to less than 10 μm, silicosis becomes a concern. Medical risk is strongly driven by exposure rates, therefore, the significance of the quartz depends on multiple factors, including quartz abundance in the feedstock, particle size distribution, and how the material is handled. Quartz is a very rare mineral on the Moon and common on Earth. It behooves users to minimize or avoid simulants with higher quartz levels, especially if the application suspends a lot of dust in the air. Please note, personal risk cannot be intelligently evaluated based on what some non-expert says about the topic. This is one place where involvement with health and safety experts is well justified.

Calcite, $CaCO_3$, is present in all three of the North American high-calcium anorthosites used to make highland simulants. It is also in the Merriam Crater material. It is mechanically softer than the major lunar minerals, and can be highly reactive in many chemical tests.

Clay minerals are a common product of both surficial weathering and hydrothermal alteration. These minerals are much richer in H_2O and OH^- than lunar materials. They are also mechanically even weaker than calcite. They have been recognized in Stillwater feedstocks and Merriam Crater ash.

Carbonates (including calcite), sulfates, and hydrated iron minerals, three groups of minerals, all commonly produced in surficial weathering, are known to exist in the Merriam Crater source material. These have much higher levels of oxygen than lunar minerals. These minerals break down at temperatures far below that of the lunar minerals, and they are mechanically soft.

While these non-lunar phases are frequently in minor or trace concentrations in simulants, their spatial distribution in the simulant can be highly biased. Thus, their significance can be much greater than otherwise expected. As a result of milling, mechanically weak minerals will be concentrated into the simulant fines. The weathering minerals, as in the Merriam Crater material, can occur dominantly on the outside of the original volcanic particles. So even though these non-lunar minerals are only ~1 wt% of the total simulant, their impact is disproportionally high in various tests.

There will be cases where the simulant-based test results in either a problem that will not be found on the Moon, or misses a problem that will occur on the Moon. Such cases can be very hard to predict.

There can be problems with phases or elements present in the parts per million, ppm, range. In 2008, Lockheed Martin was damaging their high temperature oxygen extraction equipment when an unknown greenish liquid was generated. Tests of the liquid by the USGS showed the liquid contained 10,000 ppm hydrochloric acid and 20,000 ppm of hydrofluoric acid. These were generated from the JSC-1A through the unexpected selective extraction of Cl and F, which are naturally present in the simulant in the 10s-100s of ppm. In this case, the simulant was actually reproducing lunar behavior, so the test was valid. In other words, the simulant revealed a significant problem with the experimental system.

Rock Composition

With one exception, the making of lunar simulants requires the use of terrestrial rock materials as feedstocks. Users should know a basic fact that simulant manufacturers are intimately aware of. <u>The mineralogical range of practically useful terrestrial rocks does not cover the compositional range desired for simulants!</u> While the primary lunar minerals are well represented on Earth, the rocks containing these minerals do not have the desired <u>ratios</u> of the minerals. It was this reason that caused the USGS with NASA to move from single lithology feedstocks to multiple feedstocks. For example, NU-LHT-2M used 7 natural feedstocks and 2 synthetic glasses. The down side of using multiple feedstocks is that each feedstock may drag along complexities, such as the non-lunar mineralogy in each feedstock.

The complexity of this balancing act is shown in the design evolution of NU-LHT-series. As Doug Stoeser said, the Stillwater Complex is a virtual smorgasbord of the minerals desired to make a highland simulant. One desired mineral in a highland simulant is olivine. There are two olivine bearing lithologies in at Stillwater and both are easily accessible. One is an ore of chromium (chromite + olivine). But in this rock the chromite concentration associated with the olivine is too high for a general simulant, therefore a Stillwater rock called *harzburgite* was used for NU-LHT-1M. In principle, the harzburgite is extremely desirable, as it is made of olivine + pyroxenes + plagioclase, all needed minerals in the simulant. But the harzburgite plagioclase has a lower An number than desirable. So raising the Mg and Fe content of the simulant by using the harzburgite meant lowering the average An number. This was considered less desirable than dropping the Stillwater harzburgite and using a commercially available olivine in the next generation simulant, NU-LHT-2M. And all three rock types: the ore, harzburgite, and commercial olivine, have very similar Mg to Fe ratios. Thus, limiting the possible range of Fe in the simulants.

Every simulant producer has to balance the desire for fidelity against the availability and cost of feedstocks.

Given all of the complexities, cost implications, and the unknowns associated with the minor and trace composition of the simulants, it is understandable that both users and producers generally simplify the problem by ignoring these aspects of simulants. Evolving knowledge will slowly change the situation. Most of what has been discussed here was not recognized just 4 years ago.

Particle Size, Particle Shape, and Textures

Size

The significance of particle size distribution in simulants is only partially understood. In other words, the practical engineering significance of this measure is not well constrained. This is forcefully illustrated by the general use of the term "dust", which has no standard definition. And this is commonly the only standard term that is used to designate some subset of particle size distributions. One only has many terms for something, if that something is important and understood.

Simulants are generally made to be minus 1 mm. Why? There is nothing about the lunar regolith that even suggests this is a meaningful, natural limit of some kind. It seems to derive from two sources: (1) the making of JSC-1, and (2) a misreading of a paper by David Carrier (2003) plotting size distributions measured by John Graf (1993). The significance of this artificially imposed 1 mm limit will vary with the tests. Thankfully, there is new work under way jointly at MSFC (Wesley Chambers and Anthony DeStefano) and JSC (Rostislav Kovtun, rostislav.n.kovtun@nasa.gov) to remedy this defect. It is also interesting to note that the original size distributions measured for JSC-1 are forced to terminate close to 1 mm simply by the small volume of sample used to make the measure.

There is an implicit assumption that all of the lunar regolith will have one size distribution, or the differences are small enough to be ignored. However, the multiple publications by John Lindsay (e.g. 1974) showed this may be a questionable assumption. And finally, there is a general, self-reinforcing logic chain that goes something like this – “I can only make one simulant – I’ll use the central line of Carrier as my target.” – “The simulant makers use this distribution so that is the distribution to ask for.” – “The users only ask for a single size distribution.” All of which is not a sufficient justification to use only one size distribution.

There are clearly simplifications all throughout the use of size distribution as applied to lunar simulants.

Shape

Until a few years ago particle shape distribution of both the lunar material and the simulants suffered from multiple profound problems: to acquire a statistically meaningful measurement was functionally impossible, there was no theory or guide to understand the measurements once they were made, and influential values, though clearly specious, were accepted into the literature. Therefore, it is not surprising that neither users nor manufacturers generally use shape as a useful metric. Of course, this is in itself another self-perpetuating situation. Manufacturers don’t know how to make the measurements – therefore they have no ability to control this variable – users don’t see a use of the parameter and don’t ask for it – manufacturers don’t perceive a reason to learn how to measure the parameter because users do not ask for it. It is also not surprising that at least one erroneous impression about the shape distributions of Apollo vs. simulants exists. Recent work, now being written up by Ryan Wilkerson (rwilkerson@lanl.gov), show that in a statistical sense, at least NU-LHT-4M is more angular than the Apollo samples Kevin Cannon acquired data for. Yes, it is likely there is an absolutely wider range of shapes in the lunar material, but these extrema are not statistically significant; and, there is no known reason to think the extrema have engineering significance.

It should also be noted there is aggressive work by Edward Garboczi (garboczi@nist.gov) to obtain statistically robust 3D measurements of both Apollo samples and multiple simulants.

As with knowledge of particle size, I expect the community’s knowledge and use of particle shape will change over the next few years. In other words, the simplification of ignoring shape will probably grow less and less common.

Textures

With the exception of multiple attempts to fabricate plausible lunar agglutinates, texture is a glaring void with respect to our knowledge of lunar samples and simulants. In large part this is probably driven by the same problem that blocked the meaningful use of shape for so long, the lack of an accepted, quantifiable method to express texture. Understanding texture is further handicapped by a lack of an automated measurement technology. These facts certainly stopped me. Manufacturers cannot uniformly control for something where a standard is lacking. And users cannot determine its engineering significance if a standard is lacking. There is literally no way to say something intelligible – Tower of Babel. Even though thin sections clearly reveal many lunar textures are easily distinguished, there is little if anything that people can do about it. At this time. Change may come.

Ignoring textures is another simplification.

5. Conclusions

At every step of making and using lunar simulants there are too many variables, too many unknowns, too little money to solve problems, and too little time. Simplification is mandatory. Engineering is possible by the skillful simplification of the natural world's untidy arrangements. Science depends on seeing the underlying, simple rules behind that untidiness. The art comes in recognizing when the simplifications are going to bite. Here is the "but": Just because it was a useful or necessary simplification yesterday, does not mean the simplification need apply tomorrow. The real art comes in figuring out where the past methods can be changed for maximum effect with minimum effort.

6. References

Carrier, W. David III. "Particle Size Distribution of Lunar Soil." *Journal of Geotechnical and Geoenvironmental Engineering* 129, no. 10 (2003): 956. https://doi.org/10.1061/(ASCE)1090-0241(2003)129:10(956).

Graf, John C. *Lunar Soils Grain Size Catalog*. 1265. NASA/RP-1265, 1993.

Lindsay, John F. "A General Model for the Textural Evolution of Lunar Soil." In *Lunar Science Conference (5th), March 18-22*, 861–78. Houston, Texas: Geochimica et Cosmochimica Acta, Supplement 5, Pergamon Press, 1974.

Rickman, Doug L., and Christian M. Schrader. "Figure of Merit Characteristics Compared to Engineering Parameters." Technical Memorandum. MSFC, Huntsville, AL: NASA/Marshall Space Flight Center, 2010. http://ntrs.nasa.gov/search.jsp?R=20100036343.

Sibille, Laurent, Paul Carpenter, Ron A. Schlagheck, and Raymond A. French. *Lunar Regolith Simulant Materials : Recommendations for Standardization, Production, and Usage*. September. NASA/TP—2006–214605, 2006.