Lunar Regolith Simulant User's Guide

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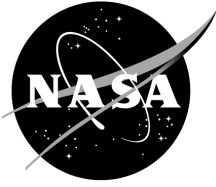
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LIST OF ACRONYMS

Ca	calcium
$CaAl_2Si_2O_8$	anorthite
CaO	calcium oxide
Cl	chlorine
EDS	energy dispersive spectroscopy
F	fluorine
Fe	iron
FeO	iron oxide
FeS	troilite
FoM	figure of merit
H_2	hydrogen
H_2O	water
HCl	hydrogen chloride
HF	hydrogen fluoride
ISRU	in situ resource utilization
JSC	Johnson Space Center
MOE	molten oxide electrolysis
MSFC	Marshall Space Flight Center
Na	sodium
$NaAlSi_3O_8$	albite

NORCAT   Northern Centre for Advance Technology Inc.

O   oxygen

OH   hydrous

PSD   particle size distribution

S   sulfur

SEM   scanning electron microscope

SiO_2 silicon dioxide

SSD   sectional size distribution

Ti   titanium

TiO_2 titanium oxide

TECHNICAL MEMORANDUM

LUNAR REGOLITH SIMULANT USER'S GUIDE

1. INTRODUCTION

This Technical Memorandum (TM) summarizes information on existing lunar regolith simulants. It focuses on primary characteristics of the simulants, which are the inherent properties of the material rather than their responses to behavioral (geomechanical, physiochemical, etc.) tests. This TM defines these inherent or primary properties to be particle composition, particle size distribution, particle shape distribution, and bulk density. When data allow, simulant properties are quantitatively compared to those of a lunar highlands regolith reference material by use of figure of merit (FoM) algorithms and software.

Some of the simulants mentioned in this TM are no longer available for use. However, if any simulant has been analyzed, used in a proof-of-concept study, or used for hardware testing, it is necessary to understand the properties of that simulant relative to the lunar regolith.

NOTE: Before choosing or using a simulant, simulant users are strongly encouraged to contact one of the members of the Marshall Space Flight Center (MSFC) simulant program listed in table 1. It is not intended for the FoM scores or the simulant use matrices to substitute for consultation with experts. Where expertise is lacking, this TM can guide the user to the appropriate resources.

Table 1. MSFC simulant program members.

Program Member	Organization/Position	Phone Number	E-Mail Address
Technical			
Dr. Douglas Rickman	NASA/Geologist	256–961–7889	Douglas.L.Rickman@nasa.gov
Jennifer Edmunson	BAE System/Geologist	256–961–7546	Jennifer.E.Edmunson@nasa.gov
Management			
Carole McLemore	NASA/VP33/Project Manager	256–544–2314	Carole.A.McLemore@nasa.gov
John C. Fikes	NASA/VP33/Deputy Project Manager	256–544–5570	John.Fikes@nasa.gov

2. DEFINITIONS

All definitions for minerals are based on Dana's New Mineralogy.[1] Definitions for rock types are based on IUGS classifications found in reference 2. Particle type definitions for the sub-millimeter portion of lunar regolith are based on Basu and McKay.[3]

3. FIGURES OF MERIT

The FoM mathematics and algorithms provide a means for formal, quantitative comparison of two particulate materials composed of geologic components.[4,5] A reference material serves as the benchmark against which a second material is compared. In this case, the reference material is an average of lunar subsamples within a lunar core (see section 4 of this TM). The simulants are compared against this reference. Though it is beyond the scope of this work, it is worth mentioning that the FoM can be used to compare multiple batches of simulant, multiple samples of lunar regolith, or any other two materials.

3.1 Objective of Figure of Merit

The FoM was designed as a practical and efficient way to characterize and compare materials. Towards this end, the parameters for evaluation are chosen to be:

- Definable: Many characteristics of materials are not yet rigorously defined. Only properties defined in reference 5 are used.
- Measurable: Parameters were chosen that could be measured economically, in a timely fashion, and with results reproducible across laboratories.
- Useful: For simplicity of design, parameters were chosen that correlate to properties important to the functioning of simulant under expected conditions.
- Primary versus derivative: This concept recurs throughout the FoM logic. All else being equal, some characteristics are inherent to a material (whether it is a mineral or glass) like the composition of its constituents, while other properties, like the behavior of a material during heating, are derivatives of the composition.

3.2 Figure of Merit Composition

Composition describes attributes of a particle that exist without regard to size or shape. Here, the term particle is used to mean a piece of solid matter mechanically separable from others, such as by using a sieve. All particles in lunar regolith or simulant will be comprised of glass and/or mineral "grains," but particles may be amalgams of grains that result in lithic fragments (rock particles) or agglutinates.

Therefore, the first order of classification of constituents includes mineral grains, glass grains, lithic fragments (which include breccia fragments), and agglutinates. Measuring proportions of particle types by volume is known as a "modal analysis" and is usually reported in modal percent by each constituent. Although not required by the FoM, it is ideal that modal analyses be obtained for a material in several different size fractions. This is because the percentages of constituents of any bulk material will tend to vary by size due to differential susceptibility to grinding and crushing.

3.3 Figure of Merit Particle Size Distribution

For the FoM, particle size is measured on a particle-by-particle basis and reported as a distribution. The number of bins and the size of the bins are defined by the user, but a more precise FoM evaluation is rendered by an approximation to the lunar regolith dataset. These data can be found in reference 6.

3.4 Figure of Merit Shape and Density

Preliminary definitions for particle shape distribution and bulk density with regard to FoMs have been developed, and algorithms and metrics are being developed. These FoMs are not included in this TM.

3.5 Figure of Merit Software

The software used here for size FoM ratings is FoM v.1.0, released in 2007, and v.2.0, released in 2009. The composition FoMs presented here were calculated using the algorithm of FoM Revision v.2 software.

4. LUNAR REGOLITH REFERENCE MATERIAL

The reference material used here for FoM calculations is the integrated suite of subsamples from Apollo core 64001/64002, which is a sample of lunar highlands regolith from Apollo 16 Station 4. A highlands sample was chosen in line with the current lunar architecture that calls for an outpost in the polar region—a region best approximated by highlands regolith (to the best of current knowledge). A lunar core was chosen as opposed to a soil sample because it provides an integration of the surface and shallow subsurface, this at least partially counters the bias lent by surface processes like "space weathering." Core 64001/64002 was specifically chosen because it is a complete and intact core, it is deemed representative of Apollo 16 site regolith, and it has been reasonably well studied.[7]

5. COMPOSITION

5.1 Lunar Regolith Data Used for Composition Figure of Merit

The FoM v.2 software combines particle type data, as described in section 3.2, with limited mineral composition data for comparison. Mineral composition data are measurements of the average chemistry of mineral phases with variable compositions. Many minerals, including the most common ones in lunar regolith (plagioclase feldspar, clinopyroxene, orthopyroxene, and olivine), have chemical compositions that vary between fixed points. This is called solid solution and it varies between end members. FoM v.2 software allows incorporation of solid solution chemistry into the composition comparison, but there is sufficient data available for reasonable comparison only for plagioclase feldspar. The other solid solution minerals are either undifferentiated, as with olivine, or grouped into subclasses, as with clinopyroxene, orthopyroxene, and the spinel minerals.

5.1.1 Literature Data

Modal particle type data was averaged for sample 64001 (the lower ≈30 cm of the core) from reference 3 and from 64002 (the top ≈30 cm of the core) from reference 7 for use as the basis for the FoM lunar reference material. Each study examined six size fractions from 20 to 500 μm of six subsamples of the core at ≈5-cm intervals. The studies classified particles according to the system found in reference 3. A weighted average (by weight percent of the size fractions) of the compositions of each subsample was calculated. These subsample averages were then combined to a single mean particle type composition of the 20–500-μm portion of the 64001/64002 core.

This particle classification has primarily been used with data generated by optical microscopy of very fine particles;[3] as a result, some mineral types are not classified to the desired level of specificity. For instance, pyroxenes are not differentiated to clinopyroxene and orthopyroxene, and all spinel minerals (chromite, spinel, and ulvöspinel), ilmenite, and sulfides are undifferentiated as "opaques."

More than 90% of the particles by weight of most lunar regolith samples fall below 500 μm.[6] An average of ≈20 wt. % of most regolith falls below 20 μm, but modal data for this fraction are scarce; therefore, this is considered to be the most reasonable available dataset for the purposes of this TM.

5.1.2 Scanning Electron Microscope/Energy Dispersive Spectroscopy Data

Modal data was generated from electron beam analysis of Apollo 16 samples from drive core 64001/64002. The analyzed lunar samples were thin sections 64002,6019 (5–8-cm depth) and 64001,6031 (50–53.1-cm depth) and sieved grain mounts 64002,262 and 64001,374 from depths corresponding to the thin sections, respectively. Four size fractions were analyzed from each grain mount sample: 500–250-μm, 150–90-μm, 75-45-μm, and <20-μm fractions. These data are not

particle type modal data, but they are total area modal percent by phase, such as by mineral type and glass.

For the lunar reference composition, ratios of certain mineral classes from these scanning electron microscope/energy dispersive spectroscopy (SEM/EDS) data are used to augment particle type modal data from the literature. For instance, when the Houck[7] and Basu and McKay[3] data report only "pyroxene," this TM subdivides these into clinopyroxene and orthopyroxene based on the electron beam-generated ratio. Furthermore, their "opaques" are divided into ilmenite, iron (Fe)-sulfide, and spinels (not further differentiated).

5.1.3 Plagioclase Composition

Plagioclase feldspar is the only mineral for which chemical compositional variability in the FoM algorithm is currently evaluated. The generally accepted composition of An_{95} is used for lunar highland regolith plagioclase,[8] which means that the plagioclase is 95 molar % of the anorthite ($CaAl_2Si_2O_8$) end-member and only 5 molar % of the albite ($NaAlSi_3O_8$) end-member. Plagioclase composition is included in the FoM because of the following:

- It is the most abundant mineral in the highlands regolith.[7]
- It is the only mineral for which there is reasonable compositional data in both the regolith and the simulants.
- Lunar highlands plagioclase is more calcic than almost any terrestrial plagioclase, and closeness to lunar plagioclase composition is viewed as a significant marker of simulant fidelity.

5.1.4 Populating the Lunar Reference for Figure of Merit

The literature and SEM/EDS data are combined to yield a highlands lunar regolith reference composition, which is shown in table 2 along with simulant data.

Table 2. Particle type modal data and plagioclase molar percent anorthite for the lunar reference material and regolith simulants.

	64001/ 64002	NU-LHT-1M	NU-LHT-2M	OB-1	JSC-1	JSC-1A	JSC-1AF	FJS-1	MLS-1
Lithic fragments	31.1	–	–	–	90.9	90.9	91.9	80.2	52.3
Glass	8.9	22.4	7.2	52.6	–	–	–	0.5	36.6
Agglutinates	32.5	29.0	23.5	–	–	–	–	–	–
Plagioclase	23.3	38.8	54.9	43.9	1.5	1.5	3.4	14.1	2.6
(*Plag. An%*)	*95*	*80*	*80*	*75*	*68*	*70*	*70*	*50?*	*47*
Olivine	–	2.9	9.5	0.0	5.6	5.6	4.1	1.1	0.0
Clinopyroxene	0.6	2.0	4.0	0.1	1.3	1.3	0.4	1.2	2.2
Orthopyroxene	3.2	4.4	0.2	–	–	–	–	–	–
Spinel minerals	0.03	0.05	0.01	0.19	–	0.04	0.02	0.05	0.03
Fe-sulfide	0.01	0.00	0.04	–	–	–	–	–	–
Ca-phosphates	0.12	–	0.43	–	–	–	–	–	–
limenite	0.1	0.3	0.2	0.0	–	0.1	0.0	0.1	1.1
Native iron	0.01	–	–	–	100	–	–	–	–
Other (sim. only)	–	0.2	0.1	3.1		0.5	0.1	2.6	5.2
Total	100	100	100	100		100	100	100	100

5.2 Simulant Data Used for Composition Figure of Merit

Particle type modal data for the regolith simulants is from electron beam analysis. Plagioclase composition is based on the limited data of feedstock analysis or, when available, electron microprobe analysis of the simulant.

5.2.1 Scanning Electron Microscope/Energy Dispersive Spectroscopy Data

All simulants analyzed have been considerably less texturally complex than the analyzed lunar regolith. Particle type data on the simulants by QEMSCAN® SEM/EDS analysis has been consistently obtained. The software used for textural analysis and particle identification is the iDiscover 4.2 package developed by Intellection Ltd. and incorporated into QEMSCAN technology. It differentiates and classifies basalt as lithic fragments in mare simulants and the pseudo-agglutinate fragments (identified as agglutinates) in the NU-LHT series highlands simulants. It is these particle type modal analyses that are used in the FoM v.2 composition routines. The data for major particle types are shown in plots with the lunar reference data in figure 1. Tabulated data are shown in table 2. In addition, the SEM/EDS analysis yields total modal area percent for the simulants as it does for the lunar material. For numerous reasons, the FoM composition definitions and algorithms use the particle type modal data; however, the area modal data for simulants and the lunar reference material are presented in figure 2 (major phases) and figure 3 (minor and trace minerals) for completeness.

There are some apparent inconsistencies between the particle type and the area modal data. For instance, the area modal data (fig. 2) show simulant OB-1 to contain measurable amounts of the mafic (Fe- and magnesium (Mg)-bearing) minerals olivine and pyroxene while the particle modal data (table 2 and figure 1) show neither as a free mineral. An examination of the phase maps indicates that this is due to pixels in the OB-1 olivine slag glass being reported as mafic phases. These may be crystals, on the scale of microns to tens of microns, formed by devitrification of the slag glass or they may be compositional inhomogeneities in the glass. The processing by the iDiscover software classified these as glass particles.

5.2.2 Plagioclase Composition

Table 2 contains the values used in the FoM analysis for plagioclase composition for simulants and lunar regolith.

The particle type composition of the Chenobi simulant is not shown in table 2 because it has not been analyzed; however, it incorporates the same anorthosite feedstock used in OB-1 and thus has plagioclase with $An_{75}\%$.
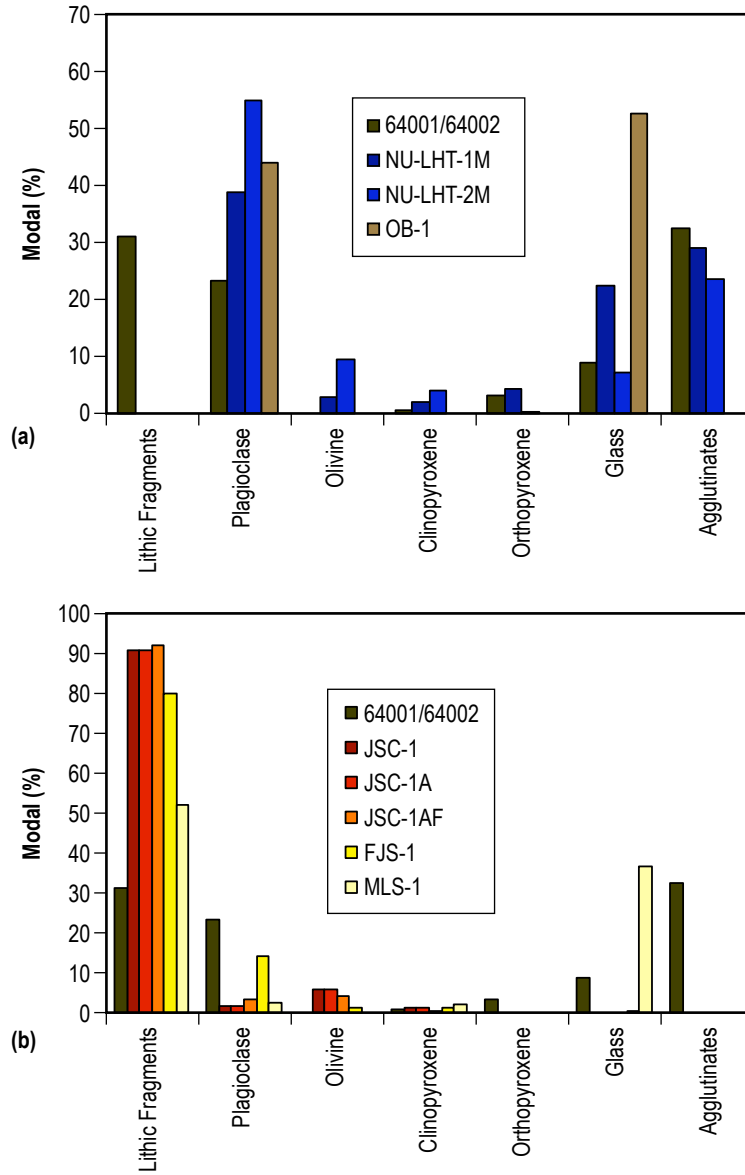
Figure 1. Particle-type compositional data for highlands regolith simulants and the lunar reference 64001/64002: (a) Contains highlands data and (b) contains modal data.
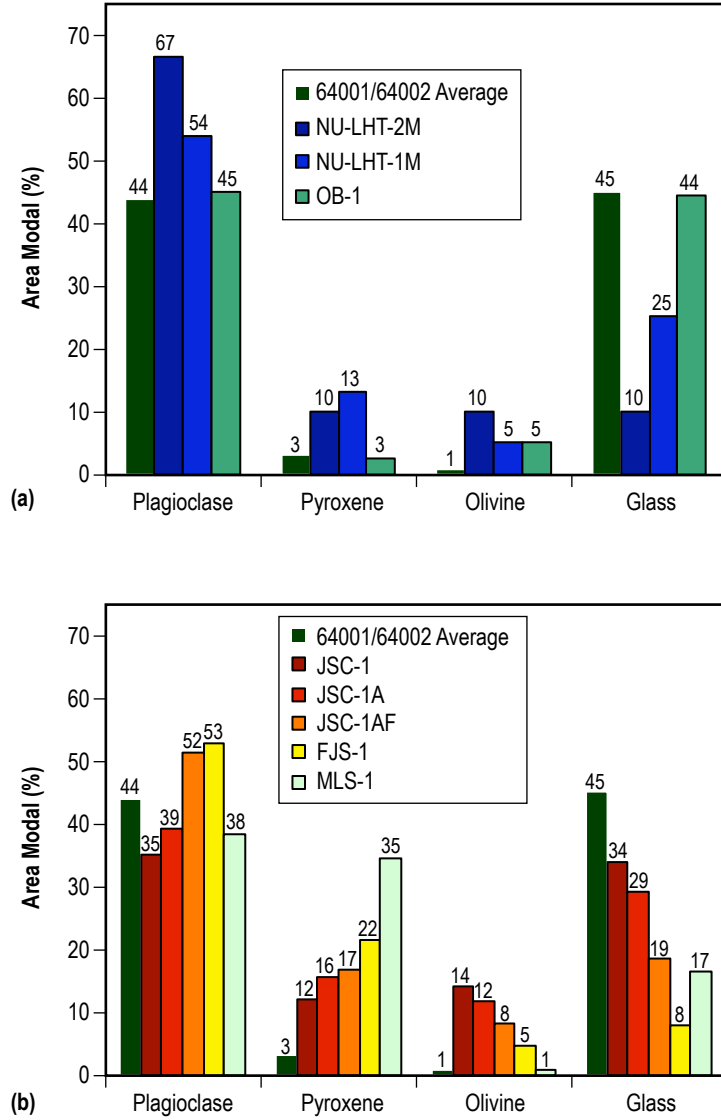
Figure 2. Area modal data for major phases in mare regolith simulants and the lunar reference 64001/64002: (a) Contains highlands data and (b) contains modal data.
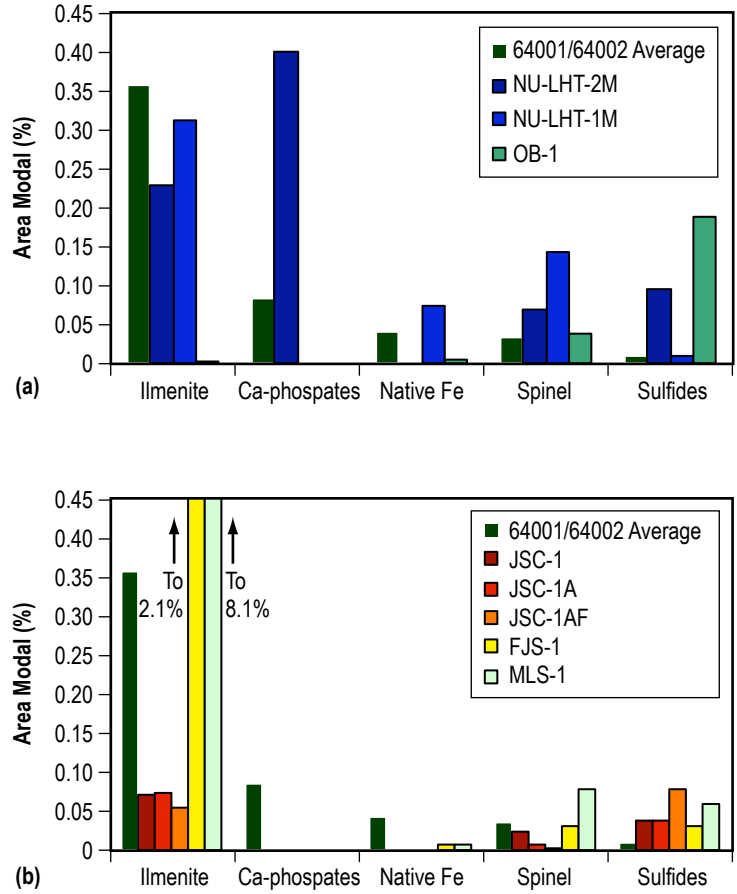
Figure 3. Area modal data for minor phases in mare regolith simulants and the lunar reference 64001/64002: (a) Contains highlands data and (b) contains modal data.

5.3 Composition Figure of Merit Results

All composition FoMs were run using FoM v.2 data entry forms and algorithms. The FoMs were calculated using Matlab software because the final user version of v.2 was not released at the time the data for this TM was produced.

See table 3 for FoM v.2 composition results for all simulants tested against the 64001/64002 lunar reference material.

Table 3. Results of FoM composition analysis.
FoM Revision 1 algorithm used with
lunar reference material 64001/64002.

Simulant	64001/64002 Reference
NU-LHT-1M	0.65
NU-LHT-2M	0.55
OB-1	0.28
JSC-1	0.33
JSC-1A	0.35
JSC-1AF	0.43
MLS-1	0.35
FJS-1	0.36

5.4 Comments

The FoM is a powerful tool still in development. Innovation and updating of the approach, algorithms, and software continues. Composition is a complicated concept for granular geologic materials as it may capture particle type and chemistry (as reflected in and controlling the mineralogy and phase assemblage), etc.

5.4.1 Lithic Fragments and Agglutinates

It is a complex problem to consistently classify fragments of rock and breccia in lunar and terrestrial material. In regolith, they form a spectrum of particle types composed of varying amounts of minerals and glass and of varying and unknown mechanical competency. For this reason, all rock fragments and breccias are classified as lithic fragments and compared to the abundance of all rock and breccia fragments in the regolith.

Agglutinates are members of the particle spectrum including lithic and breccia fragments, but they are interpreted to be sufficiently unique in their properties and abundance as to be worth differentiating. Furthermore, their characteristics as irregularly shaped, often vesicular particles composed of minerals in a glass matrix make it possible to identify them with automated beam technology.

Because the lunar regolith reference 64001/64002 is composed of ≈32-modal % agglutinates and 31-modal % lithic fragments, simulants that do not approximate these abundances will score a low composition FoM score; however, they may still be appropriate simulants for many purposes by virtue of their chemistry, shape, or size distribution. Conversely, a simulant with an appropriate abundance of these particles may be inappropriate for some uses.

5.4.2 Glass Composition

Glass is an amorphous material with no crystalline structure that can have an almost unlimited range of chemical compositions. The lunar regolith has a range of glass populations

of different origins and different chemical compositions. Various approaches for evaluating glass compositions are being evaluated for incorporation into FoM v.3. This FoM analysis (v.2) treats all glass particles as the same and compares them to the 8.9 modal % in the lunar reference material.

Most glasses behave broadly similarly for geomechanical purposes. Simulant users who need certain chemical fidelity to lunar material will need to take glass composition into consideration and consult with experts. Table 4 contains an overview of glass contained in simulants. Quantitative analyses are not available but a consideration of feedstock sources presents some constraints.

Table 4. Qualitative description of glass found in simulants.

Simulant	Qualitative Glass Description
NU-LHT series	Glass is derived by melting of noritic feedstock in a plasma stream. Si-Al-Ca with moderate Fe and Mg.
OB-1	Glass is an olivine slag, Si-Fe-Mg.
Chenobi	Glass is derived by melting of the anorthosite feedstock in a plasma stream Si-Al-Ca.
JSC-1 series	Natural basalt glass. Si-Al-Ca-Fe-Mg with lesser Na.
FJS-1	Natural basalt glass. No analyses available.
MLS-1	In the sample analyzed, glass is derived by plasma melting of basaltic feedstock, Si-Al-Fe-Mg-Ca.

6. SIZE

6.1 Lunar Regolith Data Source

The particle size distribution data (PSD) for 64001/64002 is taken from reference 6. It is an average of 12 subsamples by weight percent of each size fraction.

6.2 Simulant Data Sources

Multiple sources of simulant size-distribution data were used. In most cases, multiple data sources are represented per simulant. Data methods are clearly listed in the results.

6.2.1 Dry Sieving

Some data are from dry sieving methods and reported by weight percent. Data for OB-1 comes from Trow Analytical, Ltd. Analyses for Johnson Space Center (JSC)-1A and NU-LHT-1M were performed in the lab of Susan Batiste at the University of Colorado.

The dataset for Northern Centre for Advanced Technology Inc.'s (NORCAT's) Chenobi simulant is a combination of dry sieve data above ≈75 μm and laser diffractometry data for the finer portion.

Particle size distribution data is available for NU-LHT-2C, but the bin sizes are skewed to show the coarse fractions and are too broad to use for FoM analysis.

6.2.2 Scanning Electron Microscope and Image Processing

The authors of this TM have size data from QEMSCAN SEM/EDS analysis, reported by weight percent, for all simulants except NU-LHT-1D. It should be said that grain mounts used for SEM imaging are polished and thus provide a sectioned sample, and that most particles will not be sectioned at their plane of greatest diameter equivalent. For this reason, such results are sometimes referred to as a sectional size distribution (SSD) rather than a PSD. The high number of particles counted partially offsets this effect, but there will always be a slight bias towards finer particles in an SSD. This can be partially compensated for by stereological techniques, and this approach is being pursued. For now, users are cautioned to take this into account, but are also reminded that all simulants were measured by this method; therefore, any problems will be consistent across that portion of the dataset.

6.2.3 Liquid Dispersion and Laser Diffractometry

The authors of this TM have data for NU-LHT-1M, -2M, and -1D, and JSC-1A from liquid dispersed laser diffractometry. Susan Batiste, at the University of Colorado, measured NU-LHT-1M and JSC-1A, while the Bureau of Mines analyzed NU-LHT-2M and -1D.

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These data are presented as volume percent rather than as weight percent. If the particle composition distribution was consistent across the size fractions, the data would be equivalent, but this is not true for lunar regolith and is likely not to be true for simulants. However, it is judged likely that the deviations in density across the size fractions are of small effect. It is left to the user to evaluate these ratings until more data are gathered and analyses are presented. Again, the method is consistent for the four simulants measured and thus is of comparative value.

The <75-µm portion of the Chenobi simulant dataset is determined by laser diffractometry and converted to weight percent.

This analytical method yields more bins of data (smaller size fractions) than the FoM software allows. The bins have been summoned to best match the reference 6 bins.

6.3 Figure of Merit Particle Size Distribution Results

Table 5 contains FoM size results for all simulants against the lunar reference material 64001/64002. Several subsets of reference data are compared to simulant size datasets obtained by different methods. Simulant datasets were compared against the bulk average of 64001/64002, the <1–mm subset of the data, and the <90-µm subset of the data. Both reference subsets were recalculated to 100%. The analytical method is in parentheses.

Table 5. FoM size results for all simulants against 64001/64002 lunar reference material.

	64001/2 Bulk Average	64001/2 <1-mm Average	64001/2 Average to 90 µm
OB-1 (section image analysis)	0.23	0.54	–
NU-LHT-1M (section image analysis)	0.23	0.58	–
NU-LHT-2M (section image analysis)	0.17	0.48	–
JSC-1 (section image analysis)	0.22	0.53	–
JSC-1A (section image analysis)	0.25	0.56	–
JSC-1AF (section image analysis)	0.06	0.23	0.60
MLS-1 (section image analysis)	0.20	0.29	–
FJS-1 (section image analysis)	0.26	0.45	–
OB-1 (dry sieve)	0.59	–	–
NU-LHT-1M (dry sieve)	0.26	0.75	–
JSC-1A (dry sieve)	0.35	0.74	–
Chenobi (dry sieve + laser diffractometry)	0.77	0.73	–
NU-LHT-2M (laser diffractometry)	0.29	0.82	–
NU-LHT-1D (laser diffractometry)	–	–	0.54
NU-LHT-1M (laser diffractometry)	0.26	0.64	–
JSC-1A (laser diffractometry)	0.28	0.74	–

6.3.1 Comparison to the Entire 64001/64002 Particle Size Distribution

The range of size bins for 64001/64002 from reference 6 is broader than for any of the simulants. All simulant PSDs are compared to the entire 64001/64002 PSD and the results are shown in the first column of table 5.

6.3.2 Against Normalized Subsections

6.3.2.1 <1-mm Fraction. Most of the simulant PSDs only extend to ≈1 mm. The second column of table 5 shows comparisons of all simulants to the <1-mm fractions of 64001/64002. These fractions were recalculated to sum to 100 wt. %.

6.3.2.2 <90-μm Fraction. For the two simulants specifically intended to be dust simulants, another normalized subset of reference 6 data was used for comparison, this time recalculating the <90-μm fraction to sum to 100 wt. %. The results for this subset are shown in column 3 of table 5.

6.4 Comments

Of the simulant PSDs run in the FoM size analysis, only OB-1 sieve data and the Chenobi sieve plus laser diffractometry data had particles in the larger fraction that matched the bins of the reference data. The simulant NU-LHT-2C contains particles to 10 cm and the PSD apparently matches well with Apollo regolith; however, as mentioned in section 6.2.1, the resolution of NU-LHT-2C PSD data is insufficient for FoM analysis.

The FoM size analysis is sensitive to how data are binned. Within any one method/data type, all datasets have identical binning, so comparison within groups is reliable.

7. SHAPE

FoM Revision 1 software is capable of comparing aspect ratio and angularity of particle shape distributions, but the defining of the metrics and parameters for analysis has not yet been completed.

As part of the QEMSCAN analysis, the iDiscover software returned shape metrics for all simulants, which are shown in table 6 and compared graphically in figure 4. These are given in terms typical for geological studies but should provide a qualitative comparison between simulants. No data in these terms exist for lunar regolith. However, the Moon lacks the flowing water and wind that cause rounding in terrestrial sediments; therefore, only glass spherules are likely to be rounded or well rounded. Units in table 6 are in weight percent of typical geologic classification bins from very angular to well rounded.

Table 6. Shape parameters of simulants derived by QEMSCAN analysis.

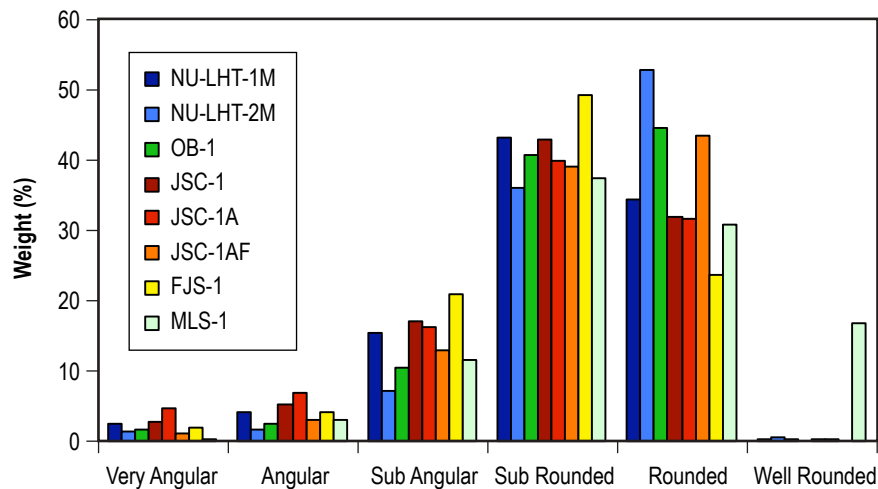| Particle Shape Classification	NU-LHT-1M (wt. %)	NU-LHT-2M (wt. %)	OB-1 (wt. %)	JSC-1 (wt. %)	JSC1A (wt. %)	JSC-1AF (wt. %)	FJS-1 (wt. %)	MLS-1 (wt. %)
Very angular	2.4	1.5	1.7	2.9	4.7	1.1	2.0	0.4
Angular	4.2	1.8	2.3	5.1	7.0	3.1	4.2	3.0
Subangular	15.3	7.3	10.4	17.0	16.3	13.0	20.9	11.5
Subrounded	43.3	36.2	40.7	42.9	40.0	39.2	49.2	37.5
Rounded	34.4	52.8	44.5	31.9	31.6	43.4	23.6	30.8
Well rounded	0.2	0.6	0.3	0.1	0.3	0.3	0.1	16.9
Total	100	100	100	100	100	100	100	100

Figure 4. Qualitative graphical comparison of shape parameters for simulants derived by QEMSCAN analysis. Units are in weight percent of typical geologic classification bins.

8. SIMULANT FIT-TO-USE MATRIX

NOTE: Before choosing or using a simulant, simulant users are strongly encouraged to contact one of the members of the MSFC simulant program listed in table 1. It is not intended for the FoM scores or the simulant use matrix to substitute for consultation with experts. Where expertise is lacking, users can be guided to the appropriate resources.

This TM represents a best estimate of appropriateness of each simulant for common types of investigations. The material behaviors important to these investigations are largely derived from the four "primary" properties captured in the FoM for simulant evaluation.[5] These material properties are particle composition, PSD, particle shape distribution, and bulk density. Table 7 is the fit-to-use matrix for excavation/flow, drilling, and abrasion/wear.

Two simulants (NU-LHT-2C and Chenobi) are included in the matrix that are not included in particle type FoM evaluations in sections 1 through 7 of this TM. Further, NU-LHT-2C is not included in the PSD section (section 6), though PSD data is presented for it. Chenobi is included in the matrix because the composition is understood to be composed of the same material as the anorthosite fraction of the OB-1 feedstock; a portion of this anorthosite was then melted to make the glass portion of Chenobi. NU-LHT-2C is derived from the same materials as NU-LHT-2M, but a portion of the material was partially fused to make a coarser fraction that is added back in after milling and grinding. Though these simulants were not analyzed in the same fashion as other simulants included in sections 1 through 7 of this TM, the authors feel that these simulants are sufficiently understood to be evaluated in the fit-to-use matrix in table 7.

In assembling this matrix, the attempt is to extrapolate from the known primary characteristics of simulants to their behavior under the relatively complex conditions of these investigative environments. For instance, the behavior of a simulant during excavation may be affected by its abrasiveness and angle of repose. These properties in turn result from the hardness and cleavage behavior of its particles (particle composition), PSD, particle shape distribution, and maximum packing density. The response of a simulant to heating in the presence of hydrogen (H_2) for oxygen (O) extraction will be largely a result of its particle type composition—neglecting reaction rates that may be due to its PSD and packing/density properties.

Researchers have a reasonably good understanding of these simulants' particle compositions and PSDs (see sections 1 through 7 of this TM), though more detail is needed in some areas. They have only a rudimentary survey of the particle shape distributions or density properties but are aided by having some initial studies on O extraction, angle of repose, and abrasiveness.

Table 7. Simulant fit-to-use matrix for excavation/flow, drilling, and abrasion/wear.

	Excavation/Flow*	Drilling*	Abrasion/Wear
NU-LHT-1M	Recommended: It has been demonstrated that pseudo-agglutinates affect geomechanical behavior that may be important to excavation.	Recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness. Presence of pseudo-agglutinates may aid fidelity to regolith.	Recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness. Presence of pseudo-agglutinates may aid fidelity to regolith.
NU-LHT-2M	Recommended: It has been demonstrated that pseudo-agglutinates affect geomechanical behavior that may be important to excavation.	Recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness. Presence of pseudo-agglutinates may aid fidelity to regolith.	Recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness. Presence of pseudo-agglutinates may aid fidelity to regolith.
NU-LHT-1D	Not recommended: Unrealistically fine PSD.	Not recommended: Unrealistically fine PSD.	Recommended with reservations: Unrealistically fine PSD for many uses.
NU-LHT-2C	Most recommended: It has been demonstrated that pseudo-agglutinates affect geomechanical behavior that may be important to excavation.	Most recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness. Presence of pseudo-agglutinates may aid fidelity to regolith, good PSD.	Recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness. Presence of pseudo-agglutinates may aid fidelity to regolith.
OB-1	Recommended: Good PSD at coarse end. Lack of lithic fragments or pseudo-agglutinates may affect flowability or angle of repose. This should be examined.	Most recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness, best PSD for coarse fractions.	Most recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness, best PSD for coarse fractions.
Chenobi	Recommended: Good PSD at coarse end. Lack of lithic fragments or pseudo-agglutinates may affect flowability or angle of repose. This should be examined.	Most recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness, best PSD for coarse fractions.	Most recommended: Fidelity to mineral and glass% should yield appropriate abrasiveness, best PSD for coarse fractions.
JSC-1, -1A	Recommended: Relatively angular particles, reasonable PSD.	Recommended with reservations: Uncertain but probably reasonable fidelity to highland abrasiveness.	Recommended with reservations: Uncertain but probably reasonable fidelity to highland abrasiveness.
JSC-1AF	Not recommended: Unrealistically fine PSD.	Not recommended: Unrealistically fine PSD.	Recommended with reservations: Unrealistically fine PSD for many uses.
FJS-1	Recommended: Low-g tests show it has a high angle of repose with relatively angular particles and reasonable PSD.	Recommended with reservations: Uncertain but probably reasonable fidelity to highland abrasiveness, low glass.	Recommended with reservations: Uncertain but probably reasonable fidelity to highland abrasiveness, low glass.
MLS-1 (processed for glass component)	Not recommended: relatively poor PSD. Shape distribution is skewed towards well-rounded particles.	Not recommended: High pyroxene/plagioclase may adversely affect particle cleavage behavior, rounded grains.	Not recommended: High pyroxene/plagioclase may adversely affect particle cleavage behavior, rounded grains.

* Quantitative data on shape is lacking, and shape is important to geomechanical behavior.

It is very important to remember that all simulants here are measured relative to the highlands lunar reference sample Apollo core 64001/64002 (see Simulant User's Guide (2008) for justification). For example, some simulants that may be appropriate for investigations pertaining to a high-titanium (Ti) mare regolith deposit will be judged poorly by the standards of the Simulant User's Guide. It is equally important to remember the necessarily speculative nature of some of these judgments. They have been made in some cases without the benefit of direct measurement. This document will be updated with input from the user community and the engineering and scientific community.

8.1 Oxygen Production

There are many approaches to O production for in situ resource utilization (ISRU), but three primary methods are currently being investigated: H_2-reduction, carbothermal reduction, and molten oxide electrolysis (MOE). The first requires heating to the point of sintering and partial melting while the latter two require total melting of the material. Table 8 presents data regarding the simulant fit-to-use matrix for O production and human health studies.

Table 8. Simulant fit-to-use matrix for O production and human health studies.

	Oxygen Production**	Human Health Studies
NU-LHT-1M	**Recommended for highlands:** Chemistry: Slightly low FeO relative to lunar reference (≈4 vs. 5 wt.%) but significantly closer than other simulants. Mineralogy: Contains ilmenite. High Fe in silicates relative to reference, which will slow reduction.	**Suitable composition:** It lacks the added phosphates and sulfides of NU-LHT-2M; reasonable PSD but too coarse in fine fraction.
NU-LHT-2M	**Most recommended for highlands:** Chemistry: Slightly low FeO relative to lunar reference (≈4 vs. 5 wt.%) but significantly closer than other simulants. Mineralogy: Contains ilmenite, phosphates, and sulfides; the presence of which is realistic but possibly hazardous to ISRU processes. High Fe in silicates relative to reference, which will slow reduction.	**Most suitable composition:** Reasonable PSD but too coarse in fine fraction.
NU-LHT-1D	**Recommended for highlands:** Should be similar to NU-LHT-1M but possibly with lower FeO.	**Suitable composition:** It lacks the added phosphates and sulfides of NU-LHT-2M; good PSD in fine fraction.
NU-LHT-2C	**Recommended for highlands:** Chemistry: Slightly low FeO relative to lunar reference ≈4 vs. 5 wt.%) but significantly closer than other simulants. Mineralogy: Contains ilmenite, phosphates and sulfides, the presence of which is realistic but possibly hazardous to ISRU processes. High Fe in silicates relative to reference, which will slow reduction	**Most suitable composition:** Good PSD.
OB-1	**Not recommended:** It is expected that the abundance of Fe-rich glass will result in unrealistically high oxygen yields per energy input; no glass analyses are available.	**Unsuitable composition:** This is due to high Fe-glass. May be acceptable for testing where abrasiveness is of primary importance.
Chenobi	**Recommended for highlands with reservations:** Will serve, in a way, as a worst-case example of the highlands regolith with the highest anorthositic fraction and that with the least mare contamination (i.e., very low FeO).	**Partially suitable composition:** It lacks added phosphates and sulfides, and it represents one end-member of regolith composition; good PSD in fine fraction.
JSC-1, -1A	**Recommended with reservations:** Chemistry: FeO is significantly high relative to lunar reference (≈11 vs. 5 wt.%). Mineralogy: Contains natural phosphates, Ti-magnetite instead of ilmenite. Use will likely result in unrealistically high oxygen yields; may be a good mare simulant (e.g., Apollo 14) for this use.	**Possibly suitable composition:** Reasonable PSD but too coarse in fine fraction.
JSC-1AF	**Recommended with reservations:** Should be similar to JSC-1A.	**Possibly suitable composition:** Good PSD in fine fraction.
FJS-1	**Recommended with reservations:** Chemistry: FeO is significantly high relative to lunar reference ≈11 vs. 5 wt.%. Mineralogy: Contains natural phosphates, Ti-magnetite instead of ilmenite. Use will likely result in unrealistically high oxygen yields; may be a good mare simulant (e.g., Apollo 14) for this use.	**Possibly suitable composition:** Poor PSD in fine fraction.
MLS-1 (processed for glass component)	**Not recommended for highlands:** Chemistry: FeO is very high relative to lunar reference (>14 vs. 5 wt.%). Mineralogy: Contains abundant ilmenite but also hydrous minerals. May result in extremely unrealistically high oxygen yields; may be an acceptable high-Ti (Apollo 11) simulant, but hydrous minerals are still problematic.	**Unsuitable composition:** Unsuitable PSD in fine fraction.

** See associated text for details on different oxygen production methods.

There are intricacies to the methods, and the O yield/energy input depends on a number of material compositional details and methodologies. It is the judgment of the researchers that a simulant to be used for O production should have reasonable compositional fidelity to the reference lunar material in the following ways:

- Chemically, it should contain iron oxide (FeO) weight percent close to the FeO weight percent of the lunar reference material. (Here, FeO is not a phase but the chemical species Fe_2+-O found in minerals, glasses, and the melt.)

  Justification: The breaking of metal-O bonds liberates O, and the amount of energy required to break them is inversely proportional to their free energy of formation. Of the major lunar chemical oxides, FeO has the highest free energy and calcium oxide (CaO) the lowest. For this reason, during H_2 reduction, O yield correlates to FeO weight percent in the starting material.[9] Some silicon dioxide (SiO_2) (chemical) and titanium dioxide (TiO_2) (chemical) are also reduced.

  In processes involving melting (i.e., carbothermal reduction and MOE), these chemical species are more completely reduced. It is generally possible to reduce all of the Fe_2+ through these methods.

- The oxidation state of the Fe in a simulant should be as close as possible to that in lunar regolith. Practically speaking, no natural rock, and thus no nonsynthetic simulant, can emulate the oxidation state of lunar rocks. It is important for users to be aware of this.

  Details: On the Moon, Fe dominantly occurs as Fe_2+ (FeO) with lesser FeO. In terrestrial rocks, Fe occurs as a combination of Fe_2+ (FeO) and Fe_3+ (Fe_2O_3).

  During H_2-reduction, Fe_2O_3 will initially reduce to FeO and thus produce more O per unit Fe than will lunar regolith. During MOE, reaction with Fe_3+ behaves parasitically with regard to electronic conduction and reduces the efficiency of the process by 20–30% relative to Fe_2+.

- The Fe-bearing phases (i.e., its assemblage of Fe-bearing minerals and glasses) should be similar in kind and abundance to the reference material. This is true especially for H_2-reduction work and less so for MOE or carbothermal.

  Justification: The O is liberated primarily from Fe-bearing phases. In the case of H_2-reduction, the O is derived most efficiently from $FeTiO_3$ then from the glass phase, and then, and only partially, from the Fe-bearing silicate minerals olivine and pyroxene.[9]

  Although O yield during H_2-reduction is proportional to FeO weight percent when run to completion (3 hours for the study in reference 9), almost 75% of the O is extracted relatively quickly due to the efficiency of liberating it from ilmenite and glass.[10] Therefore, the phases in which the Fe resides exert a strong control on yield/energy input, especially for the H_2-reduction method.

- The presence of hydrous- (OH-) or hydrated (H_2O-) bearing minerals in a simulant is undesirable, especially if it is to be used for H_2-reduction work.

Justification**:** There are no OH or H_2O materials on the Moon, except possibly in shadowed craters. In the H_2-reduction method, O is liberated as H_2O; therefore, any H_2O or OH- present will skew results of the test.

- Simulants should have an assemblage of trace minerals, especially halogen-bearing (fluorine- (F-) and chlorine- (Cl-)) and sulfur- (S-) bearing phases, similar to the lunar reference material in kind and abundance. Halogens are especially important to H_2-reduction work, while S is particularly significant for MOE.

   Justification: Fluorine and Cl occur in minor amounts in trace minerals (primarily fluorapatite) in the lunar regolith; however, at high temperatures, these elements (especially Cl) are strongly partitioned into the vapor phase yielding hydrogen chloride (HCl) and possibly hydrogen fluoride (HF). It has been demonstrated that these can have a corrosive effect on equipment, even in the short term.

   Sulfur occurs in troilite (FeS) in the lunar regolith. For MOE, S acts parasitically regarding electronic conductivity and diminishes the efficiency of the process.

9. CONCLUSIONS

There are a number of studies documenting other properties of simulants including geomechanical properties, abrasiveness, behavior during O production procedures, etc. It is recommended that users consult these studies when relevant to their needs.

Users are encouraged to contact the authors at MSFC for advisement as to simulant use. It is predicted that this document will be updated at least annually, but new information is available constantly. These evaluations are ongoing, as is FoM development. Most importantly, simulant development is continuing.

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14. ABSTRACT

Based on primary characteristics, currently or recently available lunar regolith simulants are discussed from the perspective of potential experimental uses. The characteristics used are inherent properties of the material rather than their responses to behavioral (geomechanical, physiochemical, etc.) tests. We define these inherent or primary properties to be particle composition, particle size distribution, particle shape distribution, and bulk density. Comparable information about lunar materials is also provided. It is strongly emphasized that anyone considering either choosing or using a simulant should contact one of the members of the simulant program listed at the end of this document.

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