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Figure of Merit Characteristics Compared to Engineering Parameters

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LIST OF ACRONYMS

Br	bromine
Cl	chlorine
CO_2	carbon dioxide
F	fluorine
Fe^0	iron metal
FoM	figure of merit
H_2O	water
I	iodine
ISRU	in situ resource utilization
MSFC	Marshall Space Flight Center
nFe^0	nanophase iron metal
OH	hydroxyl
P	phosphorous
TM	Technical Memorandum

TECHNICAL MEMORANDUM

FIGURE OF MERIT CHARACTERISTICS COMPARED TO ENGINEERING PARAMETERS

1. INTRODUCTION

Current NASA lunar architecture calls for permanent human habitation of the Moon by the year 2020. Due to the expense of delivering materials into orbit, technologies are being developed to use lunar regolith for building and as a material resource for fabrication, oxygen production, and other needs. Additionally, constant exposure to the finest size fraction of lunar regolith may present hazards to human health. Towards developing these technologies and mitigating hazards, lunar regolith simulants are becoming an increasingly important part of the development paradigm.

1.1 2005 Regolith Simulant Workshop

In January 2005, Marshall Space Flight Center (MSFC) hosted a workshop in Huntsville, AL, to discuss the future development of lunar regolith simulants. This meeting brought together geoscientists including some major figures in lunar geology, project managers, engineers, and simulant users from NASA centers, academia, and private enterprise. In addition to 2 days of presentations (content is available at < http://est.msfc.nasa.gov/workshops/lrsm2005_program.html >), sessions were held to identify characteristics necessary for a lunar regolith simulant to sufficiently serve the community. Regolith characteristics were discussed and votes were taken with regard to perceived importance. Following the 2005 workshop, Sibille et al. published a technical paper ranking these properties.[1]

1.2 Development of Figures of Merit

Between 2005 and 2007, the lunar regolith simulant project advanced considerably. Much of the progress and development is evident in presentations of the October 2007 MSFC-hosted Huntsville workshop < http://isru.msfc.nasa.gov/2007wksp_docs.html >. Part of the evolution was the establishment of the figure of merit (FoM) mathematics and algorithm for formal, quantitative comparison of two particulate materials composed of geologic components.[2,3] Although normally the comparison will be between a particular sample of lunar regolith and a simulant, the FoM can also be used to compare two simulants or two regolith samples.

1.3 Explanation of the 2005 Workshop Rankings With the Figure of Merit

The primary motivation for this document is to define the relationship between the four FoM measurements and other characteristics of interest. For the most part, it is shown that the characteristics of interest from the 2005 conference are either directly contained within one of the four attributes measured for and evaluated by the FoM, or they are derivative characteristics resulting from one or a combination of the FoM attributes. This information is presented along with a brief explanation in cases where the ranked characteristics from the 2005 workshop are not measurable, technically undefined, or not addressed by the FoM.

2. FIGURE OF MERIT

2.1 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 have the following characteristics:

- Definable: Many characteristics of materials are not rigorously defined. This is true even of some important physical characteristics like surface activation.
- 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. Some characteristics are inherent to a material, like the composition of its constituents, be they minerals or glass. All else being equal, other properties, like the behavior of a material during heating, are derivative of the composition.

These are positive attributes desirable in any standard.

Expressed in the negative, if something cannot be rigorously defined and measured reproducibly by multiple people, it has little value in a standard. If it cannot be practically known, a problem common with lunar materials for a host of reasons, it is not of functional utility within a standard. If a variable cannot be realistically measured in a way suitable for controlling the manufacture and the use of simulants, it has little place in a standard. If a parameter does not discriminate between materials, it has limited function to a quantitative standard.

2.2 Parameters

The FoM requires four types of measurements from both the reference material and the simulant: Particle type, particle size, particle shape, and density. These four material attributes were chosen to comply with the above objectives and because they are measurable quantities from which almost all of the 31 characteristics ranked during the 2005 conference are derived. They also are functionally useful to anyone seeking materials to make simulant, to those trying to manufacture simulant, and to those trying to use the simulant. Refer to reference 3 for a formal definition of the four characteristics.

2.2.1 Particle Type/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 use of a sieve. The 2005 report uses the term grain for several basic concepts. This is common practice for geologists who, by training and experience, understand the meaning by context. Because the majority of simulant users and developers are not geologists, the simulant development project explicitly decided to restrict grain to mean a discrete subset of a particle. 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, and agglutinates. Measuring proportions of particle types by volume is known in geologic science as a modal analysis and is usually reported in modal percent by each constituent. Although it is 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. Modal analyses for lunar highlands regolith have been published (e.g., reference 4). These data serve as the basis for the regolith simulant team's reference material in the FoM algorithm, but more precise data are being gathered to augment them.

2.2.2 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. For instance, these data can be found in The Lunar Soils Grain Size Catalog.[5]

2.2.3 Particle Shape Distribution

Particle shape is a crucial parameter in determining many geotechnical properties such as abrasiveness and bulk shear strength. The FoM calls for measurement of shape on a particle-by-particle basis, which is then reported as a distribution. Shape is described by two parameters, aspect ratio and sphericity. The specific algorithms for measuring these characteristics are being determined.

2.2.4 Density

Density as an FoM parameter refers to bulk density, and it is the only parameter that is not measured by the particle but as a bulk characteristic. The measurements that comprise the density FoM are minimum bulk density, maximum bulk density, and specific gravity. Measured as such, the bulk density FoM conveys information as to the specific gravity of the constituent particles and on the packing (i.e., the bulk relationship of the particles to one another). It is the FoM property most easily affected by handling of the simulant.

3. EVALUATION OF RECOMMENDED PROPERTIES VERSUS FIGURE OF MERIT

Table 1 contains the ranked properties from the 2005 workshop. It should be noted that neither rigorous definitions of these properties nor suggested measurement protocols or standards were provided.

Table 1. Properties from the 2005 Lunar Simulant Workshop, from table 2 in Sibille et al.[1]

Category		Category Properties Listing	
		Regolith Property	**Rank**
Geochemical (metered strength properties)		Compressive strength	10
Total number of ranked properties	11	Coefficient of friction	12
Number of properties in top 10	1	Shear strength	18
		Hardness	23
		Rheology	24
		Angle of repose	25
		Tensile strength	27
		Fracture behavior	28
		Impact resistance	32
Physical		Particle density	3
Total number of ranked properties	7	Bulk density	5
Number of properties in top 10	2	Porosity	13
		Thermal properties	20
		Surface area	21
		Friability	22
		Permeability	26
Grain specific		Grain size	1
Total number of ranked properties	6	Grain size distribution	2
Number of properties in top 10	4	Grain shape	7
		Magnetic grain properties	9
		Grain shape distribution	16
		Electrostatic charging	17
Chemical		Glass composition	4
Total number of ranked properties	6	Bulk chemistry	8
Number of properties in top 10	4	Reactivity as volatile/soluble minerals	14
		Surface reactivity (including damage)	29
Mineralogical		Mineralogical composition as function of grain size	6
Total number of ranked properties	4	Modal mineralogical composition	11
Number of properties in top 10	2	Soil texture	30
Multicategory		Implanted solar particles	15
Total number of ranked properties	2	Agglutinates with nanophase iron metal (nFe^0)	31
Number of properties in top 10	0		

The 2005 report uses the term grain for several basic concepts. The simulant development project has subsequently decided to explicitly restrict grain to mean a discrete subset of a particle.

In concept, a particle is a physically isolatable mass not chemically bonded to anything else. The grain commonly is a crystal of a mineral, but it can also be a piece of glass.

Table 2 presents relationships of properties to the FoM. Comments are provided for each parameter that is not explicitly a part of the FoM standard. In most cases the comments indicate the basic science explaining how the property is a derivative property. Also, where there are limitations to the assumptions or assertions made, some consideration of the limitations is given.

Table 2. Properties from 2005 workshop correlated to FoM properties by which they are directly addressed or from which they are derived.

Category Properties Listing Regolith Property	Particle Type	Particle Size Distribution	Particle Shape Distribution	Density	Not Addressed or Undefined
Compressive strength	▒	▒	▒	▒	
Coefficient of friction	▒	▒	▒	▒	
Shear strength	▒	▒	▒	▒	
Hardness	▒				
Rheology		▒	▒	▒	
Angle of repose		▒	▒	▒	
Tensile strength					X
Fracture behavior	▒				
Impact resistance	▒				
Particle density	▒				
Bulk density				▒	
Porosity		▒	▒	▒	
Thermal properties	▒	▒	░	▒	
Surface area		▒	▒		
Friability					
Permeability		▒	▒	▒	
Grain size		■			
Grain size distribution		■			
Grain shape			■		
Grain shape distribution			■		
Magnetic grain properties	▒	▒			
Electrostatic charging	░	░	░	░	
Glass composition	■				
Bulk chemistry	▒				
Reactivity as volatile/soluble minerals	▒	▒	▒	▒	X
Surface reactivity	▒	▒	▒	▒	X
Mineralogical composition as function of grain size	■				
Modal mineralogical composition	■				
Soil texture		▒	▒	▒	X
Implanted solar particles					X
Agglutinates with nFe^0	■				

Notes:

■	Property directly addressed by FoM
▒	Property derivative of FoM property
░	Property partially dependent on environment

3.1 Geomechanical (Mechanical Strength Properties)

3.1.1 Compressive Strength

This is a derivative property. It is a function of the particles' composition, size, shape, and how they are packed together. To the limit the FoM parameters can be measured in both the simulant and the lunar material, this property is tightly constrained by the FoM.

3.1.2 Coefficient of Friction

This is a derivative property. It is a function of the particles' composition, size, shape, and packing. To the limit the FoM parameters can be measured in both the simulant and the lunar material, this property is tightly constrained by the FoM.

3.1.3 Shear Strength

This is a derivative property. It is a function of the particles' composition, size, shape, and how they are packed together. To the limit the FoM parameters can be measured in both the simulant and the lunar material, this property is tightly constrained by the FoM.

3.1.4 Hardness

Hardness, as a geomechanical property, is ambiguous or undefined at best. In the 2005 workshop report, the context of usage is always with respect to a single particle. In the report, the usage is also with either the explicit statement or the assumption of mineral hardness as used by geologists. Assuming this is the intention of the term, the FoM particle type very tightly constrains this property. The limitation is the mechanical strength of lithic fragments and shattered particles. For this small minority of particles, the basic concept breaks down. In engineering, applications terms such as abrasiveness are substituted.

3.1.5 Rheology

Rheology is the branch of physics that deals with the deformation and flow of matter, especially the non-Newtonian flow of liquids and the plastic flow of solids. As used in the 2005 workshop report, "The rheological behavior (flow properties) of the regolith is a key property of the bulk material during excavation." The particle size and shape distribution and the bulk density largely determine the flow properties of a material.

3.1.6 Angle of Repose

The rheological behavior (flow properties) of the regolith is a key property of the bulk material during excavation. As an example, it manifests itself in the angle of repose of a regolith slope forming a trench or an erected berm. See section 3.1.5 of this Technical Memorandum (TM).

3.1.7 Tensile Strength

The varying types of tensile strength describe a material's reaction to stress and are defined as the maximum stress before rupture (breaking strength) or deformation (yield strength). The tensile strength of an individual particle is entirely constrained by the composition of the particle, although the properties may not have been adequately measured for some composite particles like breccias and agglutinates. Tensile strength of the bulk material is less well defined, but it should be a derivative of all of the four FoM characteristics.

3.1.8 Fracture Behavior

Fracture behavior of particles is driven by the particle type, specifically the hardness, cleavage, and fracture properties inherent in mineral and glass. These are addressed by the FoM and to some extent by particle shape. Whether and how particles fracture in bulk material, as a response to stress, is dependent on their size and packing.

3.1.9 Impact Resistance

Impact resistance should be akin to fracture behavior (section 3.1.8 of this TM).

3.2 Physical

3.2.1 Particle Density

If the particle type is known, this can be directly computed to high or very high precision. The limitation is for particles with large amounts of internal voids such as agglutinates and, to a lesser extent, shattered particles. The significance of this error for a bulk sample is estimated to be much less than 1%. For individual particles, it is estimated to be as high as 20%.

3.2.2 Bulk Density

This is an explicit part of the FoM standard. However, it is not rigorously defined in the 2005 recommendations.

3.2.3 Porosity

Porosity is a function of the particle type (due to vugs and voids in particles), shape and size distribution, and bulk density. It may not be uniquely constrained by these characteristics.

3.2.4 Thermal Properties

Thermal properties are derivatives of the particle type, size and shape distribution, and bulk density. Particles will have distinct conductive/insulating properties and the contact relationships between them will depend on size, shape, and bulk density.

3.2.5 Surface Area

Surface area is a function of particle size and shape distribution, and its bulk density will determine the surface area exposed in a given volume of material. Surface area is uniquely constrained by these parameters, but effective surface area defined as surface area available for contact is more largely dependent on the type of packing that may not be uniquely described by the bulk density parameter.

3.2.6 Friability

Most simulants are expected to be unconsolidated on the bulk scale and thus friability, defined as the tendency to reduce to finer particles under stress, is not applicable. Individual particles in a simulant or regolith such as breccias may be friable. Although friability and other measurements of mechanical strength are important considerations in simulant production, these properties of lunar regolith have not been measured adequately enough to simulate them.

3.2.7 Permeability

Permeability is a function of the particle shape and size distribution and bulk density. It may not be uniquely constrained by these characteristics.

3.3 Grain Specific

Size and shape are not defined by the 2005 workshop report. These concepts can only be given physical meaning by defining a specific method of measurement. Many of the measurement methods have physical meaning or are only applied to assemblies of particles.

3.3.1 Grain Size

This is an explicit part of the FoM standard.

3.3.2 Grain Size Distribution

This is an explicit part of the FoM standard.

3.3.3 Grain Shape

This is an explicit part of the FoM standard.

3.3.4 Magnetic Grain Properties

Magnetic properties derive from the mineralogy, grain or particle size, and environmental history of the particle. For example, heating above a material specific temperature will cause a radical change in magnetic response. Subsequent cooling will change it yet again. In lunar materials, particle composition should determine most of the magnetism of the bulk material, but this is complicated by the presence of nanophase iron metal (nFe^0) in the lunar regolith. At this time, nFe^0 is normally considered as a distinct solid phase independent of the commonly present Fe^0 derived from meteoritic sources. Nanophase Fe^0 is present in the agglutinates and in vapor-deposited nanoscale rims on particles. As of now, the nFe^0 in the agglutinates can only be partially reproduced, and that is at significant cost. The rims cannot be reproduced.

The FoM incorporates the mineral phase Fe^0. This was done to address both the meteoritic derived iron and the nFe^0. The FoM also explicitly incorporates the particle type agglutinate. It is concluded that when fully implemented, these two measures, with the other FoM characteristics, will reasonably cover the performance of lunar material and simulants. This is almost certainly true for first order and probably most second order measurements. It is acknowledged that this may not be the case for very high quality measurements due to the role of particle history. As there is so little applicable information of any kind on this topic for actual lunar material, inclusion of such a parameter in the current FoM would violate basic characteristics of a standard, being neither measurable nor known.

3.3.5 Grain Shape Distribution

This is an explicit part of the FoM standard.

3.3.6 Electrostatic Charging

This is not part of the FoM standard. There is little data on this parameter for lunar material. It is almost certainly dominated by the composition and size of the particles, which is addressed by the particle type and size FoM. The limitation on this is the effect of the vapor-deposited rims.

3.4 Chemical

3.4.1 Glass Composition

Glass composition is important to many applications like in situ resource utilization (ISRU) and fabrication. Theoretically, the particle type FoM measures abundance and composition of particles. The diverse populations of glass compositions in lunar regolith pose a unique problem for evaluation. In the first FoM software release, only glass abundance is included in the algorithm, though there are entry spaces for subclasses of glass. This allows the user to define populations of glass (basaltic glass, Ti-rich basaltic glass, etc.) in the reference and simulant. Future revisions to the FoM software will include a routine to compare the chemical composition of glass in the materials and the abundance of the glass.

3.4.2 Bulk Chemistry

This is an implicit part of the FoM standard. If the composition of the particles is known, the bulk chemistry of the particles is known. The limitation to this is a question of precision. The standardized list of minerals does not cover all possible minerals, nor does it attempt to specify glass composition other than to restrict it by normative mineralogy. The minor element (<1 wt. %) and trace element (<0.1 wt. %) chemistry of a material is less well determined by particle type composition, except for cases like phosphorous (P), which is specifically addressed by reporting the modal percent of phosphates—the only minerals in which it is likely to occur.

3.4.3 Reactivity as Volatile/Soluble Minerals

Although the meaning of this entry is not entirely clear in the 2005 workshop document, it seems to refer to volatile (e.g., hydroxyl (OH), water (H_2O), and carbon dioxide (CO_2))-bearing materials and halogen (fluorine (F), chlorine (Cl), bromine (Br), and iodine (I))-bearing materials.

3.4.3.1 Volatile-Bearing Materials. The presence of volatile-bearing materials in a simulant invokes a penalty to the composition FoM because correlative materials do not occur in lunar regolith. Furthermore, in revision 1 of the FoM software, these volatile-bearing minerals will populate their own subclass under the nonlunar minerals heading, and their presence will be weighted more than other nonlunar minerals due to their adverse affects on many ISRU processes.

3.4.3.2 Halogen-Bearing Materials. For halogen-bearing materials, the primary F- and Cl-bearing mineral in lunar regolith is the phosphate apatite. There is an entry for fluoroapatite on the FoM composition sheet; therefore, its presence, or lack thereof, will be assessed.

3.4.5 Surface Reactivity (Including Damage)

Surface reactivity is dependent on particle type (for reasons of chemistry) and on surface area (see section 3.2.5 of this TM). It is also dependent on the activation of a particle surface, a variable condition determined by particle lattice damage, lack or presence of adsorbates, and other characteristics. No general, measurable parameter correlates to this condition. Furthermore, it would seem to be a dynamic condition that would be difficult to impart to a bulk material by the manufacturer.

3.5 Mineralogical

3.5.1 Mineralogical Composition as Function of Grain Size

This is an explicit part of the FoM standard.

3.5.2 Modal Mineralogical Composition

This is an explicit part of the FoM standard.

3.5.3 Soil Texture

This is not defined and has many, many meanings. Some of the possible meanings are directly related to size and shape distribution and to material density.

3.6 Multicategory

3.6.1 Implanted Solar Particles

This is not addressed by the FoM as of this date. It is not considered practical or useful to add during simulant production. Reproduction of the process or result would likely be very expensive, and it seems best for the investigator to carry out treatment to replicate this property. This may change in the future.

3.6.2 Agglutinates With Nanophase Iron

The particle type FoM can address the presence of nFe^0 in the agglutinates. In version 1 of the software, data on the distributions of agglutinates are required. A subclass could be added of those agglutinates containing nFe^0 after this property is defined in the requirements document.

4. CONCLUSION

The FoM is considered to be a work in progress, both conceptually and in terms of algorithm and software development. It provides a reasonable and practical means to compare materials by addressing fundamental, inherent, measurable characteristics.

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14. ABSTRACT
A workshop held in 2005 defined a large number of parameters of interest for users of lunar simulants. The need for formal requirements and standards in the manufacture and use of simulants necessitates certain features of measurements. They must be definable, measureable, useful, and primary rather than derived. There are also certain features that must be avoided. Analysis of the total parameter list led to the realization that almost all of the parameters could be tightly constrained, though not predicted, if only four properties were measured: Particle composition, particle size distribution, particle shape distribution, and bulk density. These four are collectively referred to as figures of merit (FoMs). An evaluation of how each of the parameters identified in 2005 is controlled by the four FoMs is given.

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