MSFC ISRU & Dust Simulant Project Status

Lunar Regolith Simulant Workshop, Huntsville, AL Oct 10 – 12

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October 10, 2007

Key Logic

If we know the composition of the lunar particles, their sizes, shapes and packing density and if we can duplicate these four characteristics we will tightly constrain the performance of the simulant. Thus …

- Rather than trying to address a large number of properties as identified in the 2005 workshop we focus on a much more tractable problem.
- Rather than design a simulant to fit a user's desires we build to duplicate what is found on the Moon.

Paradigm

The simulant development effort is delivering an engineered product. Thus …

- Cost
- Schedule
- Performance
- Specifications
- Standards

Five Parallel Threads

Requirements

Figures of Merit

Characterization of Apollo Samples

Process Control

Feedstocks

Requirements Status

No change in draft text

List of minerals has been slightly modified.

Size

- Methodology has been settled on by committee
- Analysis to be done over three size ranges
- Draft text being generated by respective experts

Shape metrics also settled on by committee.

Discussion of shipping and remixing is ongoing.

Question has been raised of creating a separate “Simulant User’s Handbook” This might reduce the need for consultation with geologic experts and might incorporate a “Fit and Purpose” matrix

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Minerals

• Anorthite	- An_{90+}	• Spinel	- Low grade gem material
• Olivine	- Fo_{50-72}	• Hercynite	-
• Clinoenstatite	-	• Ulvospinel	-
• Pigeonite	-	• Chromite	-
• Hedenbergite	-	• Troilite	- Use pyrrhotite
• Augite	-	• Whitlockite	- Use beta tri-calcium phosphate
• Enstatite	- En_{70-85}	• Apatite	- Fluoro-, not hydroxy-
		• Ilmenite	- Low hematite
		• Iron	- Present in multiple forms

Figures of Merit

Led by Hans Hoelzer of TBE

Algorithm defined and logic published

Algorithm and user interface coded.

Awaiting values from Apollo and simulants for further testing and development

Expect to have first runs completed and released by end October, 2007

Apollo Samples

Lead by ARES

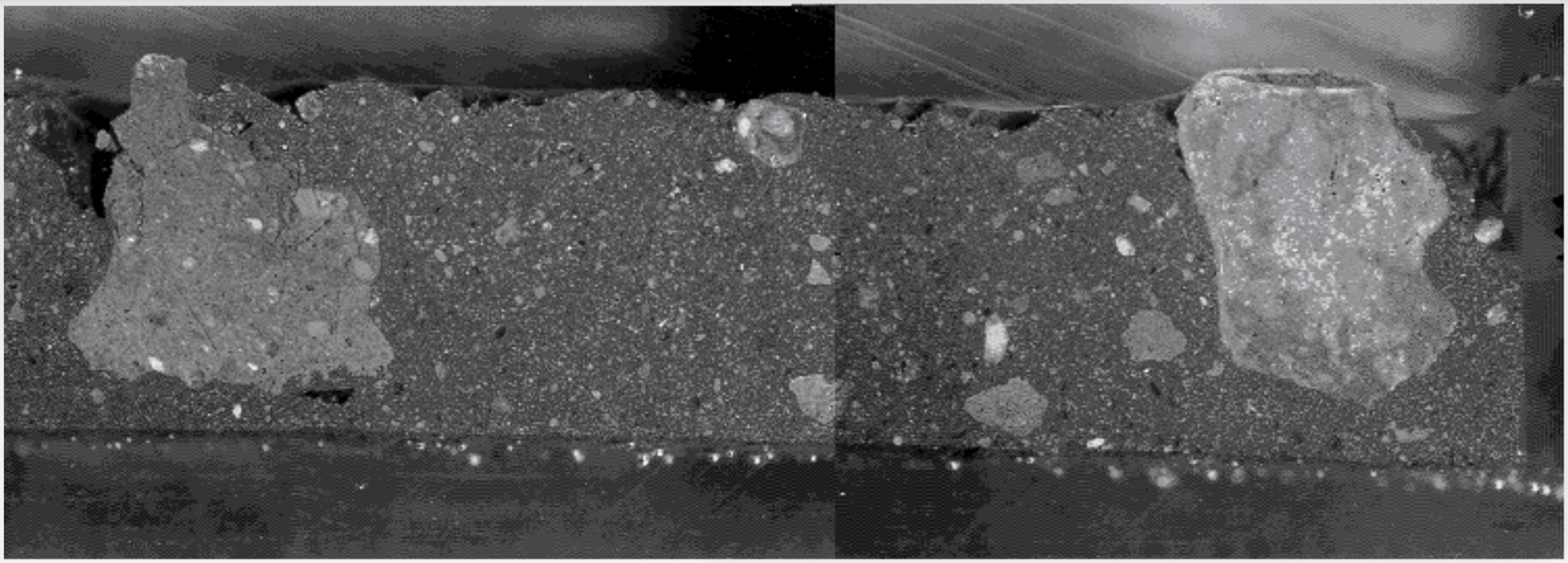
Searched and compiled existing literature and data

Curatorial staff scanning and loading data about cores to web

Discussing how to make the needed measurements

Key performance parameters discussion to begin. The requirement is to deliver a statement of what needed measurements of Apollo materials are or are not available

Apollo Drill Core



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Process Control

Led by Steve Wilson of the USGS

Glass manufacturing capability demonstrated

Pseudo-agglutinate manufacturing capability demonstrated

NU-LHT-1M – Completed, surplus released for use.

NU-LHT-2M

- Improved size distribution, trace and minor mineral fidelity
- Early December – January
- 500 – 1000 pounds, amount tbd

NU-LHT-1C – Spring 2008 ($ dependant)

Documenting methodology and process variables

High specific gravity, basaltic base, dust prototypes

Investigating synthesis processes

Naming Convention

NU	NASA/USGS (producer)
L	Lunar (Planetary body)
HT	Highlands Type (type of simulant)
1	Series (which simulant generation) 1,2,3, ...
M	Particle size (C coarse, M medium, D dust)

Thus the pilot material was named NU-LHT-1M

Size Ranges (maximum particle size)

Dust	- up to 20μm
Medium	- up to 1mm
Coarse	- ≥ 4cm

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Feedstocks

Led by Doug Stoeser of the USGS

Constrained the mineral list

Identified the Stillwater layered mafic intrusive for prototyping

Seeking commercial sources for each of the identified minerals

- Mining Industry, including quarries
- Dimension stone
- Mineral dealers (Wards, specimens, gems)

Mineral Separates

Other Major Players

Orbitec -

- JSC-1A production
- High fidelity agglutinate production

NORCAT - Developing OB-1

LASP - Geotechnical properties

GRC - Characterization

KSC - Characterization

Volunteer Contributions

Stillwater Mining Company

Iluka Exploration

Malvern Instrument

Additional Topics

ISO – International Standards Development

Synthesis of a dust simulant

Acquisition of a small quantity of pure minerals

Caveats and Warnings

Toxicity by Geoff Plumlee of USGS

Presence of P, S, Cl, F

Presence of H_2O and (OH)

Nanophase iron and vapor phase deposits

“Activation” - whatever that is

Implanted ions

Mechanical locking of multiple crystals within a particle

It is astounding how much is know in general about the lunar regolith and just as astounding how little is known in specific!

Even less is known about the dust fraction!!

Backups

BACKUPS FOLLOW

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Terms

Regolith - Broken rock of any size

Dust - Regolith smaller than 20 micrometers

Why Create Standards?

ASTM A269 Austenitic Stainless Steel vs. ASTM 3033 Aluminum

Figures of Merit, Synopsis

- Four characteristics
  1. Particle Composition
     a) Lithic Fragments
     b) Mineralogy
     c) Glass
     d) Agglutinate
  2. Size Distribution
  3. Shape (may subdivide this)
  4. Density
- Measurement methods are stipulated
- Compares simulant to specific Apollo regolith samples (core and/or surface samples)
- As needs change, requirements and FoMs may be added, deleted or modified.

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Concept

A *Figure of Merit* (FoM) is an algorithm for quantifying a single characteristic of a simulant and provides a defined measure of how a simulant and reference material compare.

Definition 1 - Composition

The *Figure of Merit* termed “composition” defines the geologic constituents of the simulant without reference to textural features, such as particle shape and particle size.

Composition includes the following constituents:

- lithic fragments,
- mineral grains,
- glasses and
- agglutinates.

Composition addresses the mineralogic and chemical makeup of the simulant. The *Simulant Requirements Document* (Rickman and Howard, 2006 draft) specifies the rock types, minerals, glass composition which may or may not be used to establish a simulant.

Vector Expression

The composition of a material (reference or simulant) may be viewed as a vector of the fractions of the various constituents of the material.

Observation 1 - The elements of a composition vector must necessarily sum to unity (the sum of the fractional parts must equal the whole) **excluding** contaminants. Mathematically, this may be stated as the L1-norm of a composition vector is always 1.

Observation 2 - A composition vector always terminates on a line (2 dimensions), a plane (3 dimensions) or hyper-plane (4 or more dimensions) which intersects the composition space coordinate frame axes at the unity coordinate points. This follows from the fact that we may write the following equation for the L1 norm of the composition vector:

$$x+y+z = 1$$

where x is the fraction of the 1st component, y is the fraction of the 2nd component, z is the fraction of the 3rd component… which is the defining equation for a hyper-plane.

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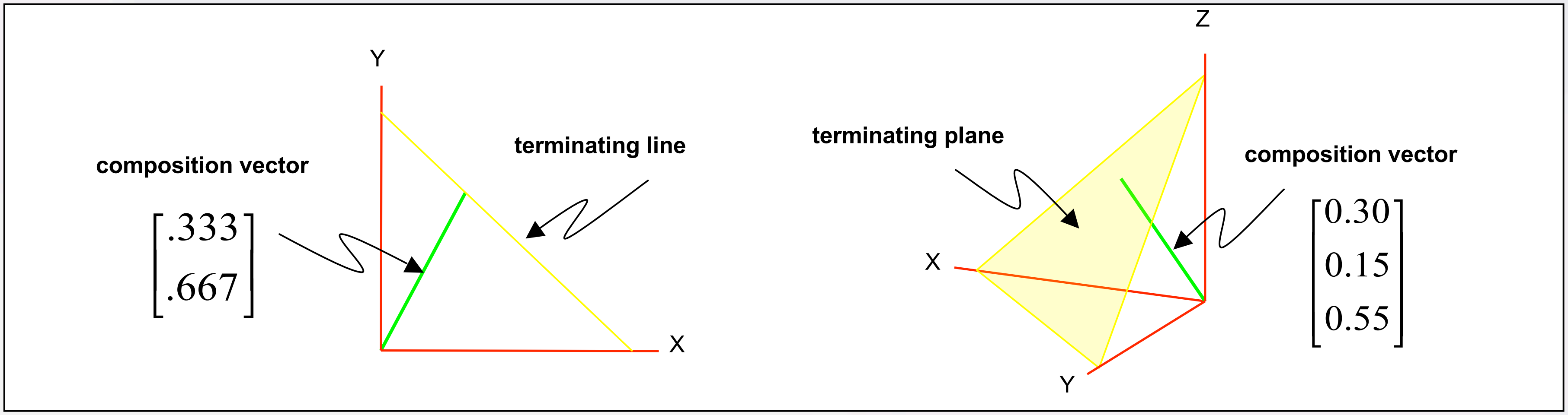
Vector Expression, part 2

Observation 3 - The components of the composition vector are always positive (negative fractions of composition are not allowed), which results in the terminating hyper-plane always lying in the first quadrant. These observations are shown geometrically for the case of 3 dimensions.



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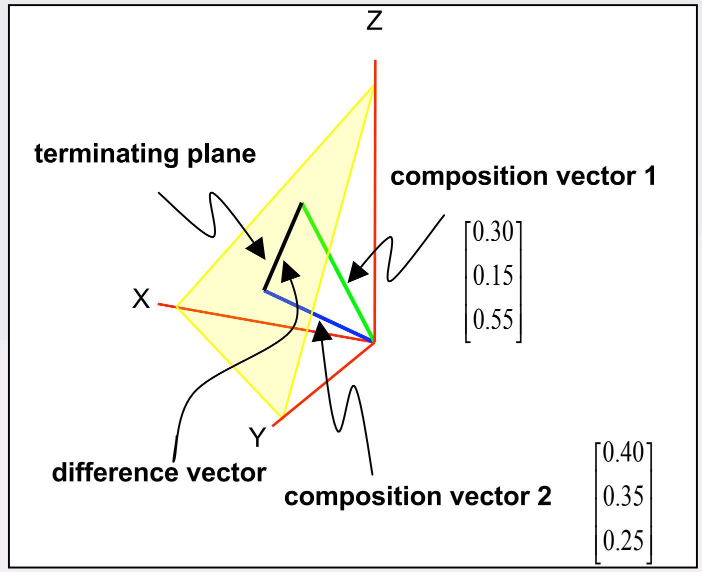
Graphical Representation

Remember a *Figure of Merit* is a comparison of a reference material to an actual material or better, the comparison of two materials.

The *Figure of Merit* (r) is defined as the normalized difference of two composition vectors subtracted from unity. Normalization forces the difference of two composition vectors to lie between 0 and 1, and subtraction from unity results in a *Figure of Merit* of 1 for a perfect match to 0 for no match at all (as opposed to the other way around).



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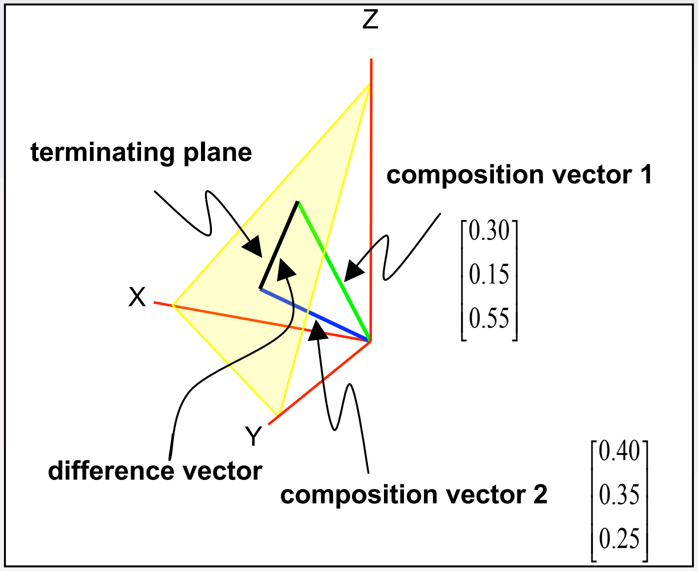
Normalization

The difference of two composition vectors must always lie in the terminating hyper-plane (because this is where both vectors terminate).

It is obvious that the maximum difference between two vectors results if one material is entirely of one composition, and the other entirely of another. The two composition vectors for such a case would lie along any two of the coordinate frame axes defining the composition coordinate space (and would necessarily be orthogonal).

Two such vectors form the sides of an isosceles triangle, whose hypotenuse is of length $\sqrt{2}$ since the length of each composition vector is 1. Thus the maximum difference between any two composition vectors is $\sqrt{2}$ and this is the normalization factor for their difference.



Weighting

The *Figure of Merit* defined for composition also has a weighting vector to weight the composition vector difference. This allows favoring certain components of composition over others. This is equivalent to scaling the axes of the composition space, which has the result that the maximum difference between two different compositions may be other than $\sqrt{2}$

However, it may be shown that in this case the maximum difference between two different composition vectors is the square root of the sum of the squares of the two largest weights:

$$\textit{normalization factor} = \sqrt{\max_1{}^2(w) + \max_2{}^2(w)},$$

Where $\max_1{}^2(w)$ is the ith largest element of the weighting vector *w* whose weighted square will be computed for the *Figure of Merit*

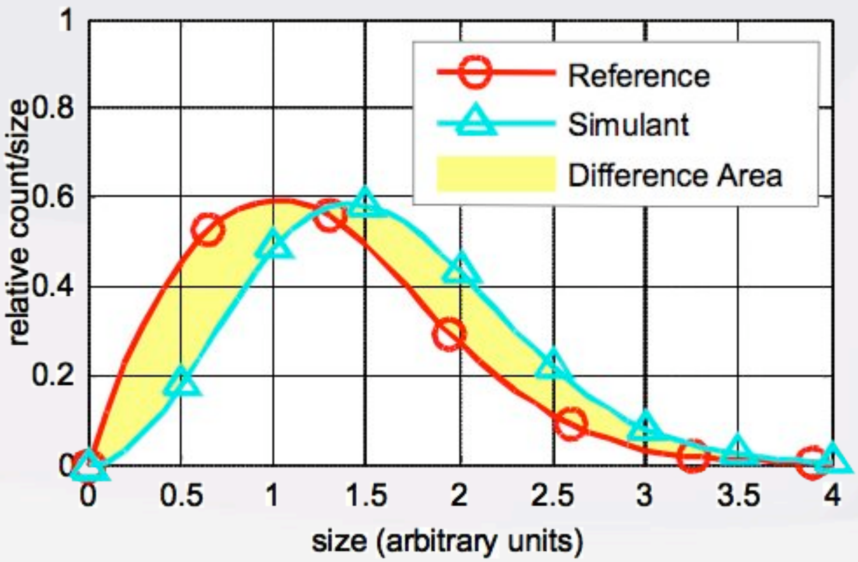
Definition 2 - Particle Size

The *Figure of Merit* for particle size distribution is similar to the one for composition. In place of composition vectors, we have particle size relative frequency distributions for the two materials under comparison.

The process is reminiscent of a least squares fit, the difference being that we compute the sum of the squares of the difference, rather than minimize it.

1. Compute the square root of a weighted sum of the squares of the difference between the two distributions (an integral),
2. normalize by the maximum possible square root of the weighted sum of the squares of the difference and
3. subtract from unity,

The figure shows the difference area in yellow.



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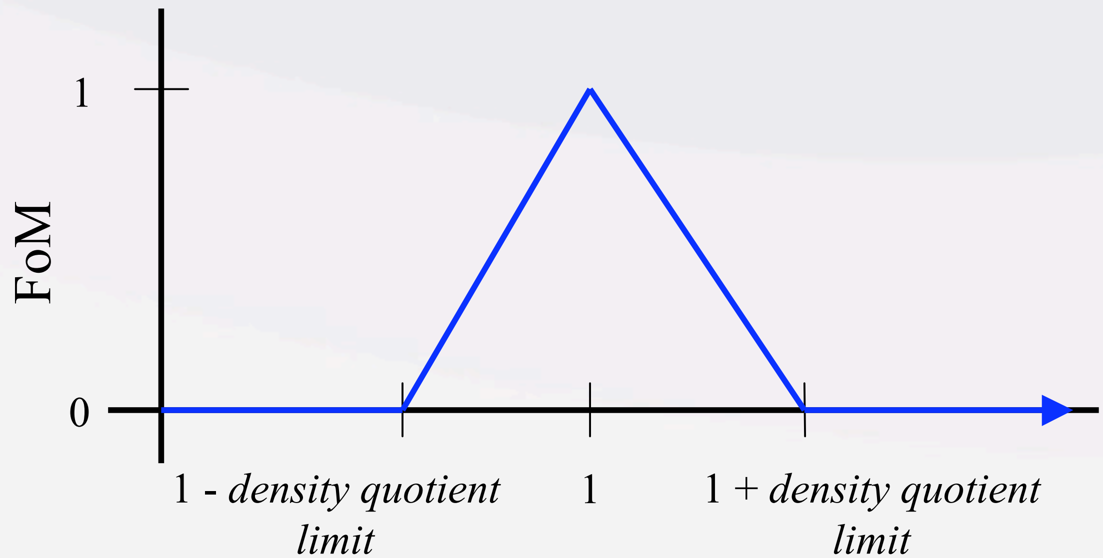
Definition 3 - Density

The *Figure of Merit* for density (there are several possible) is computed from the ratio of the densities of two materials. A penalty factor (whose magnitude is between 1 and 0 depending on the distance from 1) is used to force the quotient to go to zero at a user specified point.

The density *Figure of Merit* graphically is



Implications and Comments

FoMs are critical to defensible specifications for procurement of simulant. Some users will need higher FoMs than others. Note a FoM is a tolerance.

- Numbers approaching 1 are better reproductions of the reference material. This implies:

  - closer tolerances
  - additional quality control in
    - collection, processing, and blending,
  - and particular attention to minimizing contamination.

- Potential vendors may use offsite analytical techniques to verify the simulant FoMs.

- Tighter production tolerances or secondary processing are expected to drive higher costs to the end user.