Lunar Regolith Figures of Merit

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Agenda

- A quick review of Figures-of-Merit (FoM)
  - Composition
  - Size distribution
  - Shape
  - Density
- Software Implementation of FoM Algorithms
  - Components of the software
  - Inputs to the software
- Demonstration of the software
- Backup slides

A Quick Review of Figures-of-Merit

Characterization of Simulant Materials

- A method is needed to specify simulant requirements and simulant suitability for a given purpose and to compare simulants to reference materials and other simulants.

- D. Rickman has postulated that a simulant may be characterized by the following four quantities:
  - material composition
  - particle size distribution
  - particle shape
  - material density.

- This leads to the search for methods of specifying and comparing materials in terms of these four quantities.

Figures of Merit (FoM)

- A FoM is conceptually an algorithm for quantifying a single characteristic of a simulant and provides a clear measure of how well a simulant and reference material compare.
- The human mind can only compare and rank scalars. Thus, to compare more complex quantities, a method (algorithm) must be devised that boils the complex quantity down to a scalar.
- In our context a FoM is a measure of how well a characteristic of a simulant material compares to a reference material.
- For simulant specification and comparison, there are four FoMs for the quantities *composition*, *size*, *shape,* and *density*.

Modal Composition

- Composition defines the geologic constituents of a simulant without reference to textural features, such as particle shape and particle size.

- Composition includes the following classes of constituents:
  - lithic fragments
  - mineral grains
  - glasses
  - agglutinates

- Conceptually, composition addresses the chemical makeup of individual particles.

- Composition may be a function of the size of the particles.

Size Distribution

- Size distribution refers to the distribution of particle sizes.
- We will use the term Relative Frequency Distribution (RFD) to refer to the particle size distribution of a material.

Shape

- Measures for shape are still under development but may include:
  - mean width
  - mean shape factor
  - mean aspect ratio
  - convexity
- A FoM for shape is still under development and may influence how shape is defined and measured.

Density

- Density refers to the average weight per unit volume of a material.

Figures-of-Merit Usage

- The FoMs have been constructed to lie in the range 0 to 1, with 0 indicating a poor or no match and 1 indicating a perfect match.
- The FoM may be used for specification by stating the value a simulant's FoMs must attain to be suitable for a given application.
  - As an example, for composition, an FoM of 0.75 might be quite suitable for road building experiments, while an FoM of 0.98 might be required for chemistry experiments
- The FoM methodology may be used to compare various simulants from different vendors, production runs, and different kinds of simulant.
- The FoM of a simulant may be used during production for quality control.

Algorithms for the FoMs - Some Preliminaries

Reference Material

- Reference material refers to the *desired* composition, size, shape, or density of a material.

- The composition, size, shape, or density of a reference material usually mirrors that of an actual material but does not have to.
  - A reference material may be completely hypothetical

- As such, a reference material may be used for specification of a simulant.

- A simulated material may also be compared to the reference material.
  - The simulated material should match to the degree specified, the reference material.

Modal Composition

- The composition of a material (reference or simulant) is defined as a *vector* of the fraction of the various constituents of the material.

- Composition may be defined at multiple levels of granularity, starting with the composition in terms of the four basic classes of constituents, lithic fragments, minerals, glasses, and agglutinates.
  - Each class may be sub-divided into sub-constituents as necessary for a particular application.
  - This process may be repeated for multiple levels, but the level of detail need not be uniform across the various classes and sub-constituents or between two materials.
  - The elements of a composition vector must necessarily sum to unity (the sum of the fractional parts must equal the whole) excluding contaminants.

- Composition may also be defined as a function of size, so that a composition definition for a substance consists of a set of vectors for various different particulate sizes, one vector for each of the various particle sizes or range of particle sizes.

Modal Composition FoM

- The Figure-of-Merit is defined as the scaled L1 Norm of the difference of two composition vectors subtracted from unity.

- Scaling (normalization) forces the norm of 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).

$$FoM = 1 - \frac{\left\| w_{adjusted} \left(c_{adjusted\ reference} - c_{adjusted\ simulant} \right) \right\|_1}{\left\| w_{adjusted}\, c_{adjusted\ reference} \right\|_1 + \left\| w_{adjusted}\, c_{adjusted\ simulant} \right\|_1}$$

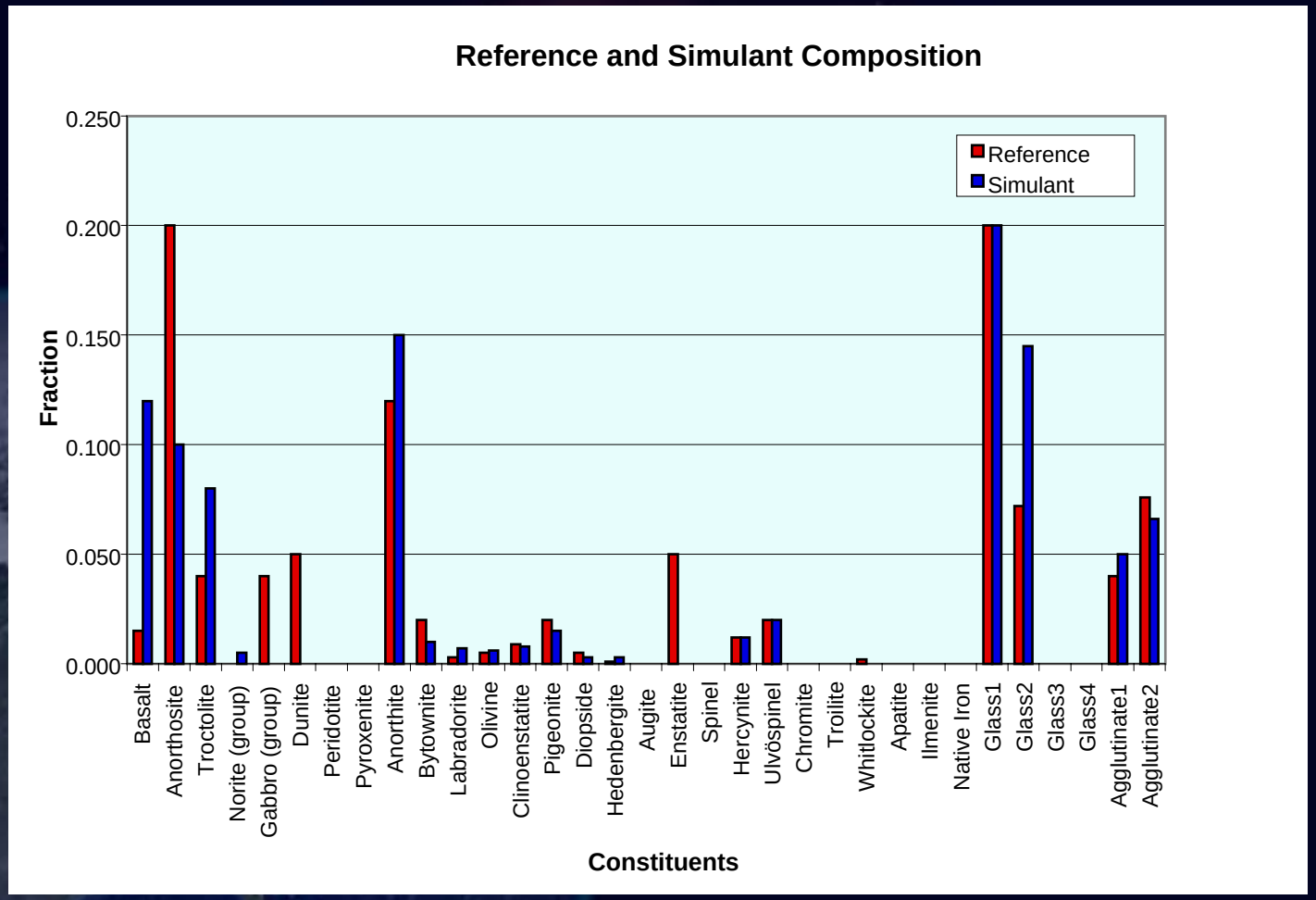
$$= 1 - \frac{\sum_i w_{adjusted_i} \left| \left(c_{adjusted\ reference_i} - c_{adjusted\ simulant_i} \right) \right|}{\sum_i w_{adjusted_i} c_{adjusted\ reference_i} + \sum_i w_{adjusted_i} c_{adjusted\ simulant_i}}$$

$\|w\|_1$ *denotes the L1 norm of vector w*

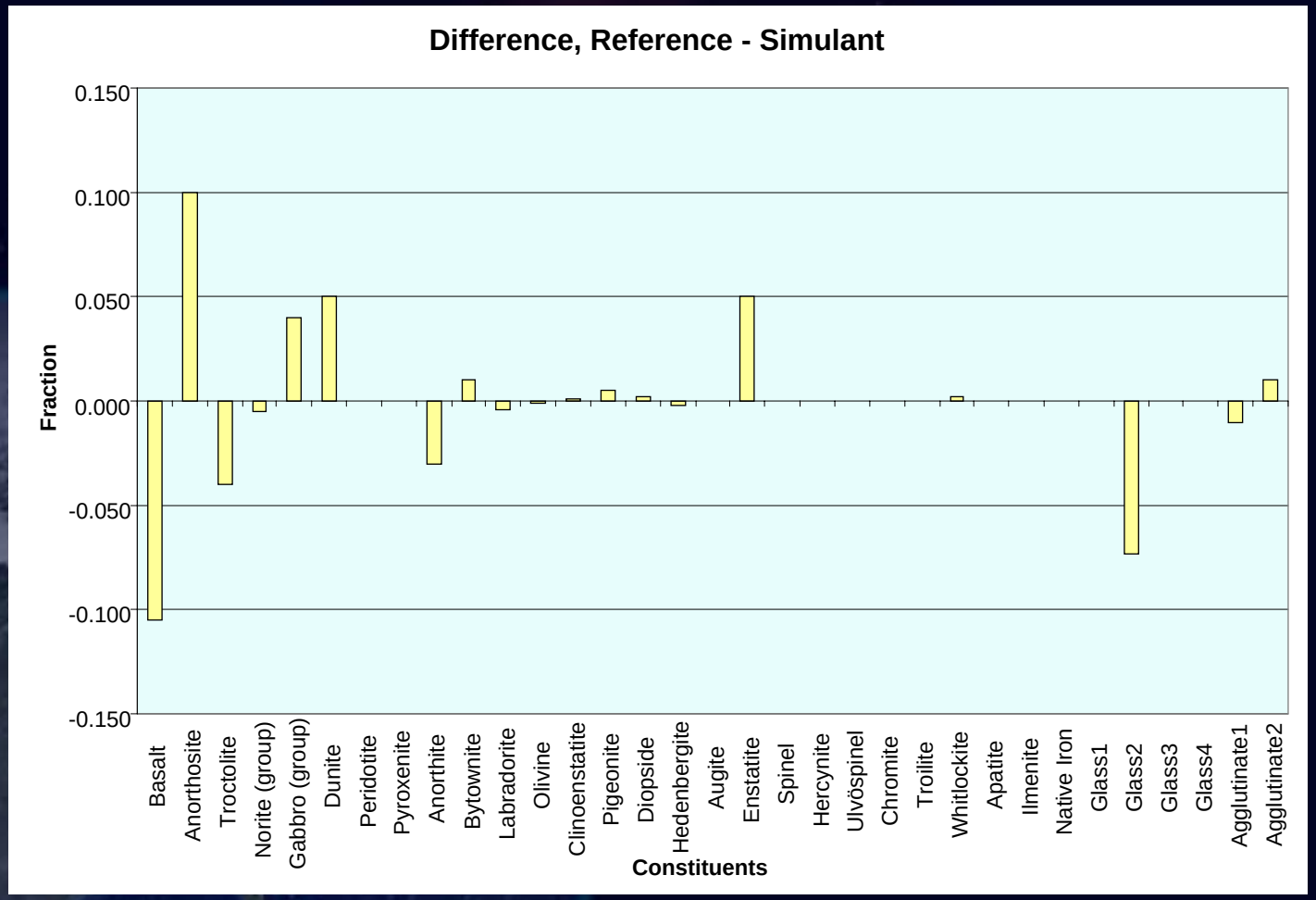
- The L1 Norm of a vector is defined as the sum of the absolute values of the elements of the vector.

Composition FoM

Composition vectors displayed as a bar chart (example)



Composition FoM
Difference of composition vectors (example)



Modal Composition FoM Interpretation

- The Figure-of-Merit for modal composition may be interpreted as:

"the fraction of material that is the same in both materials".

- As an example suppose you had a reference material which consists of 60 red marbles, 30 green marbles 10 blue marbles and a simulant material which consist of 40 red marbles, 10 green marbles and 50 blue marbles. How do these compare? Well, the figure-of-merit would be 0.6

- Now, of the red marbles, each material had at least 40, of the green marbles, each material had at least 10 and of the blue marbles each material had at least 10, so the two materials have 60 marbles in common out of 100 marbles, or, 0.6 of the marbles in each material are the same.

Size Distribution FoM

- The Figure-of-Merit is defined as the scaled L1 Norm of the difference of two RFDs subtracted from unity.

$$FoM = 1 - \frac{\left\| w\left(RFD_{reference} - RFD_{simulant} \right) \right\|_1}{\left\| wRFD_{reference} \right\|_1 + \left\| wRFD_{simulant} \right\|_1}$$

$$FoM_{before\ constraints} = 1 - \frac{\int w \left| RFD_{reference} - RFD_{simulant} \right|}{\int w \left| RFD_{reference} \right| + \int w \left| RFD_{simulant} \right|}$$

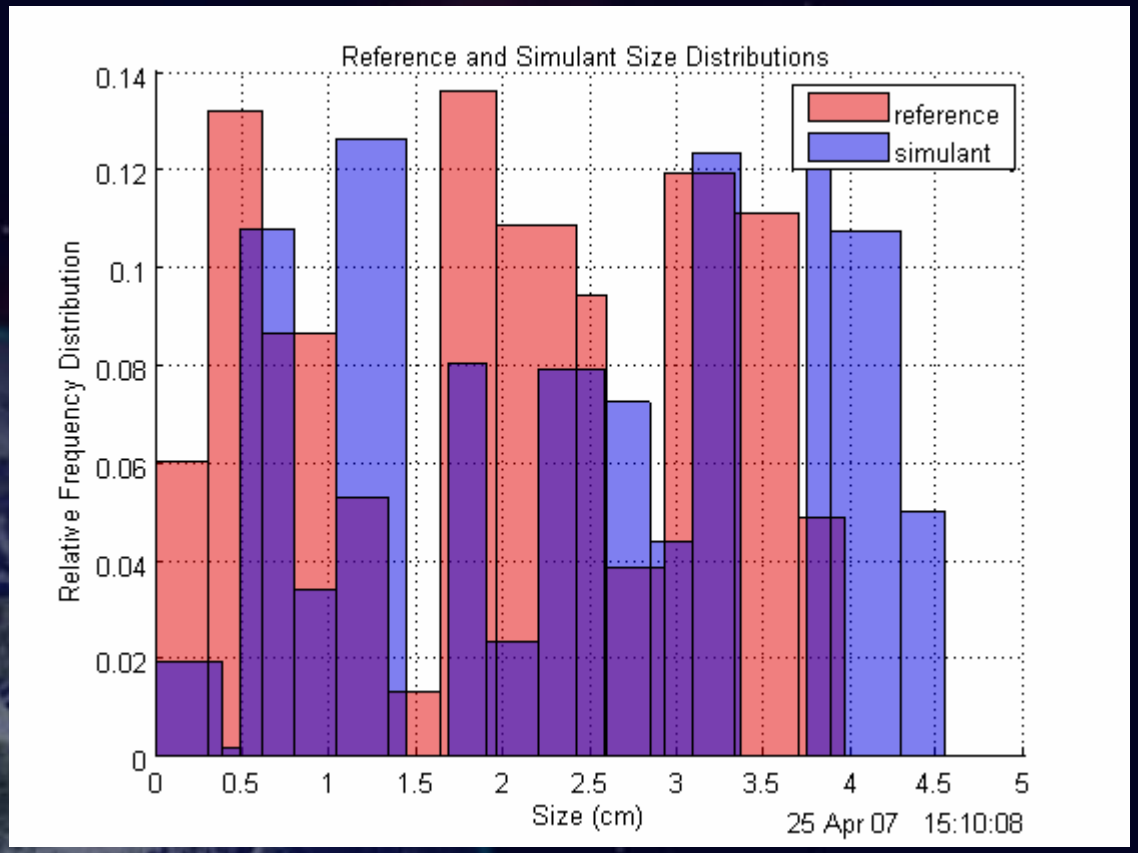
- The FoM is further subject to a maximum error constraint:

$$FoM = \begin{cases} FoM_{before\ constraints} & if \quad \left| RFD_{reference} - RDF_{simulant} \right| \le max_RFD_difference \\ 0 & otherwise \end{cases}$$

- The L1 Norm of a function is defined as the integral of the absolute value of the function.

Size Distribution FoM

Histogram of relative frequency as a function of size



Size Distribution FoM Interpretation

- The Figure-of-Merit for size distribution may be interpreted as:

“the fraction of particle sizes that both materials have in common”.

Density

- Density refers to the average weight per unit volume of a material.

- Density shall be measured by taking a sufficiently large enough sample so that the sample follows the particle size distribution of the material as defined in the slides on Size Distribution.
  - This avoids biasing the value of the density to the density of an aggregate of small particles that may pack more closely or an aggregate of large particles that may pack more loosely than an aggregate of particles that follows the particle size distribution as defined in the slides on Size Distribution.

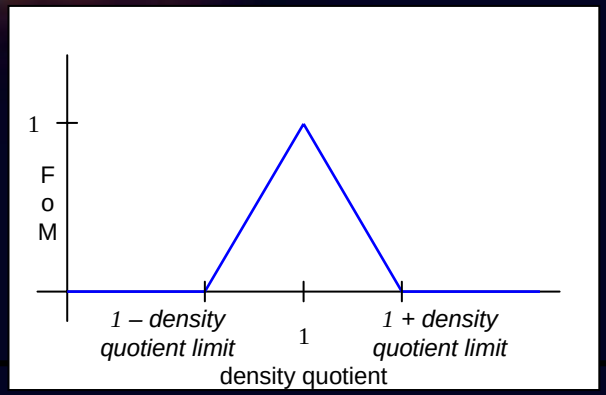
Density FoM

- The Figure-of-Merit for how closely a simulant matches a reference is proportional to the ratio of the densities.

- Ratios of less than 1 – *density quotient limit* or greater than 1 + *density quotient limit* correspond to an FoM of 0, while a ratio of 1 corresponds to an FoM of 1.

- Mathematically and graphically this may be expressed as:

$$FoM = \begin{cases} \dfrac{1}{density\ quotient\ limit}\left(\dfrac{simulant\ density}{reference\ density}\right) + \dfrac{density\ quotient\ limit - 1}{density\ quotient\ limit} \\ \quad for\ 1 - density\ quotient\ limit \le \dfrac{simulant\ density}{reference\ density} < 1 \\ \\ \dfrac{-1}{density\ quotient\ limit}\left(\dfrac{simulant\ density}{reference\ density}\right) + \dfrac{density\ quotient\ limit + 1}{density\ quotient\ limit} \\ \quad for\ 1 \le \dfrac{simulant\ density}{reference\ density} < 1 + density\ quotient\ limit \\ \\ 0 \quad otherwise \end{cases}$$



Software Implementation of FoM Algorithms

Components of the Software

The software that implements the Figures-of-Merit consists of three parts:

- An input editor – we use Microsoft Excel for this purpose.
- A back end that computes the Figures-of-Merit – we use The MathWorks Matlab for this purpose.
- A front end with which the user interacts that opens and reads the Excel input files, performs checks on the inputs, and calls the Matlab routines for computation of the FoMs – this is custom code.

What the FoM Software Is and Is Not

- Given input data on the composition, size distribution, shape, and density of two materials, the FoM software computes the Figures-of-Merit discussed in this presentation.

- The software itself DOES NOT contain any data; it is not a database, only a computational engine.

Inputs - Composition

Microsoft Excel - FOM Template.xls

Composition

Short Instructions

	Size Range 1		Size Range 2		Size Range 3		Size Range 4		Size Range 5		Size Range 6		Size Range 7		Size Range 8	
	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit
size																
units																
Sum of Components (computed - must sum to unity)																
	fraction	importance	fraction	importance	fraction	importance	fraction	importance	fraction	importance	fraction	importance	fraction	importance	fraction	importance
Lithic Fragments	0.000		0.000		0.000		0.000		0.000		0.000		0.000		0.000	
Total (no further breakdown)																
Basalt																
Anorthosite																
Troctolite																
Norite (group)																
Gabbro (group)																
Dunite																
Peridotite																
Pyroxenite																
Mineral Grains	0.000		0.000		0.000		0.000		0.000		0.000		0.000		0.000	
Total (no further breakdown)																
Anorthite																
Bytownite																
Labradorite																
Olivine																
Clinoenstatite																
Pigeonite																
Diopside																
Hedenbergite																
Augite																
Enstatite																
Spinel																
Hercynite																
Ulvöspinel																
Chromite																
Troilite																
Whitlockite																
Apatite																
Ilmenite																
Native Iron																
Glasses	0.000		0.000		0.000		0.000		0.000		0.000		0.000		0.000	
Total (no further breakdown)																
Glass1																
Glass2																
Glass3																
Glass4																

Units		
µm	micrometer	10
mm	millimeter	10
cm	centimeter	10

Short Instructions

For up to 8 Size Ranges
the following data (a Figu
for each Size Range):

1) The lower and upper li
25, 50).

2) The units for the sizes
down menu. (e.g. micron

3) The fraction of each co
B. If only level A composit
specified, enter the fractio
further breakdown).

4) For Reference sample
component should be sp
theses fields are not use

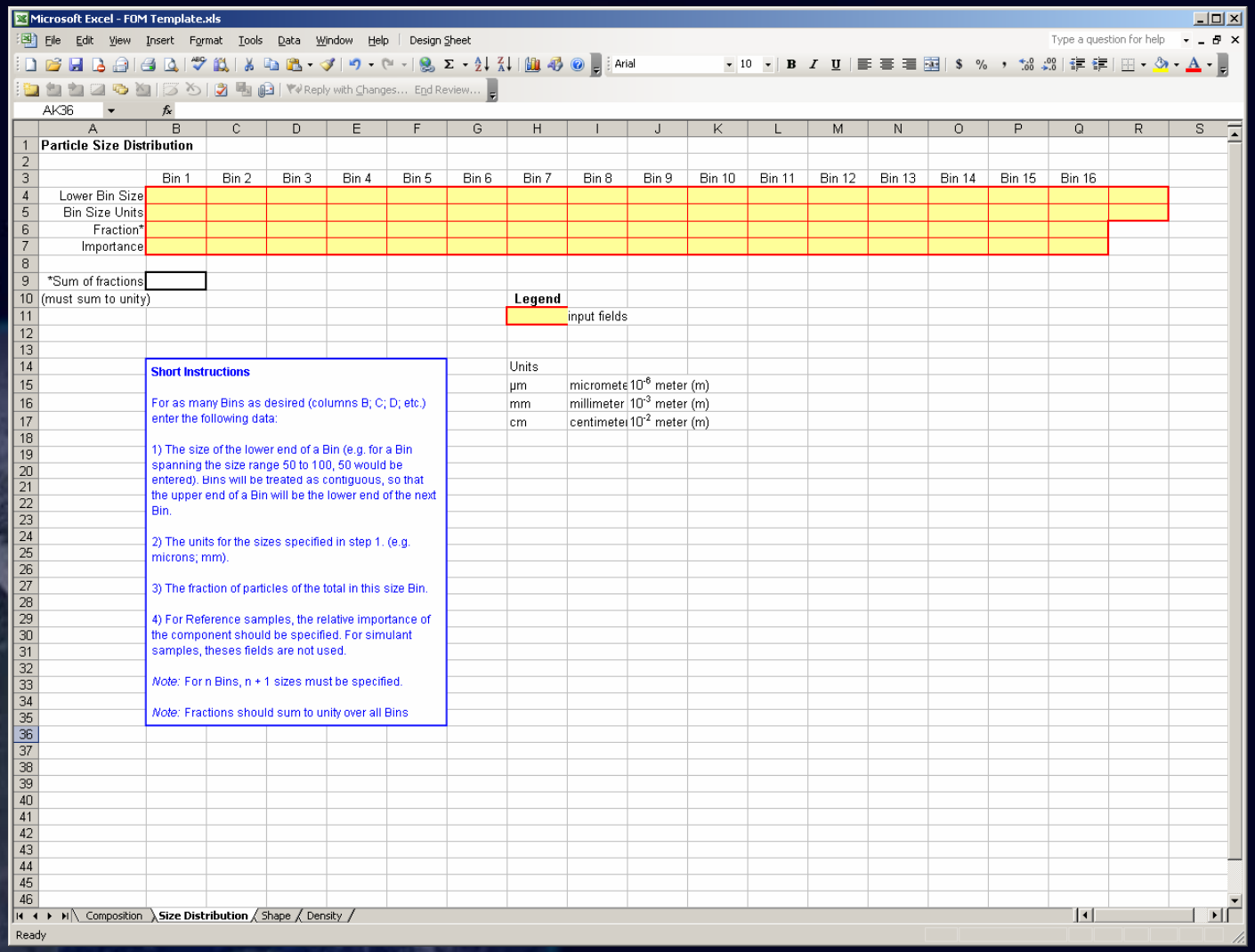
5) For Glasses and Aglut
etc. with a more detailed

Note: Only fractions at th
higher levels are comput

Composition | Size Distribution | Shape | Density

Ready

Inputs – Size Distribution



Microsoft Excel - FOM Template.xls

Particle Size Distribution

	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10	Bin 11	Bin 12	Bin 13	Bin 14	Bin 15	Bin 16
Lower Bin Size																
Bin Size Units																
Fraction*																
Importance																

*Sum of fractions (must sum to unity)

Legend

input fields

Units		
µm	micromete	10^{-6} meter (m)
mm	millimeter	10^{-3} meter (m)
cm	centimeter	10^{-2} meter (m)

Short Instructions

For as many Bins as desired (columns B; C; D; etc.) enter the following data:

1) The size of the lower end of a Bin (e.g. for a Bin spanning the size range 50 to 100, 50 would be entered). Bins will be treated as contiguous, so that the upper end of a Bin will be the lower end of the next Bin.

2) The units for the sizes specified in step 1. (e.g. microns; mm).

3) The fraction of particles of the total in this size Bin.

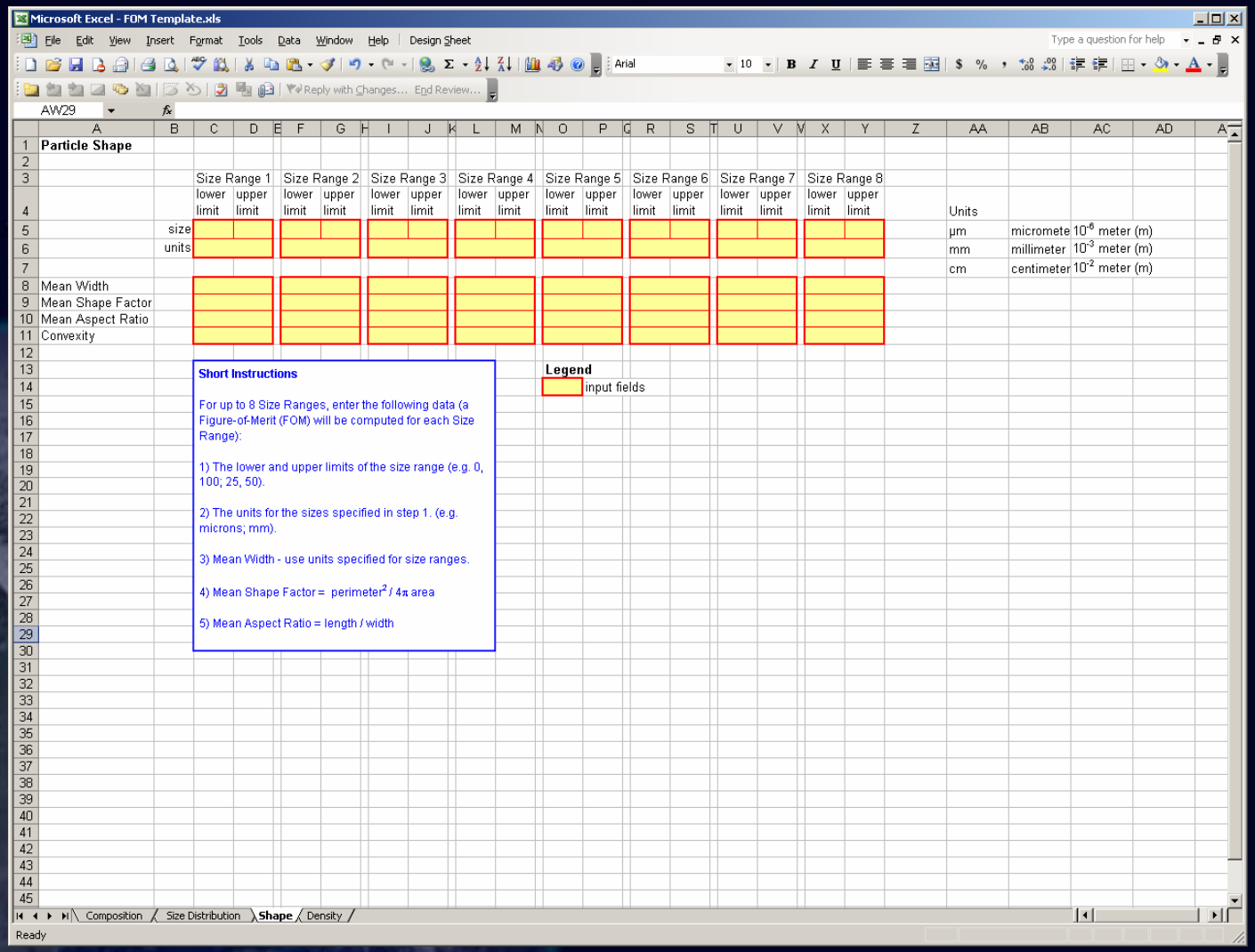
4) For Reference samples, the relative importance of the component should be specified. For simulant samples, theses fields are not used.

Note: For n Bins, n + 1 sizes must be specified.

Note: Fractions should sum to unity over all Bins

Composition | Size Distribution | Shape | Density

Inputs - Shape



Microsoft Excel - FOM Template.xls

Particle Shape

	Size Range 1		Size Range 2		Size Range 3		Size Range 4		Size Range 5		Size Range 6		Size Range 7		Size Range 8	
	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit
size																
units																
Mean Width																
Mean Shape Factor																
Mean Aspect Ratio																
Convexity																

Units		
µm	micromete	10^{-6} meter (m)
mm	millimeter	10^{-3} meter (m)
cm	centimeter	10^{-2} meter (m)

Short Instructions

For up to 8 Size Ranges, enter the following data (a Figure-of-Merit (FOM) will be computed for each Size Range):

1) The lower and upper limits of the size range (e.g. 0, 100; 25, 50).

2) The units for the sizes specified in step 1. (e.g. microns; mm).

3) Mean Width - use units specified for size ranges.

4) Mean Shape Factor = perimeter^2 / 4π area

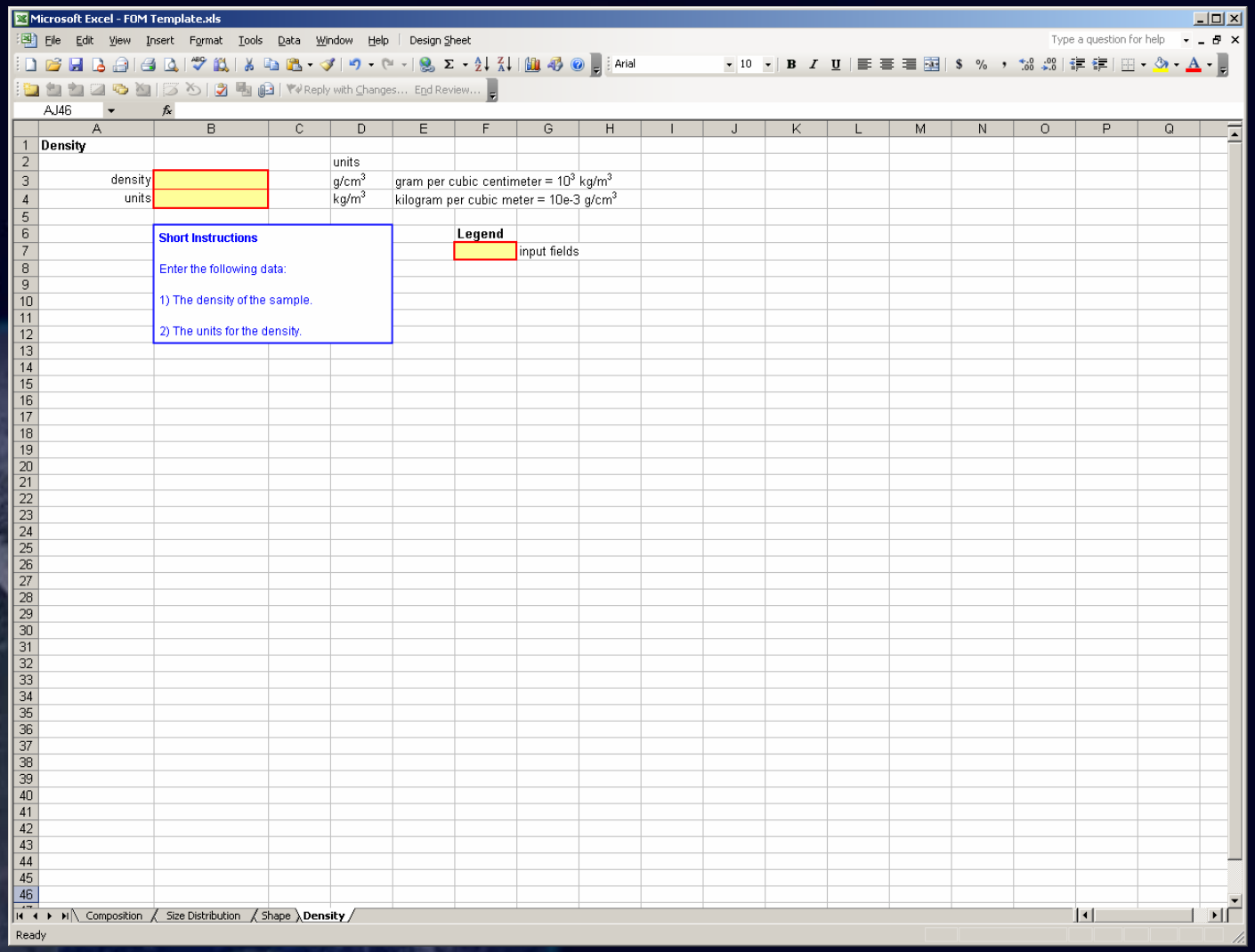
5) Mean Aspect Ratio = length / width

Legend

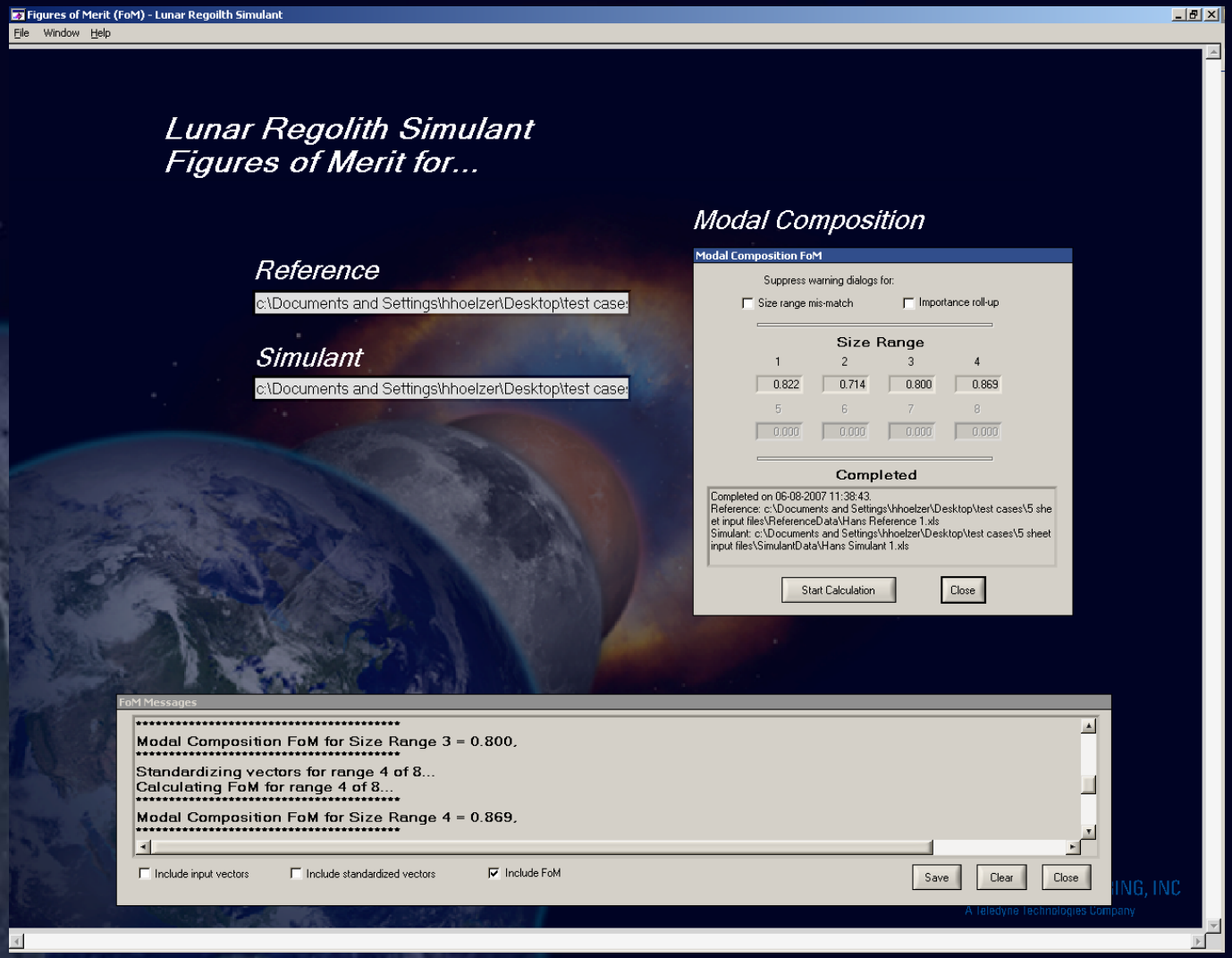
input fields

Composition / Size Distribution / Shape / Density

Inputs - Density

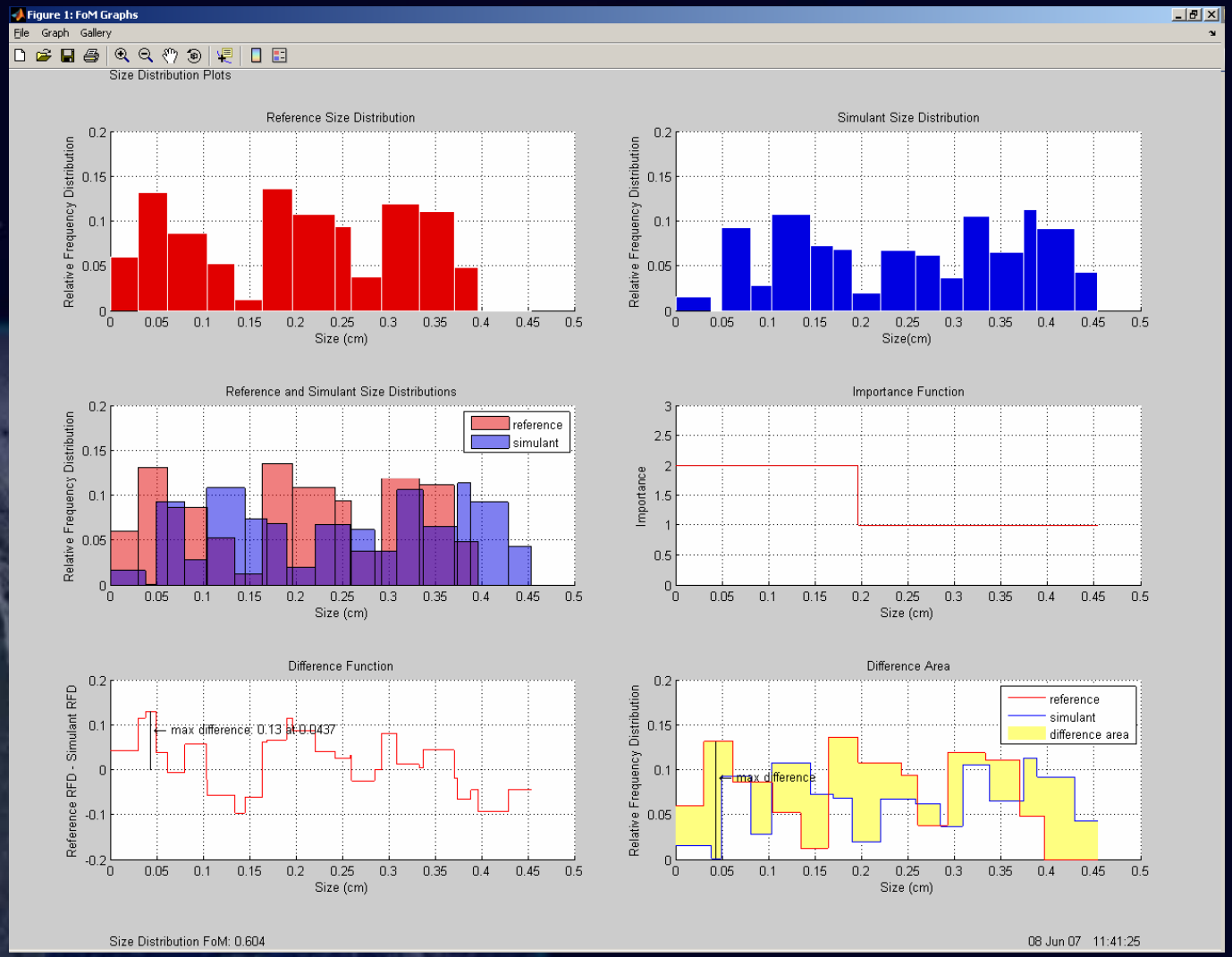


FoM – Modal Composition

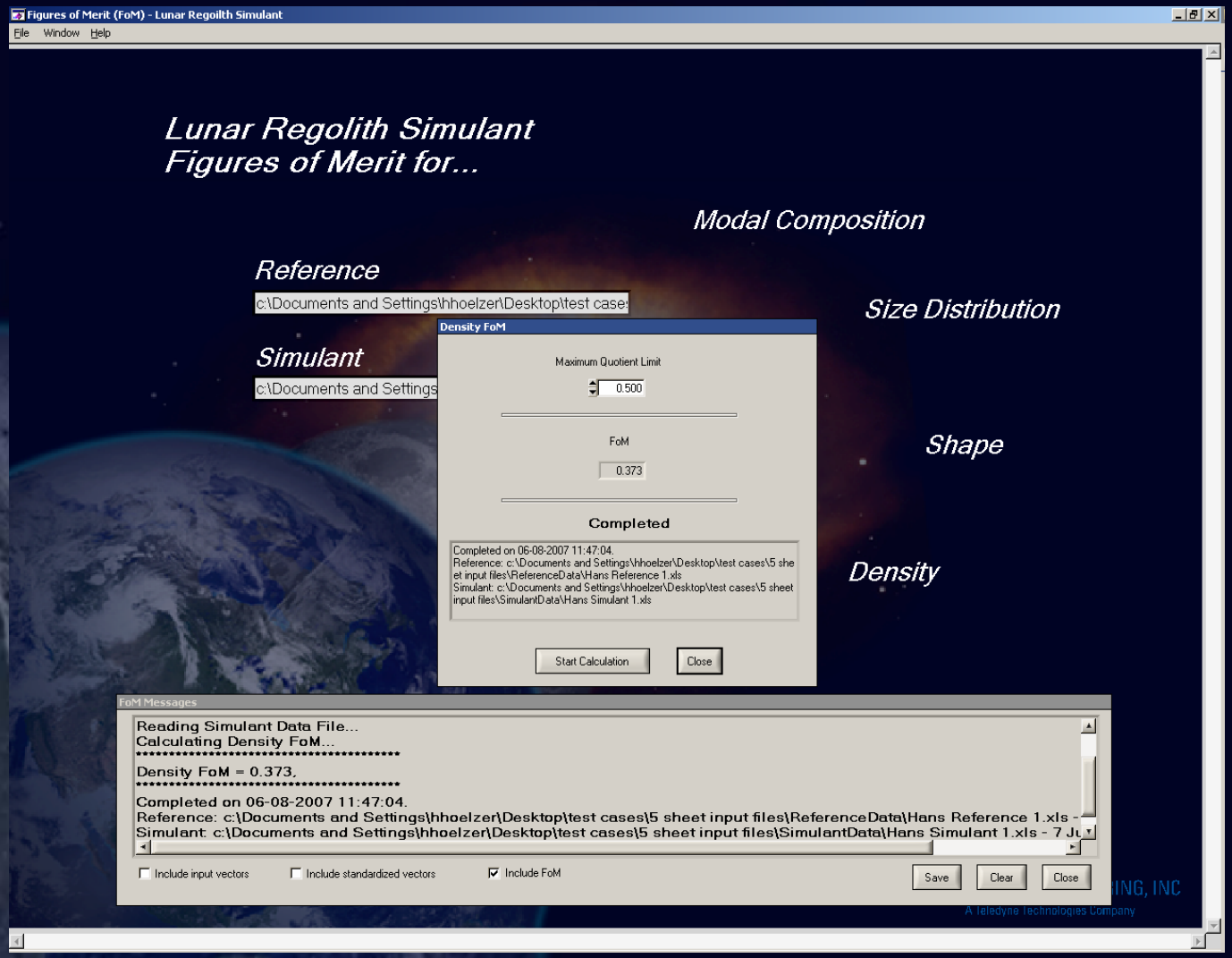


FoM – Size Distribution - 1

FoM – Size Distribution - 2



FoM – Density


Figures of Merit (FoM) - Lunar Regoilth Simulant
File Window Help
Lunar Regolith Simulant
Figures of Merit for...
Modal Composition
Reference
c:\Documents and Settings\hhoelzer\Desktop\test case
Size Distribution
Simulant
c:\Documents and Settings
Density FoM
Maximum Quotient Limit
0.500
FoM
0.373
Completed
Completed on 06-08-2007 11:47:04.
Reference: c:\Documents and Settings\hhoelzer\Desktop\test cases\5 sheet input files\ReferenceData\Hans Reference 1.xls
Simulant: c:\Documents and Settings\hhoelzer\Desktop\test cases\5 sheet input files\SimulantData\Hans Simulant 1.xls
Start Calculation
Close
Shape
Density
FoM Messages
Reading Simulant Data File...
Calculating Density FoM...
Density FoM = 0.373,
Completed on 06-08-2007 11:47:04.
Reference: c:\Documents and Settings\hhoelzer\Desktop\test cases\5 sheet input files\ReferenceData\Hans Reference 1.xls -
Simulant: c:\Documents and Settings\hhoelzer\Desktop\test cases\5 sheet input files\SimulantData\Hans Simulant 1.xls - 7 Ju
Include input vectors
Include standardized vectors
Include FoM
Save
Clear
Close
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Backup Slides

Regolith Properties To Be Simulated And Their Relationship to the Figures Of Merit

Figures of Merit / Simulant Properties	Composition	Size	Shape	Density
1. Grain Properties	X	X	X	
2. Electrostatic Charging Properties	X	X		
3. Magnetic Properties	X	X		
4. Geomechanical Mechanical				
a. Fatigue	X	X	X	X
b. Strength				
i. Tensile	X	X	X	X
ii. Compressive	X	X	X	X
iii. Shear	X	X	X	X
iv. Grain Hardness	X			
v. Coefficient of Friction	X	X	X	X
c. Flexural Strength – Bending Resistance	X	X	X	X
d. Fracture Properties	X	X	X	X
e. Impact Resistance	X	X	X	X
f. Rheology (flow properties)	X	X	X	X
g. Angle of Repose		X	X	X

Regolith Properties To Be Simulated And Their Relationship to the Figures Of Merit

Simulant Properties \ Figures of Merit	Composition	Size	Shape	Density
4. Geomechanical (cont'd)				
Physical				
h. Thermal Properties	X	X	X	X
i. Bulk Density	X	X	X	
j. Particle Density	X			
k. Porosity	X	X	X	X
l. Surface Area	X	X	X	
m. Permeability (gas)	X	X	X	X
5. Agglutinate-specific				
a. Friability				
b. With single-domain iron				
6. Chemical Reactivity				
a. From surface damage				
b. As volatile / soluble minerals				
7. Chemical Properties				
a. Bulk	X	X	X	X
b. Mineral	X	X	X	

Regolith Properties To Be Simulated And Their Relationship to the Figures Of Merit

Simulant Properties \ Figures of Merit	Composition	Size	Shape	Density
7. Chemical Properties (cont'd)				
c. Glass	X	X	X	
8. Modal Composition				
a. Total	X			
b. As a function of grain size		X		
9. Texture	X	X	X	
10. Implanted solar particle–specific (e.g. H, C, N)	X			