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Creation of Sediment Models (Appendix to Task 3 Technical Report)

Mechanisms Leading to Co-Existence of Gas and Hydrate in Ocean Sediments

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Office of Fossil Energy

APPENDIX

Summary of Properties

For convenience we reproduce Table 1 from the body of this report here.

Table 1. Summary of Properties of Model Sediments								
	Grain sizes (arbitrary units)				Porosity (fraction)	Sorting Index		Notes*
Packing No.	Minimum Radius	Maximum radius	Mean radius	Standard deviation	· · · · ·	Number fraction basis	Volume or weight fraction basis	
1	0.32	2.58	2.18	0.11	0.37	1.04	1.04	LN
2	1.84	2.64	2.18	0.11	0.36	1.03	1.03	LN
3	1.80	2.60	2.18	0.11	0.37	1.03	1.03	LN
4	0.32	2.59	2.18	0.11	0.35	1.03	1.03	LN
5	1.82	2.52	2.15	0.11	0.41	1.03	1.03	LN
Average	1.22	2.59	2.17	0.11	0.37	1.03	1.03	
6	1.50	3.22	2.17	0.22	0.36	1.07	1.07	LN
7	1.50	3.08	2.16	0.22	0.36	1.07	1.07	LN
8	1.48	2.99	2.17	0.22	0.36	1.07	1.07	LN
9	1.47	3.06	2.16	0.22	0.37	1.07	1.07	LN
Average	1.49	3.09	2.16	0.22	0.36	1.07	1.07	-
10	0.96	4.12	2.12	0.42	0.35	1.14	1.14	LN
11	0.93	4.64	2.12	0.43	0.34	1.14	1.14	LN
12	1.07	4.49	2.11	0.42	0.35	1.14	1.14	LN
13	0.99	4.27	2.11	0.43	0.35	1.14	1.14	LN
Average	0.99	4.38	2.11	0.43	0.35	1.14	1.14	
14	4.24E-03	7.05	1.90	0.80	0.32	1.31	1.32	LN
15	3.44E-03	6.44	1.90	0.79	0.35	1.31	1.31	LN
16	3.91E-01	6.38	1.91	0.78	0.33	1.31	1.29	LN
17	7.81E-03	7.01	1.90	0.79	0.32	1.31	1.30	LN
18	1.59E-03	7.62	1.91	0.79	0.32	1.31	1.29	LN
Average	8.17E-02	6.90	1.90	0.79	0.33	1.31	1.30	
19	1.86E-03	11.30	1.31	1.16	0.29	1.72	1.48	LN; Trn
20	2.39E-03	10.16	1.31	1.17	0.25	1.72	1.54	LN; Trn
21	7.85E-03	11.26	1.31	1.15	0.30	1.72	1.53	LN; Trn
22	1.17E-03	11.17	1.30	1.16	0.30	1.69	1.53	LN; Trn
Average	3.32E-03	10.97	1.31	1.16	0.29	1.71	1.52	-
23	3.45E-05	11.31	0.69	1.25	0.31	3.11	1.32	LN; Trn
24	1.63E-05	11.19	0.71	1.26	0.30	3.12	1.38	LN; Trn
25	3.80E-05	11.28	0.70	1.25	0.37	3.16	1.30	LN; Trn
26	1.44E-05	12.16	0.72	1.23	0.32	3.07	1.46	LN; Trn
Average	2.58E-05	11.49	0.71	1.25	0.33	3.11	1.37	

 * LN = log normal distribution of sphere sizes. N = normal distribution of sphere sizes. Trn indicates that the actual distribution of sphere sizes in the packing was truncated.

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27	8.10E-06	18.29	0.30	1.07	0.31	3.63	1.38	LN; Trn
28	2.04E-06	21.32	0.30	1.04	0.29	3.77	1.37	LN; Trn
29	6.94E-06	22.46	0.31	1.04	0.32	3.95	1.41	LN; Trn
Average	5.69E-06	20.69	0.31	1.05	0.31	3.79	1.39	,
30	1 24E-03	11.93	1 01	1 20	0.29	2.00	1 50	I N [.] Trn
31	6.31E-04	11.00	1.01	1.20	0.20	2.00	1.56	
31	0.31E-04	10.04	1.04	1.22	0.32	2.00	1.00	
32	5.70E-04	12.34	1.02	1.21	0.30	2.03	1.48	
33	4.21E-05	12.57	1.07	1.22	0.31	1.94	1.51	LN; Im
34	5.47E-04	11.63	1.03	1.19	0.34	2.01	1.49	LN; Trn
Average	6.06E-04	12.09	1.03	1.21	0.31	2.00	1.51	
35	4.62E-04	9.67	1.63	1.03	0.30	1.51	1.40	LN
36	1.89E-03	9.70	1.61	1.04	0.30	1.50	1.43	LN
37	1.35E-03	9.30	1.59	1.04	0.27	1.49	1.46	LN
38	3 98F-03	9 41	1 60	1.05	0.27	1 51	1 44	IN
	1 92F-03	9.52	1.60	1.04	0.20	1 50	1 / 3	
20	1.920-03	2.02	2 10	0.07	0.29	1.00	1.40	N
<u> </u>	1.97	2.40	2.19	0.07	0.34	1.02	1.02	N
40	1.97	2.41	2.13	0.07	0.33	1.02	1.02	N
41	1.95	2.33	2.17	0.07	0.30	1.02	1.02	N
Averages	1.97	2.40	2.13	0.07	0.36	1.02	1.02	· · · · · ·
43	1.07	3.20	2.10	0.35	0.36	1.02	1 10	N
44	1.07	3.20	2.14	0.35	0.36	1.12	1.10	N
45	1.07	3.20	2.14	0.36	0.35	1.12	1.11	N
46	1.07	3.20	2.14	0.35	0.37	1.12	1.11	N
Averages	1.07	3.20	2.14	0.35	0.36	1.12	1.10	
47	5.64E-05	4.01	2.01	0.68	0.34	1.27	1.17	N
48	4.20E-05	4.01	2.01	0.66	0.33	1.25	1.17	Ν
49	3.59E-05	4.03	2.01	0.67	0.34	1.25	1.18	Ν
50	3.22E-05	4.04	2.02	0.66	0.33	1.25	1.17	N
Averages	4.16E-05	4.02	2.01	0.67	0.34	1.26	1.17	
51	1.27E-03	4.59	1.85	0.90	0.32	1.42	1.21	N
52	1.10E-03	4.51	1.85	0.91	0.34	1.42	1.21	N
53	5.94E-04	4.44	1.86	0.89	0.35	1.40	1.21	N
54	2.94E-03	4.59	1.86	0.90	0.32	1.42	1.20	<u> </u>
Averages	1.48E-03	4.53	1.86	0.90	0.33	1.42	1.21	
55	6.34E-04	5.00	1.73	1.04	0.32	1.60	1.23	<u>N</u>
50	3.30E-04	5.06	1./1	1.05	0.31	1.64	1.22	
51	8 76E 04	5.07	1.71	1.00	0.30	1.02	1.22	
50		5.00	1.71	1.05	0.34	1.00	1.20	
Averanes	8 98F-04	5.01	1 71	1.05	0.33	1.03	1.22	
60	3 81F-03	4 56	1.84	0.91	0.32	1 43	1 21	N
61	4.85F-03	4.82	1.77	1.00	0.31	1.53	1.22	N
62	4.93E-03	4.85	1.76	1.00	0.35	1.53	1.23	N
63	4.47E-04	4.81	1.76	1.00	0.33	1.53	1.22	N
64	2.51E-03	4.82	1.77	0.99	0.33	1.51	1.22	N
65	4.94E-03	4.88	1.76	1.00	0.34	1.54	1.23	N
Averages	3.58E-03	4.79	1.78	0.98	0.33	1.51	1.22	
66	3.31E-03	5.36	1.60	1.15	0.33	1.89	1.24	Ν
67	1.88E-04	5.38	1.61	1.14	0.32	1.85	1.24	N

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68	2.30E-03	5.44	1.60	1.15	0.33	1.94	1.23	Ν
69	2.37E-03	5.43	1.60	1.14	0.33	1.91	1.24	Ν
70	2.43E-04	5.32	1.59	1.14	0.33	1.90	1.25	Ν
Averages	1.68E-03	5.39	1.60	1.14	0.33	1.90	1.24	
71	2.88E-04	5.46	1.54	1.19	0.33	2.12	1.23	N
72	2.93E-03	5.47	1.53	1.20	0.33	2.20	1.23	Ν
73	2.86E-04	5.49	1.52	1.20	0.32	2.27	1.24	Ν
74	2.52E-03	5.64	1.53	1.20	0.33	2.18	1.24	N
75	8.97E-04	5.65	1.53	1.19	0.33	2.13	1.26	Ν
76	7.35E-04	5.52	1.53	1.20	0.32	2.23	1.24	N
Averages	1.28E-03	5.54	1.53	1.20	0.32	2.19	1.24	

Definition of Sorting Index

Two sorting indexes are used in Table 1, depending on the basis used for computing the cumulative distribution function. Sorting index on the basis of **number fraction** is exactly the same as what is used in developing CDF (Cumulative Density Function). It is calculated as follows. Suppose that we have a sorted set of data set as $R = [r_1, r_2, r_3, ..., r_n]$ (If it is not sorted it can be easily sorted using different algorithms in the literature). We can easily develop a table as follows. The second column includes the numbers of the data that are smaller or equal to every corresponding r_i . In the case that we don't have any repeated number we would have:

R	No. of data <= r _i	F (CDF according on the basis of number fraction)
r ₁	1	<u>1</u>
		n
r ₂	2	2
		n
r ₃	3	3
		n
		•••
r _{n-1}	n-1	n-1
		n
r _n	n	1

The cumulative density function on the basis of number fraction for run number 38 is plotted in the following figure:



Figure A-1. CDF (No. Fraction) for run #38

The next step would be to use this CDF and calculate the sorting index. Sorting index is defined as:

Sorting index =
$$\sqrt{\frac{d_{75}}{d_{25}}}$$

 d_{75} : Radius at which CDF(d) = 0.75 d_{25} : Radius at which CDF(d) = 0.25

The other basis for computing CDF is the volume fraction of spheres. Values of So using this basis can also be seen in Table 1. It is a kind of weighted CDF and differs from the mathematical definition of CDF. To calculate the sorting index using the latter definition one can develop a table as follows:

R	V (Volume)	Cumulative Vol.	CDF (on volume fraction basis)
r ₁	$V_1 = \frac{4}{3}\pi r_1^3$	$\sum_{k=1}^{1} V_k$	$\frac{\displaystyle\sum_{k=1}^{1} V_k}{\displaystyle\sum_{k=1}^{n} V_k}$

r ₂	$\mathbf{V}_{2}=\frac{4}{3}\pi r_{2}^{3}$	$\sum_{k=1}^{2} V_k$	$\frac{\displaystyle{\sum_{k=1}^2} V_k}{\displaystyle{\sum_{k=1}^n} V_k}$
r ₃	$V_3 = \frac{4}{3}\pi r_3^3$	$\sum_{k=1}^{3} V_k$	$\frac{\displaystyle\sum_{k=1}^{3} V_k}{\displaystyle\sum_{k=1}^{n} V_k}$
r _{n-1}	$V_{n-1} = \frac{4}{3}\pi r_{n-1}^{3}$	$\sum_{k=1}^{n-1} V_k$	$\frac{\displaystyle{\sum_{k=1}^{n-1}}V_k}{\displaystyle{\sum_{k=1}^{n}}V_k}$
r _n	$V_n = \frac{4}{3}\pi r_n^3$	$\sum_{k=1}^{n} V_k$	1

The next step to calculate the sorting index is exactly the same as what we did for CDF on the basis of number fraction:

Sorting index =
$$\sqrt{\frac{d_{75}}{d_{25}}}$$

 d_{75} : Radius at which CDF(vol. frac.) = 0.75 d_{25} : Radius at which CDF(vol. frac) = 0.25

The cumulative density function on the basis of volume fraction in comparison with that of number fraction for run number 38 is plotted in the following figure:



Figure A-2. CDF (Vol. fraction and number fraction)

It is obvious from the above figure that the sorting indexes drawn form the two definitions are not the same. Nevertheless, Table 1 shows that in a well sorted packing the two sorting indexes are close to each other. As the sorting becomes poorer, the two values deviate more and more from each other.

Verification of statistics of individual realizations

If one can see the radius and volume of the spheres in a packing is log normally distributed one can compare the mean and standard deviation of the radius and volume values for the realization to the formula for log-normal distribution CDF (Cumulative density function). This is a useful check especially as the sorting becomes poorer. We have done this for both radius and volume values. The results are as follows: Looking at the following two graphs one can easily see that CDF calculated from the lognormal model matched to the radius is very well matched with the actual CDF of the radius distribution. So the radius and volume is perfectly log normally distributed. CDF of a log normally distributed quantity x is:

$$C(x) = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left[\frac{\ln(x) - \mu}{\sigma\sqrt{2}}\right]$$

Where in μ is the average of natural log of the quantity and σ is the standard deviation of the natural log of the quantity.



Figure A-3. Matching a Lognormal model to the volume distribution



Figure A-4. Matching a Lognormal model to radius distribution

But actually what geologists mostly work with is a graph that presents the weight percent or weight fraction distribution of the grains. Such a distribution can be achieved form the radius distribution of the grains as follows:

Supposing that all the grains are made of the same material and so of the same density, we can easily work with the volume distribution of the grains to calculate the weight distribution since weight is equal to the product of volume and density. If we divide natural Log of Volume into some bins, store the centers of such bins in an array x and store the frequency corresponding to those bins in an array N we would have:

$$Weight\% = \frac{N.e^x}{\sum N.e^x} \times 100$$

We prefer to plot the histogram of weight percent vs. natural log of radius, so we need the natural log of radiuses corresponding to each volume bin center:

$$x = Ln(\frac{4}{3}\pi r^3) \Longrightarrow Ln(r) = \frac{1}{3}(x - Ln(\frac{4}{3}\pi))$$

Visual confirmation of limits on statistical validity of individual realizations

To visualize the computer generated packings the following figures are presented in the ascending order of sorting index. For every packing different cubes inside the packing has been chosen, to better show how the spheres are located in the packing. The distribution of grain sizes in the realization is plotted with each set of visualizations. As the sorting index increases beyond $S_o = 1.5$, large spheres are under-represented and the packings become more porous than they should be.





Spheres with X, Y and Z between 35 and 50



Spheres with X, Y and Z between 45 and 70



Figure A-5. Visualization of the a packing with sorting index of 1.03





Spheres with X, Y and Z between 35 and 50



Spheres with X, Y and Z between 45 and 70



Figure A-6. Visualization of the a packing with sorting index of 1.3



Spheres with X, Y and Z between 35 and 50





Spheres with X, Y and Z between 45 and 70



Figure A-7. Visualization of the a packing with sorting index of 1.5



Spheres with X, Y and Z between 35 and 50



Spheres with X, Y and Z between 45 and 70



Figure A-8. Visualization of the a packing with sorting index of 1.7

Spheres with X, Y and Z between 20 and 30



Spheres with X, Y and Z between 35 and 50



Spheres with X, Y and Z between 45 and 70



Figure A-9. Visualization of the a packing with sorting index of 2

Spheres with X, Y and Z between 20 and 50



Spheres with X, Y and Z between 35 and 70



Spheres with X, Y and Z between 45 and 70



Figure A-10. Visualization of the a packing with sorting index of 3.8

A closer view of the left down corner image of the above visualization (sorting index of 3.8) is shown below.



Figure A-11. A close look at a sub cube out of one of the packings with sorting index of 3.8



Figure A-12. A close look at another sub cube out of one of the packings with sorting index of 3.8

Over viewing the above visualizations, together with the weight percent graphs, it is seen that the outputs of the packing generator code is realistic up to a sorting index of about 1.5 (well sorted packing).

Saadatfar et al.¹ (2007) directly measured rock fabric and texture from 3D digital images of core fragments. They did the experiments for unconsolidated soils and sands, homogeneous consolidated core samples and more complex consolidated hydrocarbon reservoir core. Since we are going to work on unconsolidated sands, we just study their

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¹ Saadatfar, M., A. Sheppard and M. Knackstedt. "Measurement of rock fabric and texture from microtomographic images," *J. Geophys. Res.*, in press, 2007.

results related to unconsolidated sand packs. The following figure shows 2D slices of the unconsolidated sand samples after grain partitioning.

Images and Grain Size Distributions of Several Natural Sediments

For reference in examining the geometric properties of the model sediments, we reproduce here 2D slices from 3D digital images (CT scans) through four unconsolidated sand packs (Saadatfar et al., 2007). The authors applied a grain partitioning algorithm to identify and color the individual grains. The measured grain size distribution are also reproduced below.



Sample (a) is very well sorted, Sample (b) is moderately sorted, Sample (c) is well sorted and Sample (d) is barely moderately sorted



Histogram at upper left was measured on the sample corresponding to the 2D slice in the upper left in the preceding figure. The other histograms are arranged similarly.

The grain size distributions above use the "phi" scale, where $\phi = -\log_2(d_{grain})$ and d_{grain} is in mm. The results indicate that the sand system shown in the upper left of each set of images is well to very well sorted; the grain size distribution is near symmetrical. Laser particle size measurement was conducted on a sister core of the soil samples correspond to the upper pair of images. The match of the particle size data with the histograms, which were inferred from the CT images, indicates that the latter are reasonably accurate. The soil system in the upper right image is moderately sorted and strongly positively skewed. The bottom row of images shows the increase in width of the grain size distribution as the sorting becomes poorer.

Radial Distribution Functions

The radial distribution function (RDF) is convenient measure of structure in a packing. The function measures the probability of finding another sphere at a prescribed distance from an arbitrary test sphere. Peaks in the function correspond to common arrangements of spheres, while valleys indicate relatively rare arrangements. At sufficiently large distances within a random packing, the function approaches the average number density of spheres in the packing. For reference, the RDF for the dense random packing of equal spheres built and painstakingly characterized by Finney² is shown below. The very large peak in the function at a separation of 2 sphere radii, which corresponds to pairs of grains in point contact, has been truncated so that the other structures are more easily visible. The valley between 2.1 and 3.2 sphere radii is the consequence of the common occurrence of adjacent triangles mutually touching spheres, which establishes the peak at 3.46 sphere radii. Similarly the peak at 4.0 sphere radii corresponds to a line of three touching spheres. The peaks and valleys decay rapidly when the separation between

spheres exceeds 6 sphere radii, and the function approaches the number density $\frac{3(1-\phi)}{4\pi}$.

A regular, crystalline packing of equal spheres would continue to exhibit peaks and valleys at greater distances, though eventually it would be impossible to resolve them and the function would approach the sphere number density.

² Finney, J. Random packings and the structure of simple liquids. I. The geometry of random close packing. *Proc. Roy. Soc. Lond. A*, 319:479–493, 1970.



The features of the Finney pack RDF are readily apparent in the very well sorted model sediments ($S_o < 1.2$), but they disappear as the grain size distribution becomes broader. The distance scale in the RDFs in the following plots is normalized to the arithmetic mean grain size in each packing.



• Packings with Log-Normal radius distribution

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• Packings with Normal radius distribution





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Pore Throat Size Distribution



• **Packings with** Log-Normal radius **distribution**


















Mechanisms Leading To Co-Existence Of Gas And Hydrate In Ocean Sediments























Packings with Normal radius • distribution









































Grain Size Distributions



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