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Compute Critical Curvatures for Pore-level Events (Task 5.1 Technical Report)

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

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MECHANISMS LEADING TO CO-EXISTENCE OF GAS AND HYDRATE IN
OCEAN SEDIMENTS

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Deliverable 5.1:
Report on Task 5.1 “Compute critical curvatures for pore-level events”

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Objective of Task 5.1

In the conceptual model to be examined in this project, hydrate formation depends upon the location and geometry of the gas/water interface. First will be a determination of the critical capillary pressure (equivalently, critical curvature of the meniscus) for drainage in each throat identified in Task 3. This will be done with the level set method (LSM) using a speed function that equilibrates capillary pressure and interface curvature^[2]. Then the critical capillary pressure for imbibition of each pore body will be determined. The critical value depends on which grain contacts support pendular rings of wetting phase and which pore throats contain a meniscus, so these values will be catalogued for the different possible combinations for each pore body.

We have developed and produced a final draft catalog of critical curvatures for model sediments based on the results of this work. Files containing the curvatures are described in this report have been uploaded to a public-accessible website. Statistical descriptions of the drainage curvatures appear in Appendix A of this report. Statistical descriptions of the imbibition curvatures appear in Appendix B.

Summary of Findings in Task 5.1

Geometric Properties of the Model Sediments

In previous reports we have described the results of more than 75 runs of our cooperative rearrangement code for creating model sediments. The models consist of randomly arranged, densely packed sphere of different radii. Here we summarize the features of these model sediments. In the next section, we describe the critical curvatures for drainage and for imbibition in each model.

The packings each contain 5000 spheres. All are periodic, with a cube as the unit cell. The mean sphere size in each packing is reported in the same units as the unit cube size. Because these units are arbitrary, it is natural to normalize all lengths (in the model sediments by the mean sphere size. The sphere radii in a packing are distributed either normally or log-normally (see Table 1) with different means and standard deviations and consequently different sorting indexes S_o . The sorting index is commonly used by sedimentologists and is defined by

$$S_o = \sqrt{\frac{d_{75}}{d_{25}}} \quad (1)$$

where d_{75} is the grain size that is larger than 75% of all grains, and d_{25} is the grain size larger than 25% of all grains. The sorting index is essentially a proxy for the standard deviation of the grain size distribution. The percentage can be calculated on a number fraction basis or on a volume fraction basis. We report both measures. The index can be correlated to the qualitative terminology in customary use as follows:

Extremely well sorted:	$1.0 \leq \text{sorting index} \leq 1.1$
Very well sorted:	$1.1 \leq \text{sorting index} \leq 1.2$

Well sorted: $1.2 \leq \text{sorting index} \leq 1.4$
 Moderately sorted: $1.4 \leq \text{sorting index} \leq 2$
 Poorly sorted: $2 < \text{sorting index}$

A summary of the packings is tabulated below. Several realizations were created for each value of sorting index. The shaded rows marked “average” give the average values for the set of realizations immediately above that row. The column labeled “Notes” indicates whether the packing grain size distribution is log normal (LN) or normal (N) and whether the realization exhibits a truncated distribution (Trn) because of the number of spheres used to create the packing.

Table 1. Summary of Properties of Model Sediments								
Packing No.	Grain sizes (arbitrary units)				Porosity (fraction)	Sorting Index		Notes*
	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	
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	LN; Trn
31	6.31E-04	11.99	1.04	1.22	0.32	2.00	1.56	LN; Trn
32	5.70E-04	12.34	1.02	1.21	0.30	2.03	1.48	LN; Trn
33	4.21E-05	12.57	1.07	1.22	0.31	1.94	1.51	LN; Trn
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	3.98E-03	9.41	1.60	1.05	0.27	1.51	1.44	LN
Average	1.92E-03	9.52	1.60	1.04	0.29	1.50	1.43	
39	1.97	2.40	2.19	0.07	0.34	1.02	1.02	N
40	1.97	2.41	2.19	0.07	0.35	1.02	1.02	N
41	1.95	2.39	2.17	0.07	0.38	1.02	1.02	N
42	1.97	2.40	2.19	0.07	0.37	1.02	1.02	N
Averages	1.97	2.40	2.18	0.07	0.36	1.02	1.02	
43	1.07	3.20	2.14	0.35	0.36	1.12	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	N
49	3.59E-05	4.03	2.01	0.67	0.34	1.25	1.18	N
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	N
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	N
56	3.30E-04	5.06	1.71	1.05	0.31	1.64	1.22	N
57	1.56E-03	5.07	1.71	1.05	0.35	1.62	1.22	N
58	8.76E-04	5.08	1.71	1.05	0.34	1.65	1.23	N
59	1.09E-03	5.01	1.70	1.05	0.33	1.63	1.22	N
Averages	8.98E-04	5.04	1.71	1.05	0.33	1.63	1.22	
60	3.81E-03	4.56	1.84	0.91	0.32	1.43	1.21	N
61	4.85E-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	N
67	1.88E-04	5.38	1.61	1.14	0.32	1.85	1.24	N
68	2.30E-03	5.44	1.60	1.15	0.33	1.94	1.23	N
69	2.37E-03	5.43	1.60	1.14	0.33	1.91	1.24	N
70	2.43E-04	5.32	1.59	1.14	0.33	1.90	1.25	N
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	N
73	2.86E-04	5.49	1.52	1.20	0.32	2.27	1.24	N
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	N
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	

*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.

There are four sets of text files available for the 76 packings produced by the cooperative rearrangement algorithm and summarized in Table 1. These files define completely the geometric characteristics of the packings.

- **Listing of sphere centers and radii for each packing**

The file name for this category is “Coordinates_PackingNN.txt” where NN indicates the number of the packing in Table 1. For example the file named “Coordinates_Packing12.txt” includes the X, Y and Z coordinates of the centers of the spheres making up the packing and also the radius of the spheres for the 12th packing. The coordinates are in the same arbitrary but self-consistent units used to report grain sizes. There are 4 columns in each of these text files. The first 3 columns are XYZ coordinates of the sphere centers respectively and the fourth column contains the radius of the corresponding spheres. The ID number for each sphere is the number of the row the data of that specific sphere is mentioned. This ID number is used to refer to the spheres in the Delaunay tessellation (see next file type).

Example: the first ten lines of Coordinates_Packing1.txt are shown below

```

2.9510300e+001 2.1302500e+001 4.0295900e+001 2.2783500e+000
5.3711700e+001 1.2861000e+001 4.3209600e+001 2.2168100e+000
6.6300900e+001 6.5553900e+001 1.8227200e+001 2.1118800e+000
9.6867900e+000 6.1662900e+000 2.9074100e+001 2.2594700e+000
2.4610100e+001 2.4928900e+001 1.6943900e+001 2.1263300e+000
1.3072500e+001 2.2058300e+001 1.2149000e+001 2.1046600e+000
5.0956900e+001 3.7340800e+001 2.4290000e+000 2.3653800e+000
7.0123200e+000 4.4366600e+001 2.6550400e+001 2.1209200e+000
2.5703100e+001 1.4560700e+001 6.3361000e+001 2.1258700e+000
6.6219300e+001 3.4782600e+001 5.1609200e+001 2.1561500e+000

```

Thus sphere 1 in this packing has radius 2.27835 and its center is located at (29.5103, 21.3025,40.2959).

- **Listing of sphere IDs corresponding to Delaunay tessellation for each packing**

The file name is “Tes_Matrix_PackNN.txt” where NN indicates the packing number in Table 1. It includes four columns. Each row in this text file represents a Delaunay cell. The four numbers mentioned in each row indicate the IDs of the spheres that make up a Delaunay cell. The number of each row is the ID number for the corresponding Delaunay cell. This ID number is used in the topology file (see next file type).

Example: the first ten lines of Tes_Matrix_Pack1.txt are shown below.

```

2.8910000e+003  3.2660000e+003  2.5230000e+003  4.8480000e+003
2.4040000e+003  4.3260000e+003  1.2230000e+003  2.5280000e+003
3.3540000e+003  1.2910000e+003  3.9550000e+003  4.9920000e+003
1.7380000e+003  4.8110000e+003  7.0900000e+002  4.4200000e+002
6.6900000e+002  1.3730000e+003  3.8360000e+003  4.5170000e+003
6.3000000e+001  3.4640000e+003  4.6450000e+003  1.7090000e+003
1.2460000e+003  3.4640000e+003  4.6450000e+003  1.7090000e+003
1.2460000e+003  2.1210000e+003  3.4640000e+003  1.7090000e+003
2.8360000e+003  2.8910000e+003  3.2660000e+003  2.5230000e+003
4.3630000e+003  3.5390000e+003  4.5110000e+003  2.5380000e+003

```

Thus the first Delaunay cell corresponds to spheres 2891, 3266, 2523 and 4848. By inspecting the corresponding lines of file Coordinates_Packing1.txt, we could determine the spatial location of each corner of this tetrahedron, and thus the radii of each pore throat in this cell. Note that cells 6 and 7 both contain spheres 3464, 4645 and 1709. This means that cells 6 and 7 will be neighbors (see topology file next). Similarly, cell 1 and cell 9 have three spheres in common, namely 2891, 3266 and 2523.

- **Listing of network topology (which cells in the above file are the neighbors of each cell)**

The file name is “Neighbors_Matrix_PackNN.txt” where NN indicates the packing number in Table 1. This file contains four columns. Each row corresponds to one cell in the tessellation. Each column contains the ID number of a cell that neighbors the given cell. There are four columns, because all cells are tetrahedral and therefore have four neighbors. Though the packings are periodic, this listing treats the packing as though it were finite and limited to the cubic domain used by the cooperative rearrangement algorithm. Thus cells on the outer face of the packing will have less than four neighbors *within* the packing. The exterior face(s) of these cells are assigned a neighbor index of zero (0).

Example: the first ten lines of Neighbors_Matrix_Pack1.txt are shown below.

```

9.0000000e+000  1.5300000e+002  0.0000000e+000  0.0000000e+000
1.2000000e+003  3.8980000e+003  3.9410000e+003  3.8130000e+003
1.9750000e+003  8.8300000e+002  0.0000000e+000  0.0000000e+000
2.9000000e+002  1.3110000e+003  4.0350000e+003  8.7830000e+003
1.2400000e+002  1.2200000e+002  5.8490000e+003  0.0000000e+000
7.4500000e+002  7.4800000e+002  3.0400000e+002  7.0000000e+000
2.7220000e+003  1.4300000e+002  8.0000000e+000  6.0000000e+000
6.9680000e+003  7.0000000e+000  2.8850000e+003  3.0300000e+002
1.5400000e+002  2.9100000e+003  2.5000000e+001  1.0000000e+000
1.6000000e+002  7.3600000e+002  4.5000000e+001  2.1762000e+004

```

Thus the first Delaunay cell has as neighbors cells 9, 153, 0 and 0. The latter two mean that the first cell has two faces on the exterior of the packing. The ninth line

indicates that cell 9 has neighbors 154, 2910, 25 and 1. The presence of cell 1 in this list serves as a consistency check; we have carried out this check on the topology file for every packing. Similarly, cell 7 is the fourth neighbor of cell 6, and cell 6 is the fourth neighbor of cell 7. To determine the size of the pore throat connecting cells 6 and 7, one would identify the sphere IDs that are common to the Delaunay cell definitions for cells 6 and 7 (see previous section.) The spatial locations and radii of these spheres can be extracted from the file of coordinates. This information is sufficient to determine the radius of the inscribed circle (and any other geometric information desired), which we use as a measure of the pore throat size (see next file type).

- **Listing of pore throat radii associated with each throat connecting neighboring cells**

The file name is “Normalized_Pore_Throat_Size_Matrix_PackNN.txt” where NN indicates the packing number in Table 1. It includes the normalized pore throat radii associated with each throat connecting neighboring cells throughout the packing. The throat radii in each packing are normalized by the mean sphere radius (see Table 1). Thus the normalization factor differs from packing to packing, but after normalization all quantities involving length are comparable between packings. A radius of -1 indicates a throat that is connected to the exterior of the packing. The treatment of such throats depends on the algorithm to be used for drainage and imbibition. If the actual geometric value is needed, it can be readily extracted from the other three data files as discussed above.

The throat radii file is constructed in exactly the same order as the topology file above. The line number of each row corresponds to the Delaunay cell number. For a given row, the first column contains the radius of the throat connecting the given cell to its first neighbor. (The first neighbor is identified in the corresponding line of the topology file). The second column contains the radius of the throat connected the given cell to the second neighbor, and so on.

Example: the first ten lines of Normalized_Pore_Throat_Size_Matrix_Pack1.txt are shown below.

```

1.7554545e-001  1.6062099e-001  -1.0000000e+000  -1.0000000e+000
4.2141740e-001  2.5307557e-001  3.0896714e-001  2.4233366e-001
3.7456316e-001  3.7354064e-001  -1.0000000e+000  -1.0000000e+000
3.1531876e-001  2.2893521e-001  3.1233790e-001  3.7145802e-001
1.4884367e-001  1.5176807e-001  4.1038120e-001  -1.0000000e+000
2.6542254e-001  1.6435000e-001  3.7279741e-001  4.1491201e-001
2.7451845e-001  2.0055349e-001  3.8093278e-001  4.1491201e-001
5.3127678e-001  3.8093278e-001  4.2109478e-001  5.0433782e-001
2.2256290e-001  2.2367991e-001  1.7227901e-001  1.7554545e-001
3.6117889e-001  2.8125971e-001  1.7008389e-001  2.9634619e-001

```

Thus the first Delaunay cell has throats of radius $0.175545R$, $0.160621R$ and two throats connected to the exterior of the packing. Here R is the mean radius of spheres in packing No. 1, which is 2.18 (cf. Table 1). Cell 10 is connected to its neighbors through throats of radius $0.361179R$, $0.28126R$, $0.170084R$ and $0.296346R$. Cell 6 is connected cell 7 through a throat of radius $0.414912R$, i.e. through the fourth throat of cell 6.

Drainage Curvatures for Model Sediments

To compute drainage curvature for each throat in a packing we use Mason and Mellor critical curvature estimate

$$C_{drain}^* = \frac{2R_{avg}}{r_{inscribed}} - 1.6 \quad (2)$$

The result is stored in `Drainage_Curvatures_PackingNN.txt`, which are stored in folder ‘Drainage Curvatures’. Note that the throat inscribed radius in the above formula is stored in previously described files

“`Normalized_Pore_Throat_Size_Matrix_PackNN.txt`”.

Statistical description (histogram, cumulative distribution function) of the drainage curvatures for each packing are given in Appendix A.

Imbibition Curvatures for Model Sediments

For computing the imbibition curvature we use two of the geometric data files described above:

`Coordinates_PackingNN.txt`
`Tes_Matrix_PackNN.txt`

where NN is the packing number, ranging from 1 to 76.

In the first type of data files are the coordinates of the spheres in each pack. The line number in the file corresponds to the index number of the sphere. There are 4 records in each line, which from left to right stores x coordinate, y coordinate, z coordinate and the sphere radius of the corresponding sphere, respectively.

In the second type of the data files are the sphere indices of the tetrahedra generated by using Delaunay tessellation. Each row corresponds to one tetrahedron, and the 4 numbers are the indices of the spheres that define this tetrahedron. The line number of the file is the index of the tetrahedron. The void space within each tetrahedron corresponds to a pore body.

In each tetrahedron, there may be an inscribed sphere, that is, a sphere that is tangent to all 4 spheres defining the tetrahedron. The radius of this so-called insphere can be used to calculate the imbibition curvature based on Mellor’s theory^[1].

The first step is to compute the insphere radii for the pores in each pack. The computation is based on the following nonlinear equation system:

$$\begin{aligned} (x_{inscribed} - x_1)^2 + (y_{inscribed} - y_1)^2 + (z_{inscribed} - z_1)^2 &= (r_{inscribed} + r_1)^2 \\ (x_{inscribed} - x_2)^2 + (y_{inscribed} - y_2)^2 + (z_{inscribed} - z_2)^2 &= (r_{inscribed} + r_2)^2 \\ (x_{inscribed} - x_3)^2 + (y_{inscribed} - y_3)^2 + (z_{inscribed} - z_3)^2 &= (r_{inscribed} + r_3)^2 \\ (x_{inscribed} - x_4)^2 + (y_{inscribed} - y_4)^2 + (z_{inscribed} - z_4)^2 &= (r_{inscribed} + r_4)^2 \end{aligned} \quad (3)$$

where $(x_{inscribed}, y_{inscribed}, z_{inscribed}, r_{inscribed})$ are the coordinates and radius of the inscribed sphere, and (x_i, y_i, z_i, r_i) are the coordinates and radii of the spheres forming the tetrahedron, where i ranges from 1 to 4.

We solve the above nonlinear equation system numerically. Iteration is a powerful tool to deal with this kind of problem. A relaxation factor of $2/3$ was used to stabilize the solution and a maximum iteration count of 10,000 was imposed.

The results showed that in some tetrahedra, there were no inscribed inspheres. This happens in some kinds of specific geometry. Examples include when 4 spheres have similar radii and their centers lie almost on a plane (Figure 1), and when a very big sphere is surrounded by 3 smaller spheres (Figure 2). The possibility of not finding inscribed sphere increases as the packing gets worse sorted. For the well sorted packing (e.g. packing 1), this situation only happened around 10 times in our calculation; however in the less well sorted packings (e.g. packing 19), the situation happens thousands of times.

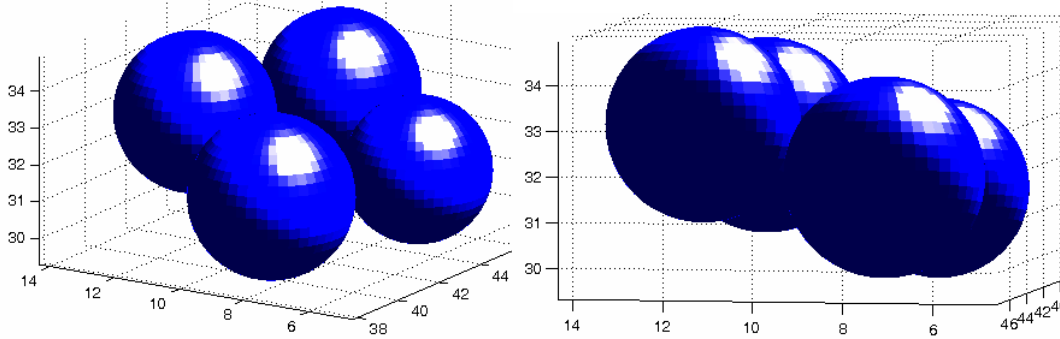


Figure 1, A pore (Delaunay tetrahedron) for which an inscribed sphere does not exist. The left and right figures show the same pore from different points of view.

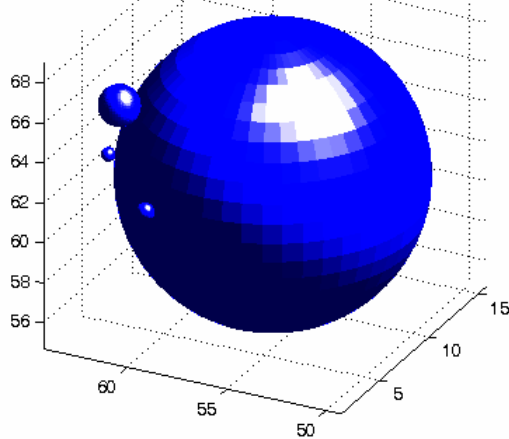


Figure 2, A pore (Delaunay tetrahedron) formed by one large sphere and three smaller spheres. No inscribed sphere exists for this pore.

The estimate of dimensionless imbibition curvature due to Mason and Mellor^[1] is given by:

$$C_{imb}^* = \frac{2R_{avg}}{r_{inscribed}} - 1.6 \quad (4)$$

where R_{avg} is the average radius of spheres in the packing. This equation was derived from monodisperse sphere pack. The constant -1.6 is introduced in the equation in order to preserve the imbibition hysteresis. However, as it was originally developed from the monodisperse pack, this equation turn out not to be applicable to packings with sufficiently broad distribution of sphere radii. We have therefore developed a modified equation using insights gained from application of the level set method.

Prodanović and Bryant^[2] developed a novel way to calculate the imbibition curvature by using Level Set Method. All pores can have a multiplicity of imbibition curvatures, depending on which menisci and/or pendular rings merge to trigger the imbibition event. For a given pore, the largest curvature of these curvatures, and therefore the curvature most likely to apply during an imbibition process, is found when menisci in two throats merge. The merger of menisci is physically and geometrically analogous to Haines' original concept, namely, that a pore imbibed when the gas/water meniscus forms a sphere contained within the pore. Consequently there is a strong correlation between this curvature and the Haines' estimate of $C_{imb}^* = \frac{2R_{avg}}{r_{inscribed}}$. For a monodisperse packing, the imbibition curvatures, which are dependable, can be approximately fit by the following equation:

$$C_{imb}^* = \frac{1.25R_{avg}}{r_{inscribed}} + 0.8 \quad (5)$$

Equation(5) eliminates the possibility of negative imbibition curvatures and is simple to use. In the report, the imbibition curvature calculations are all based on equation(5).

The final results include the following two kinds of data files:

`Insphere_Coordinates_PackingNN.txt`, which are stored in folder 'Insphere Coordinates';

`Imbibition_Curvatures_PackingNN.txt`, which are stored in folder 'Imbibition Curvatures'

where `NN` is the packing number, ranging from 1 to 76.

In `Insphere_Coordinates_PackingNN.txt`, we stored the coordinates and radii of the inscribed spheres. In each row, there are four numbers, corresponding to x, y and z coordinates of an inscribed sphere and its radius, the row index of these numbers corresponds to the row index of `Tes_Matrix_PackNN.txt`.

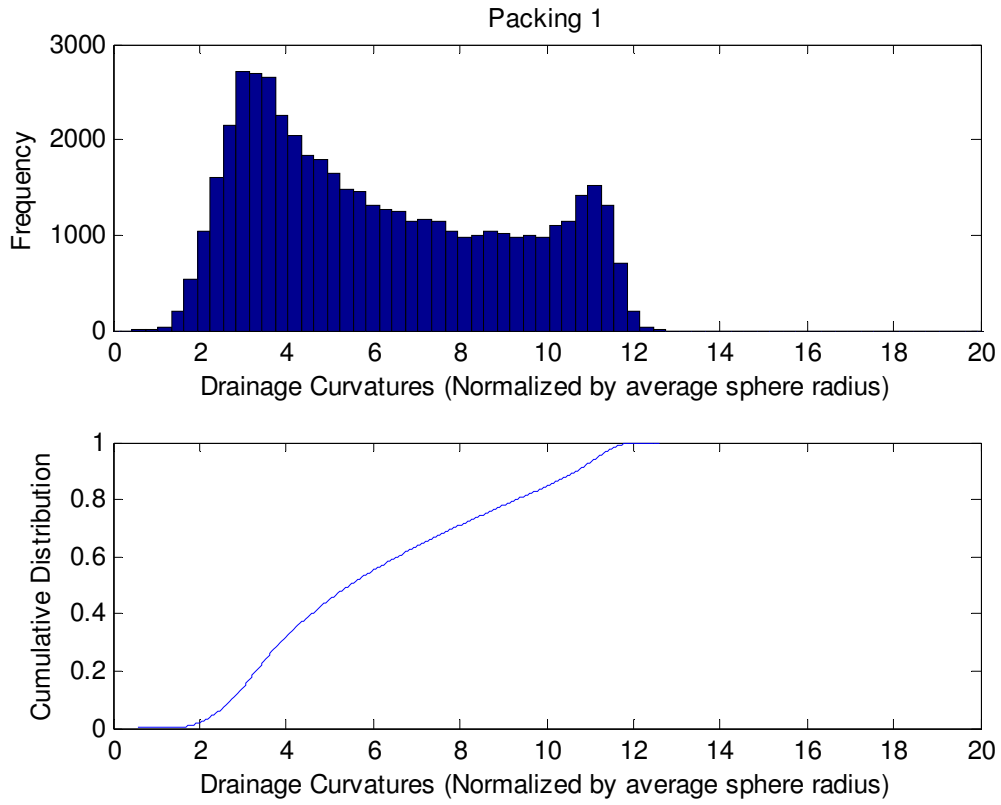
In `Imbibition_Curvatures_PackingNN.txt`, we stored the imbibition curvatures, computed from equation(5). The row index of these numbers corresponds to the row index of `Tes_Matrix_PackNN.txt`.

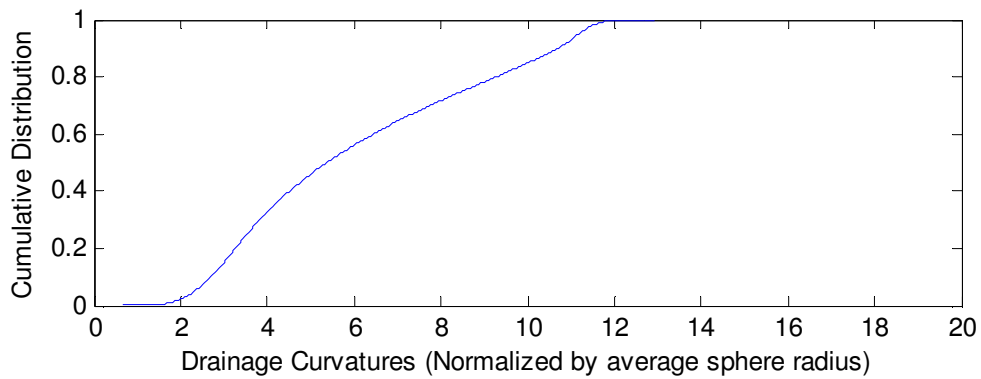
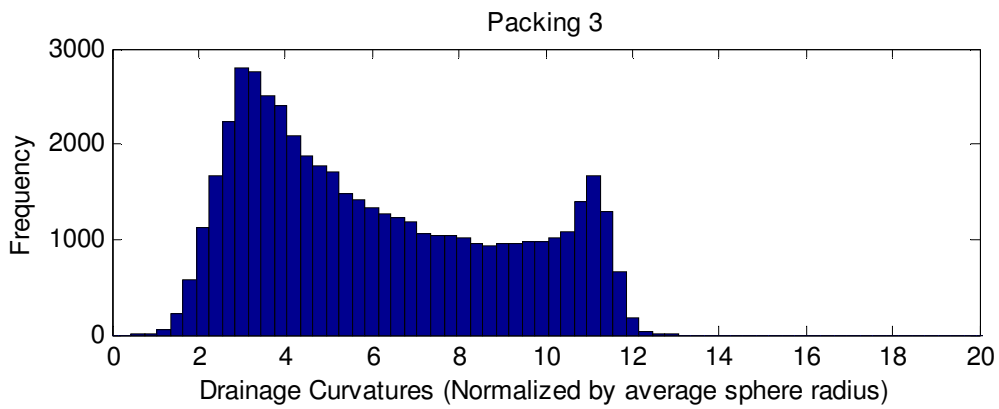
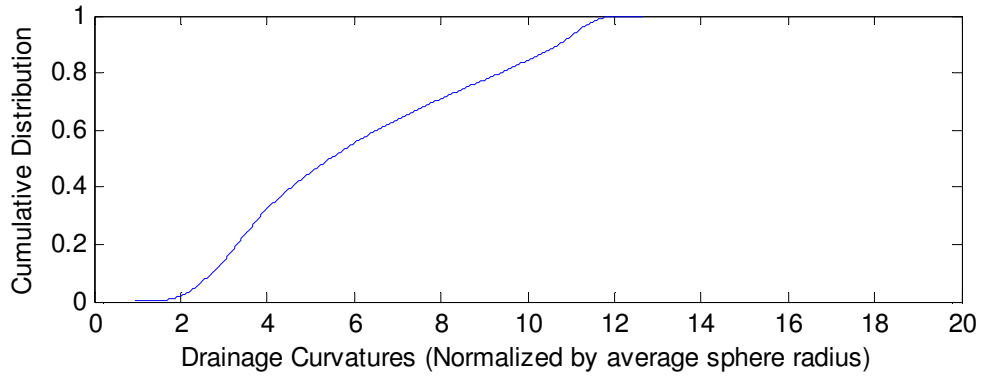
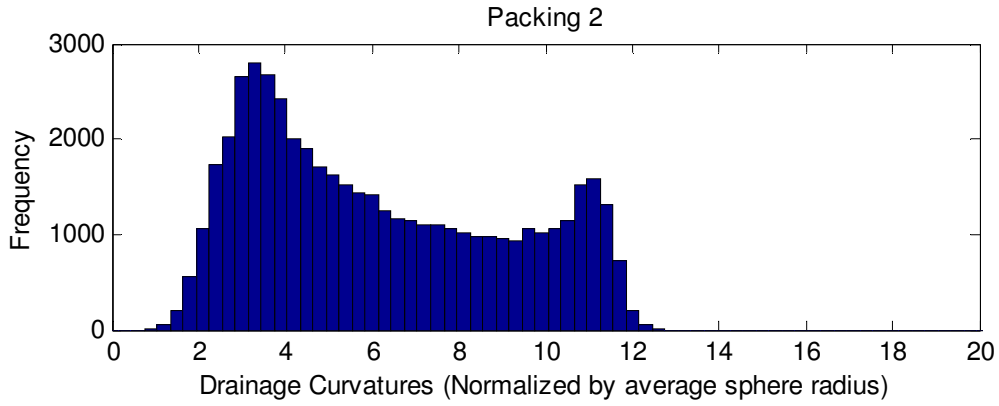
For both kinds of data files, the string 'NaN' corresponds to the situation where there is no inscribed sphere in a tetrahedron (and therefore no imbibition curvature).

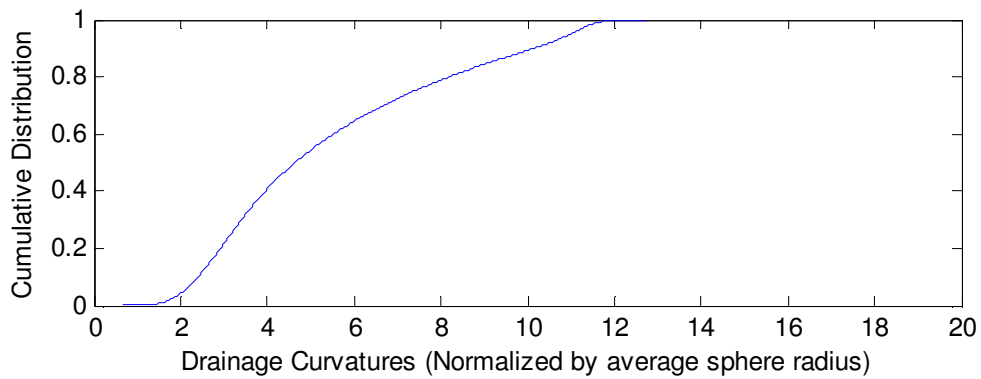
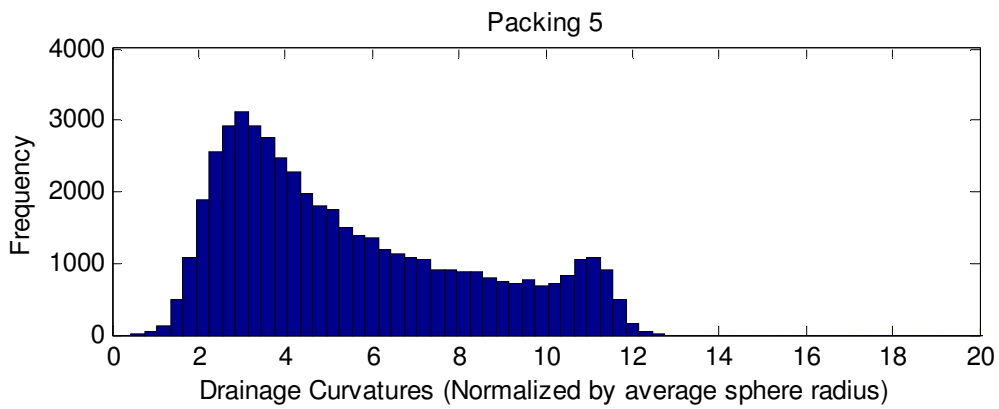
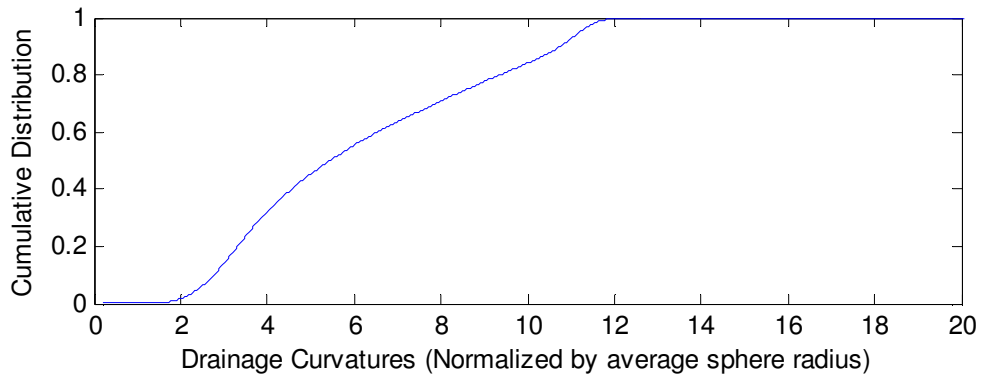
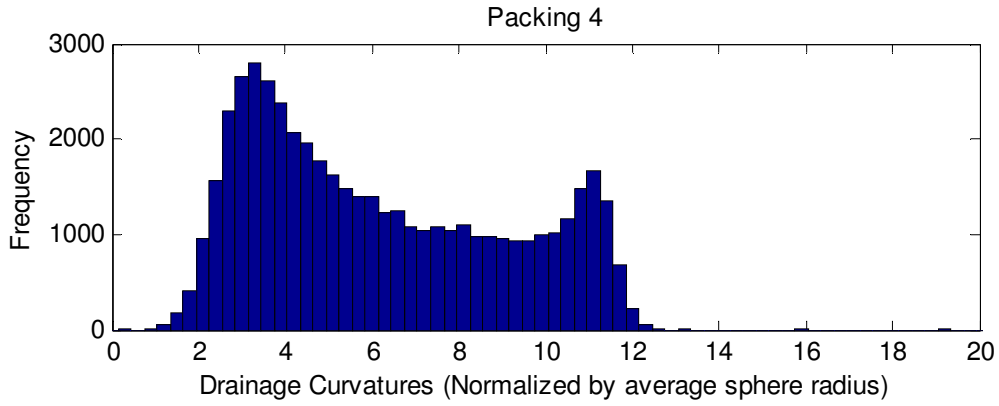
Statistical description (histogram, cumulative distribution function) of the curvatures for each packing are given in Appendix B.

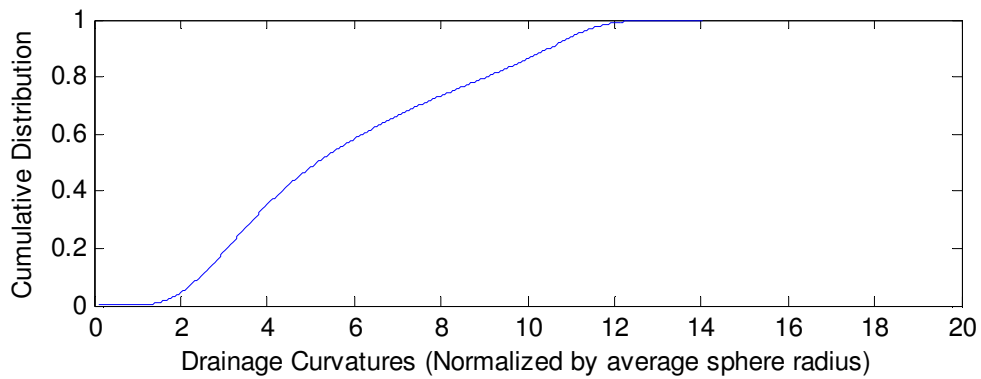
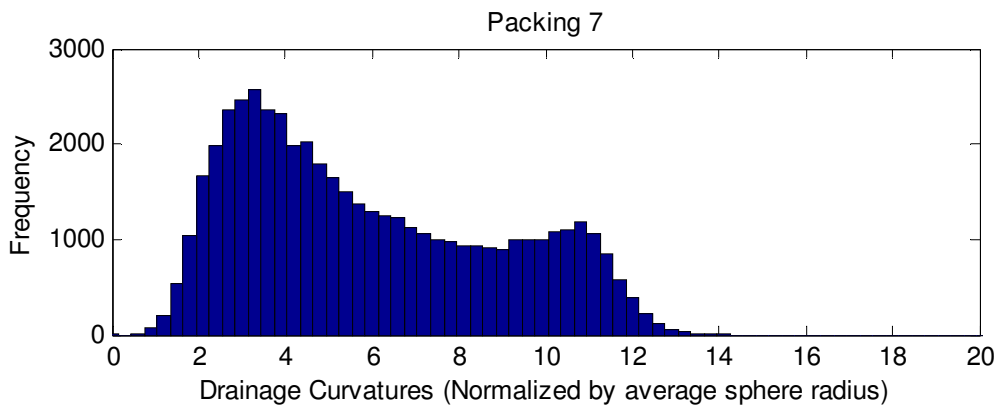
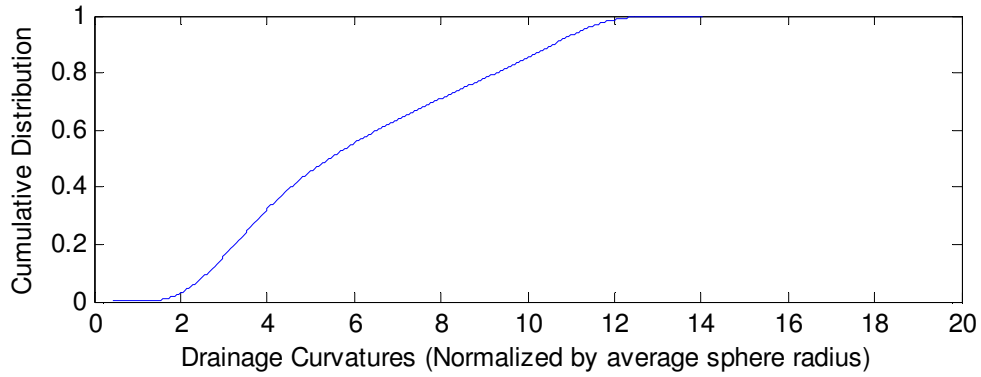
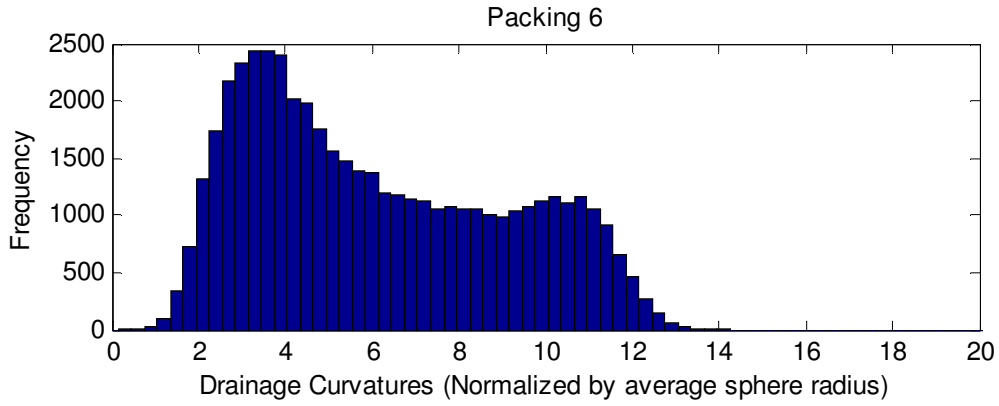
APPENDIX A

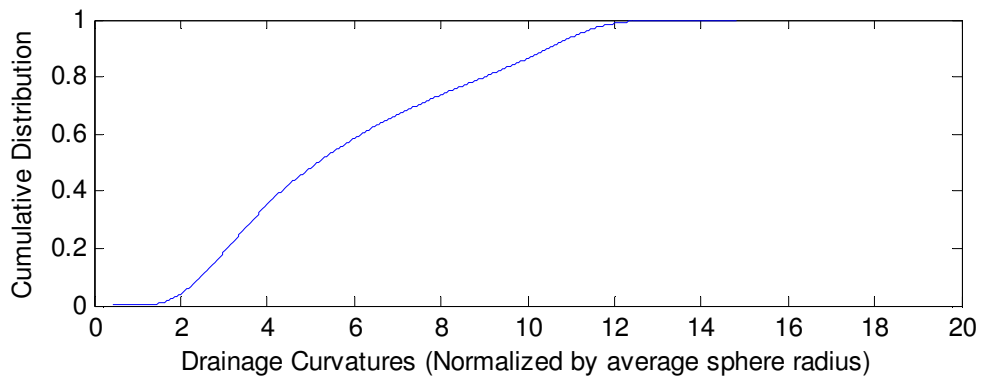
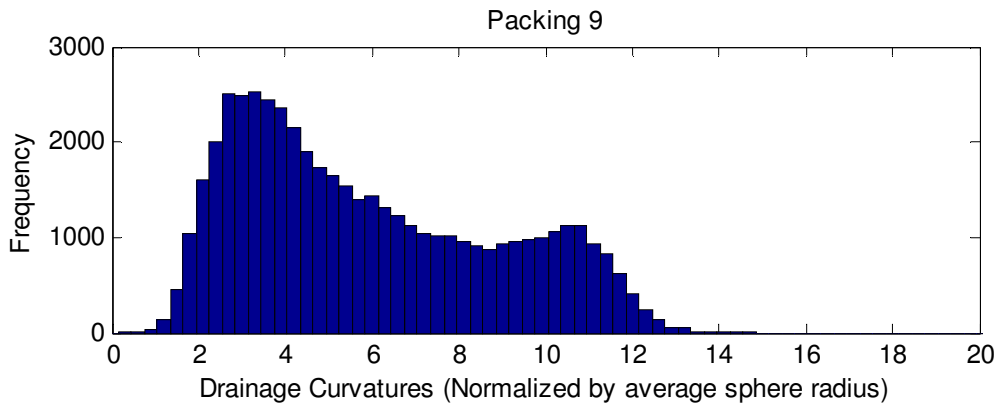
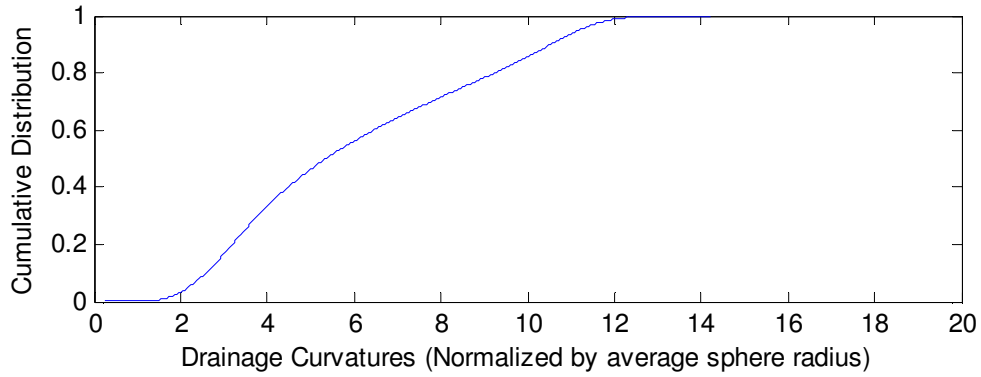
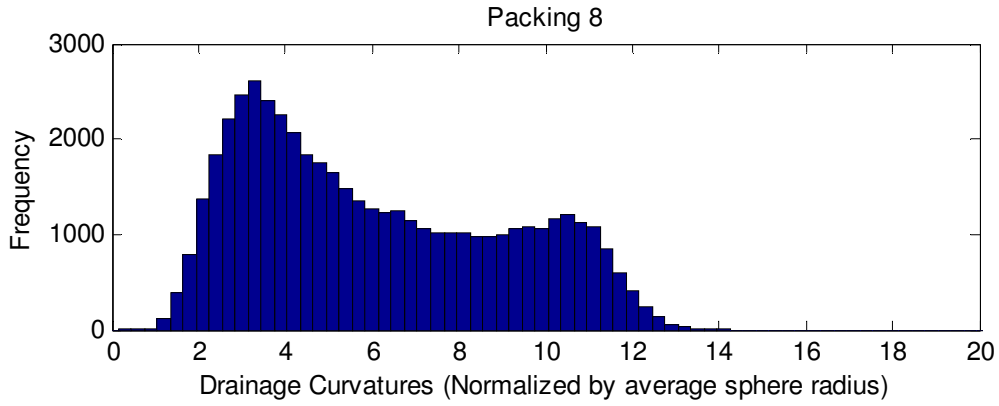
Statistical Information on Drainage Curvatures

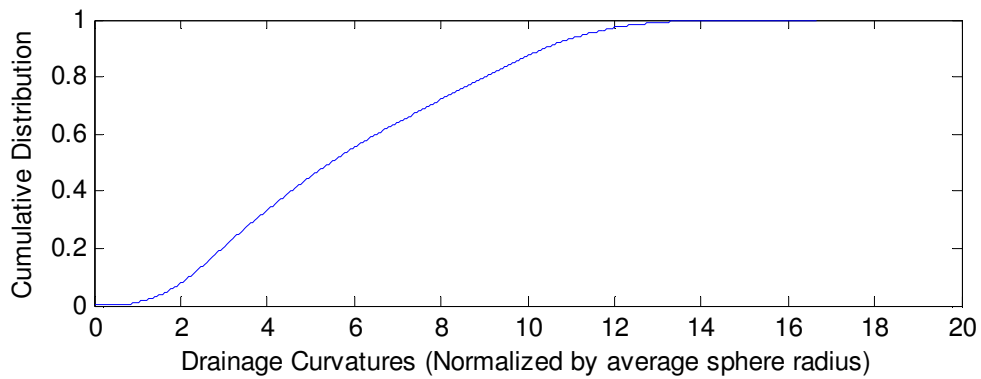
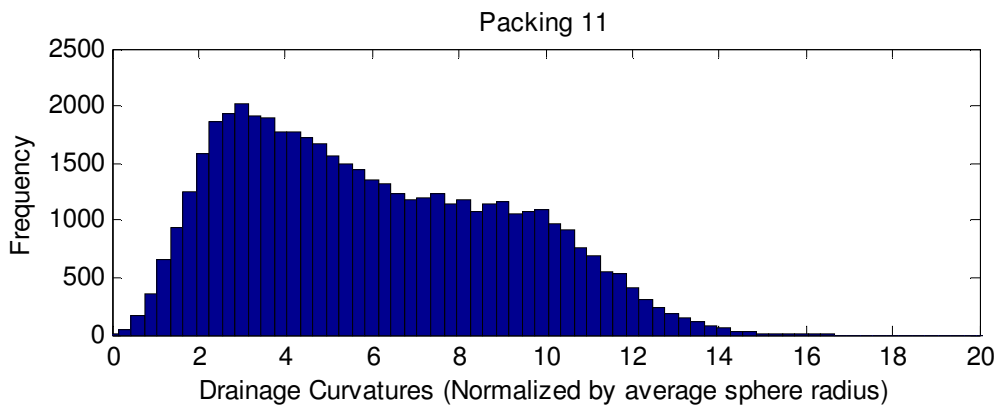
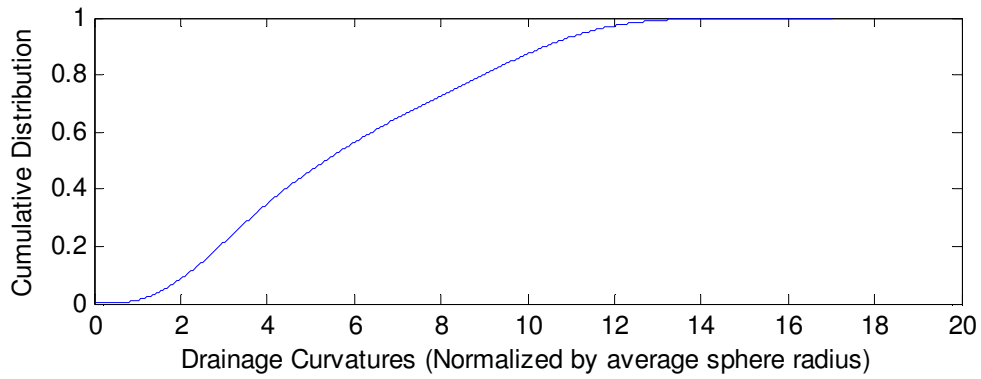
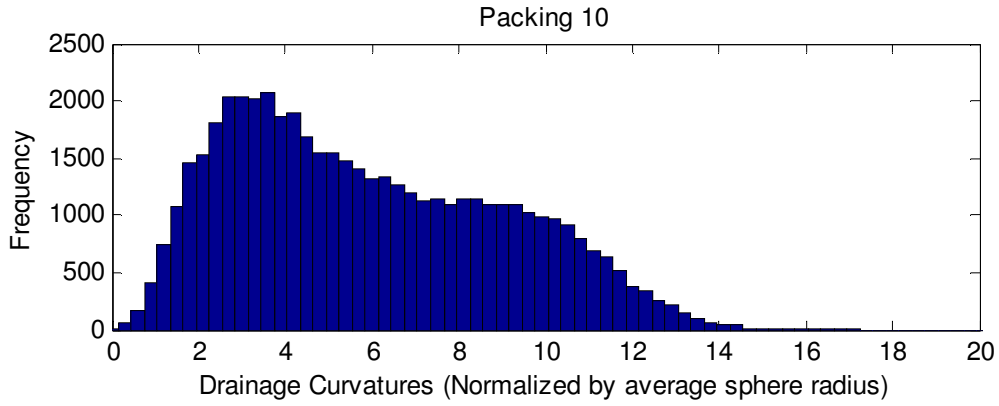


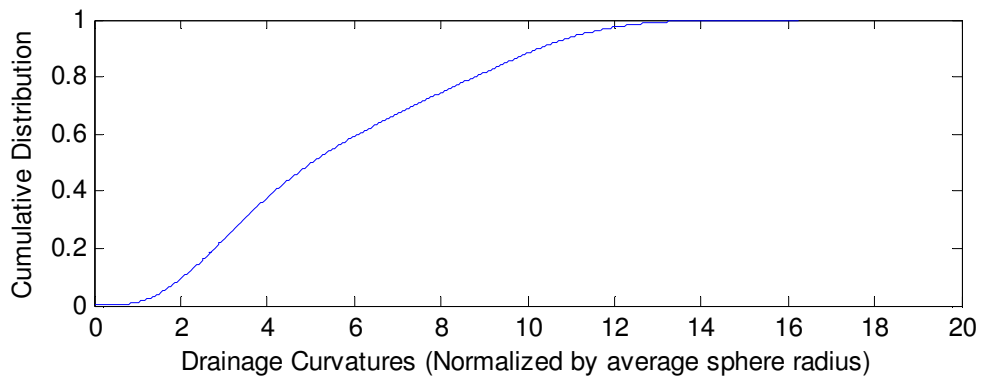
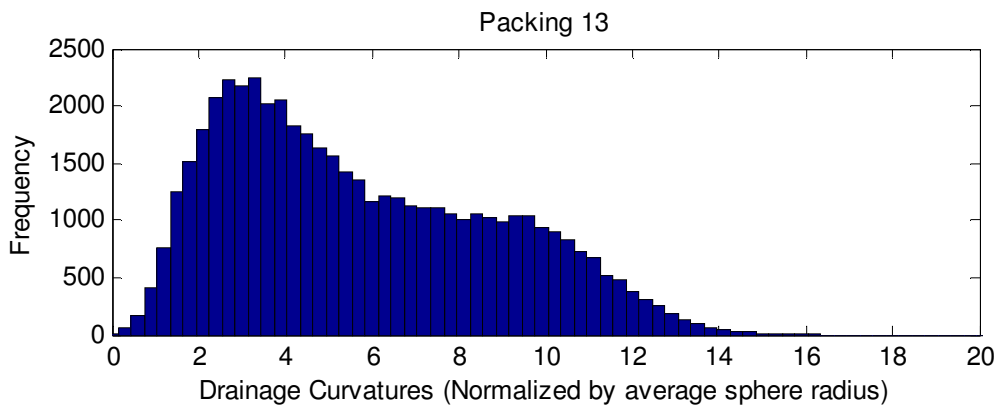
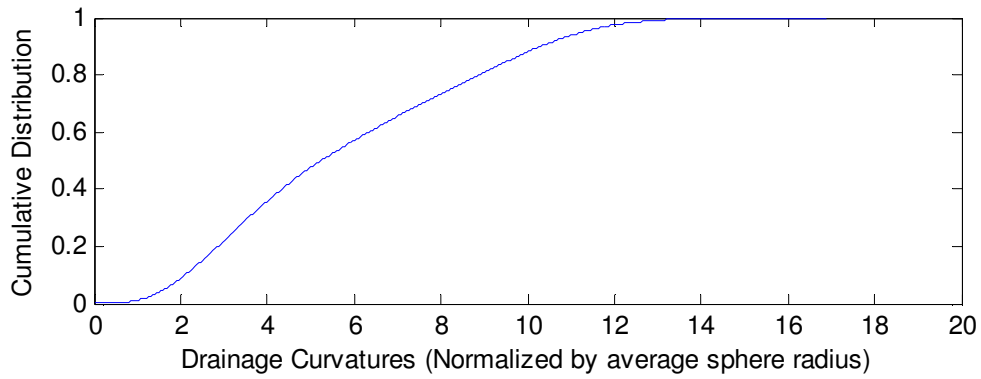
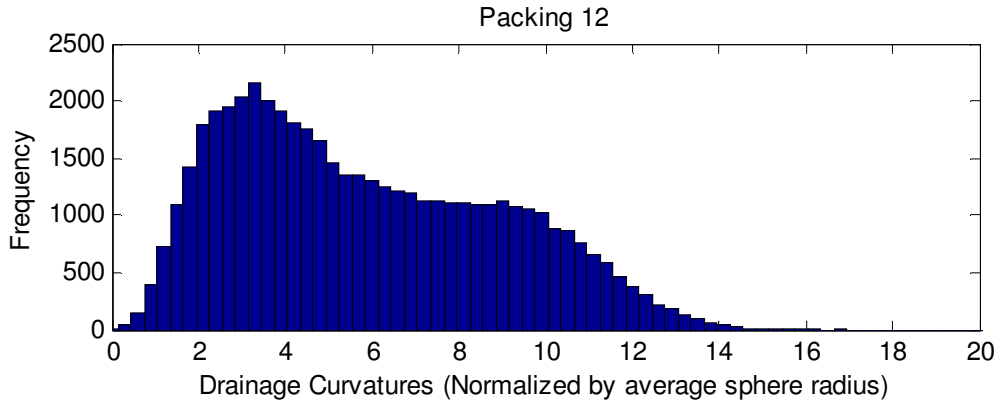


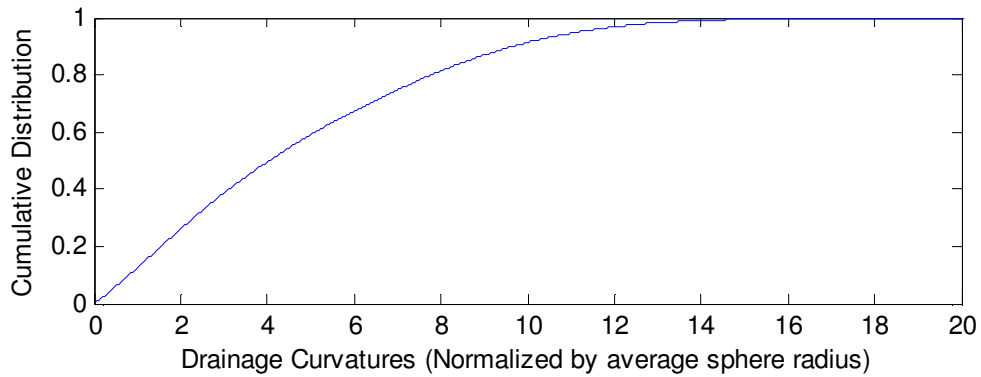
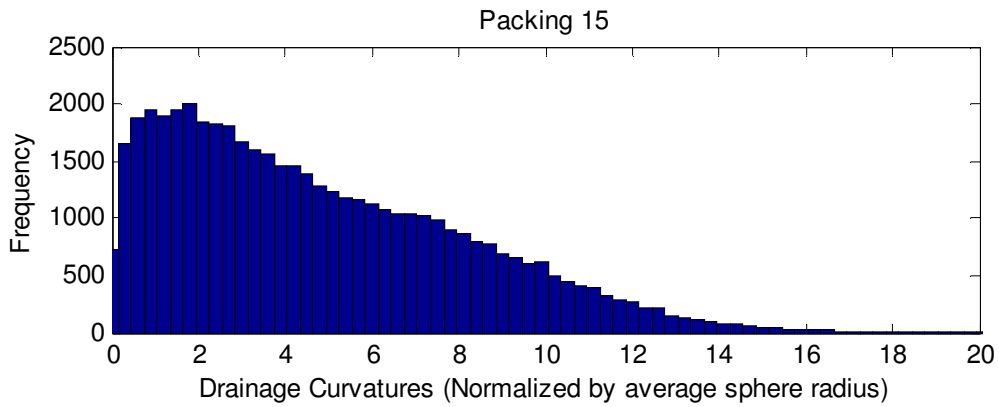
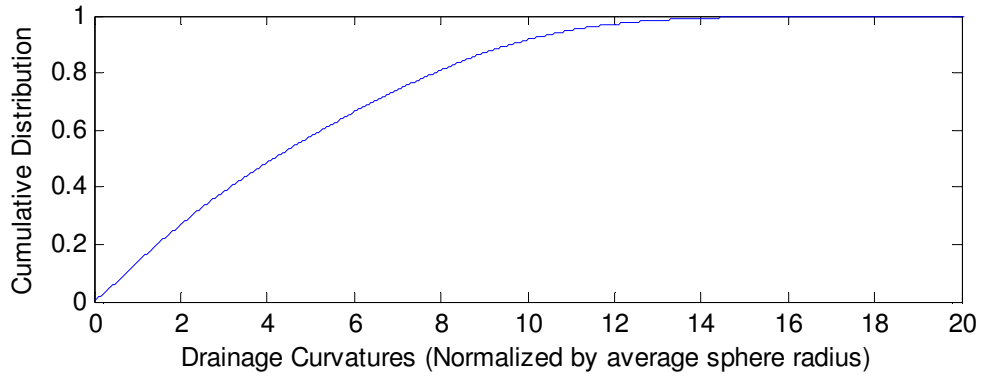
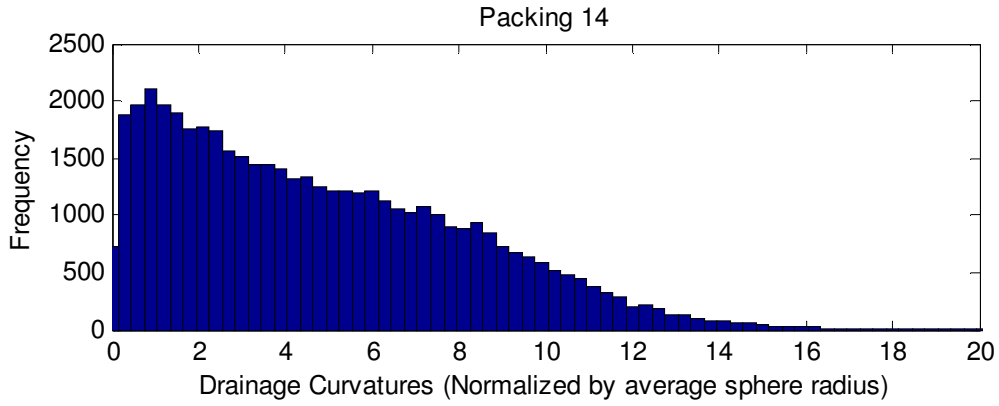


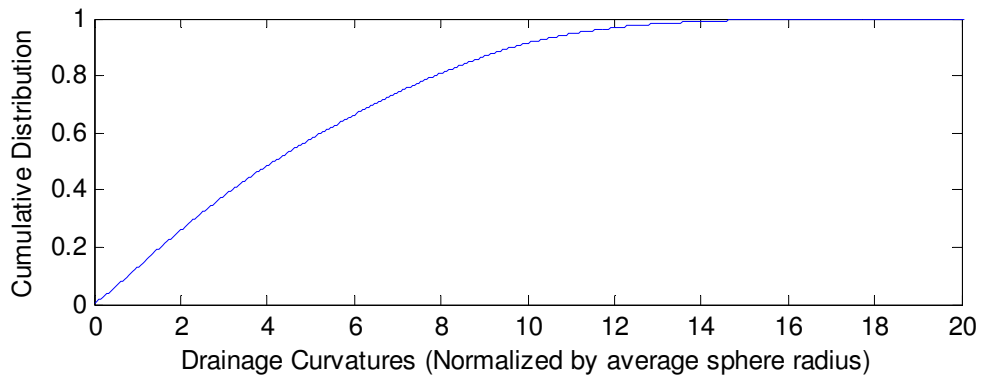
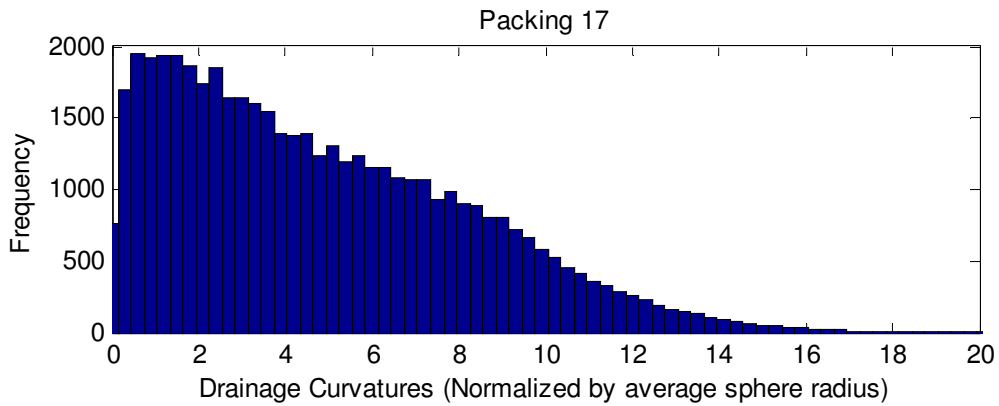
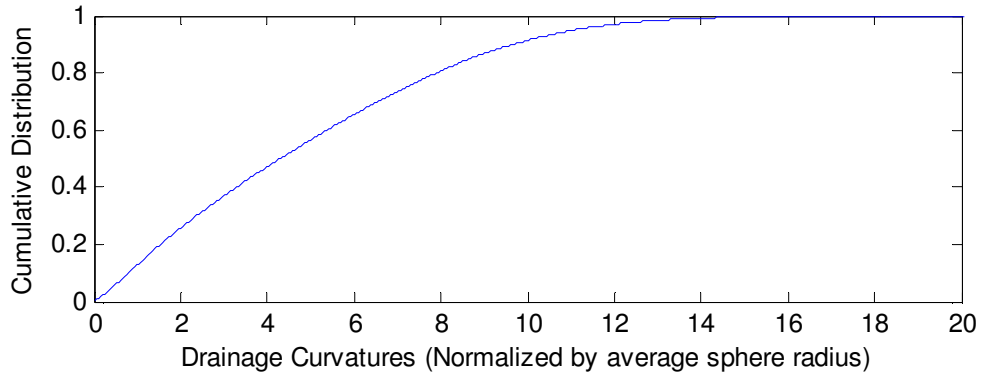
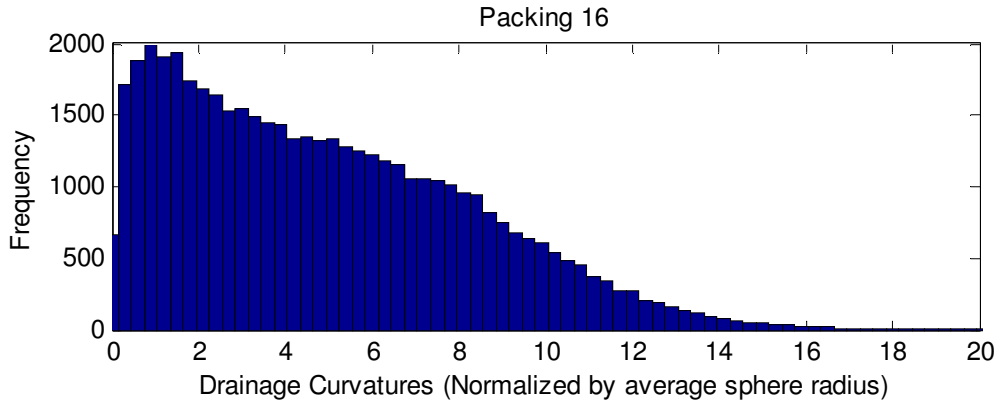


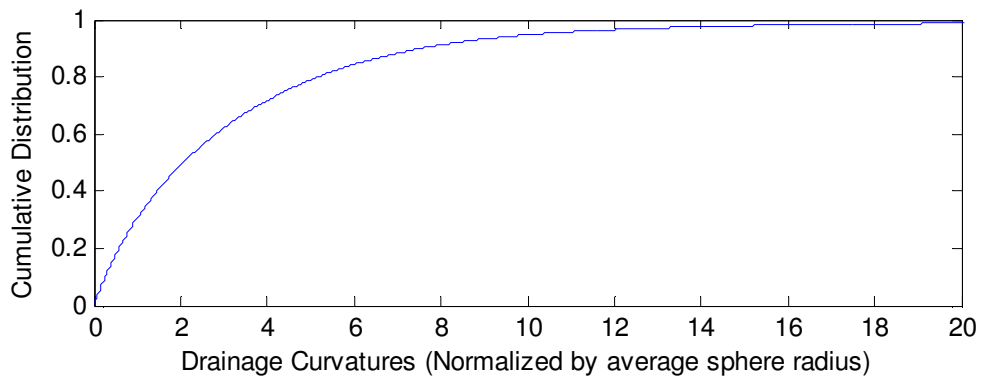
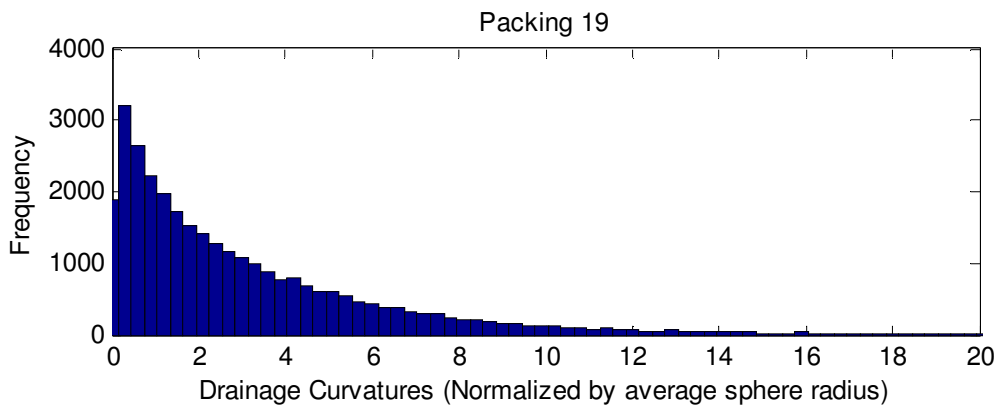
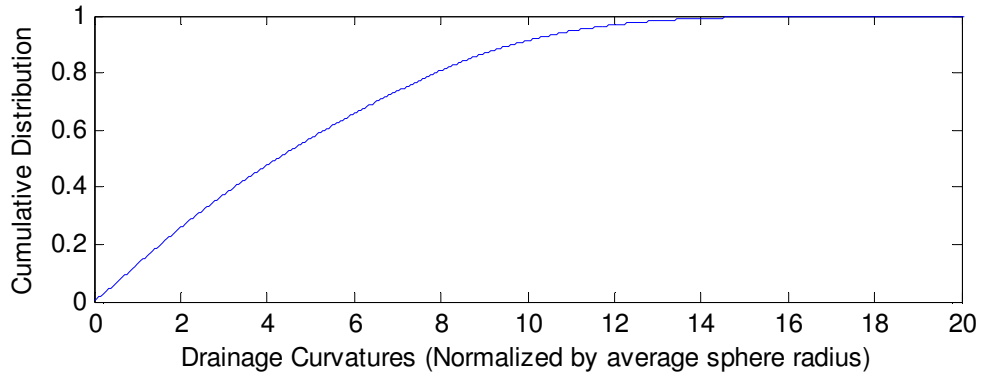
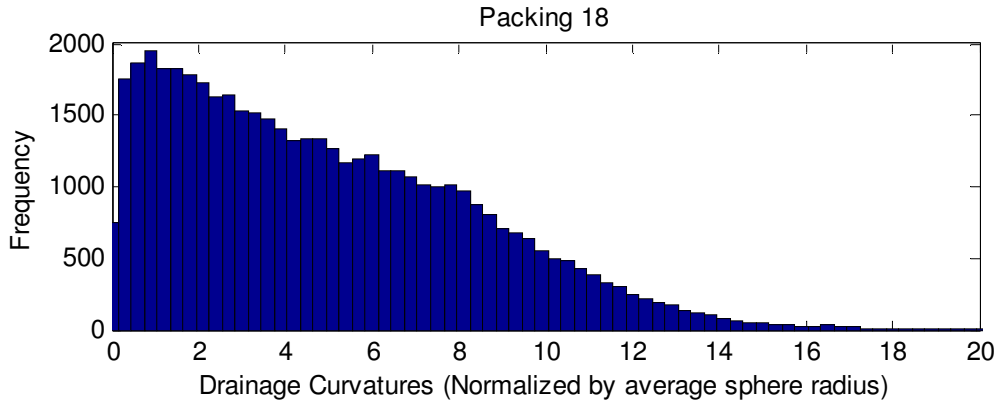


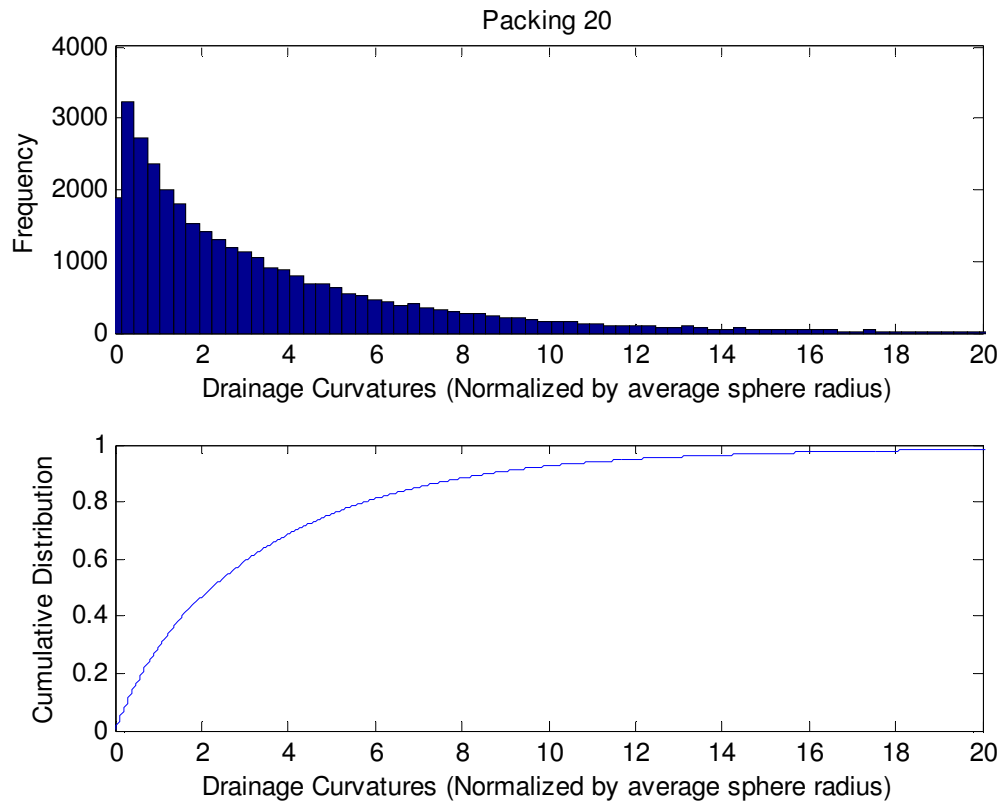


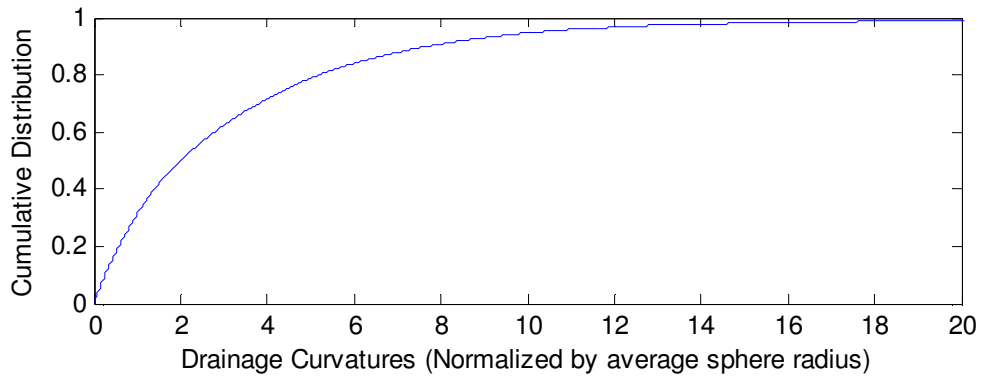
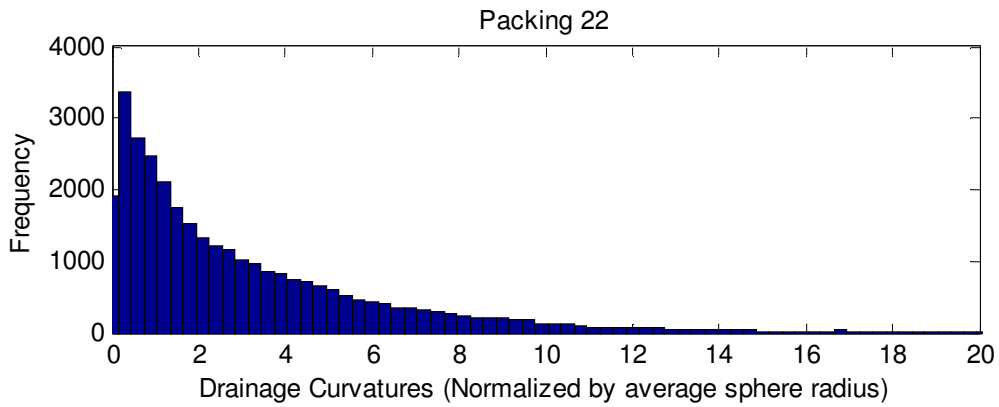
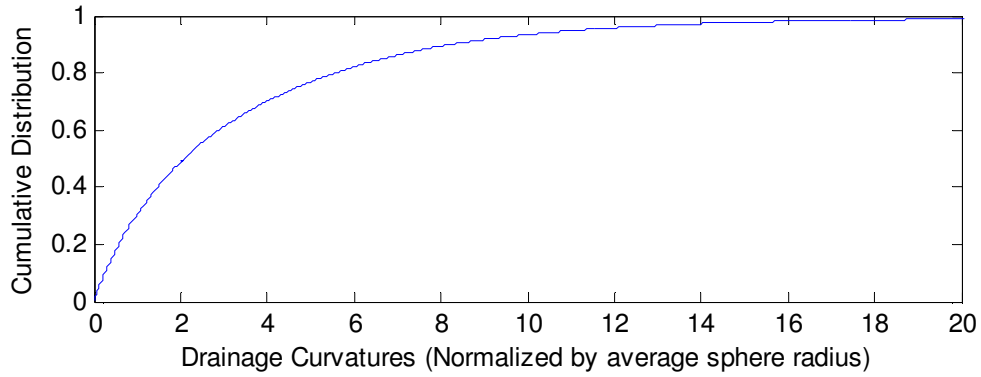
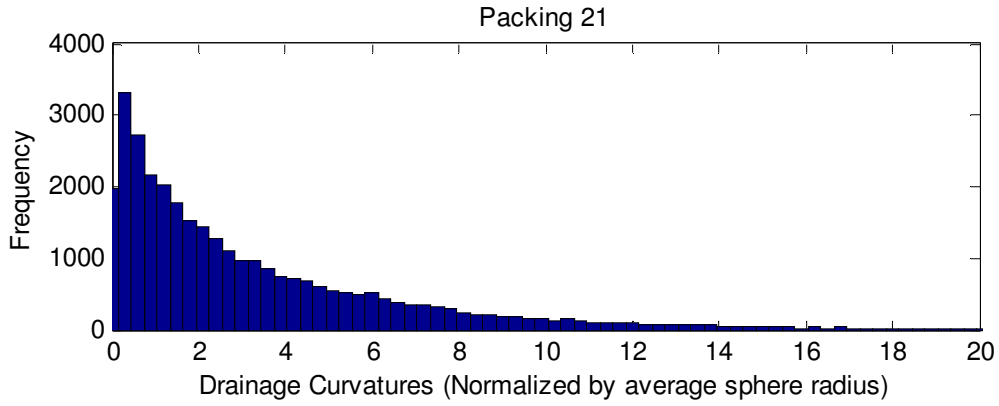


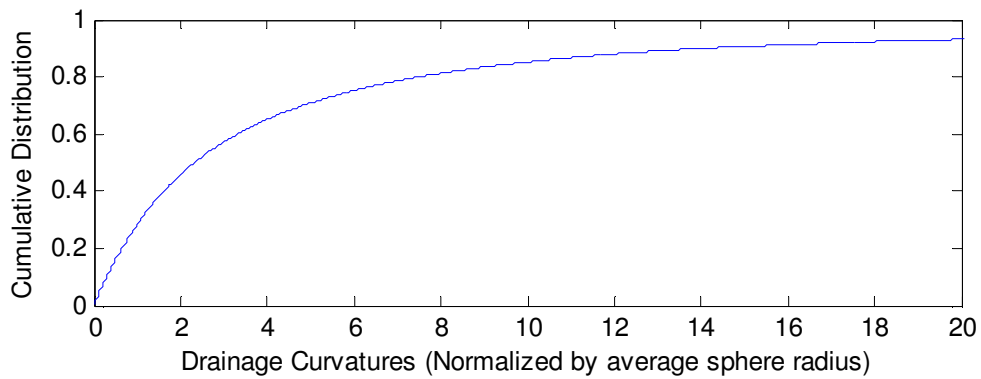
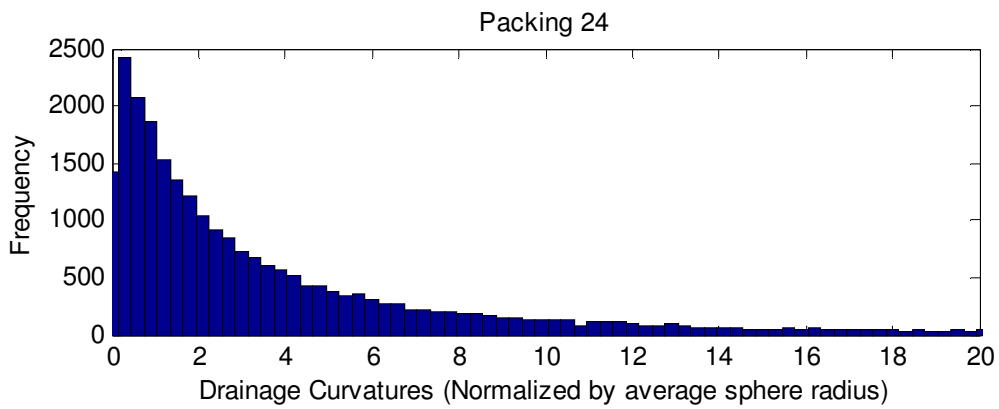
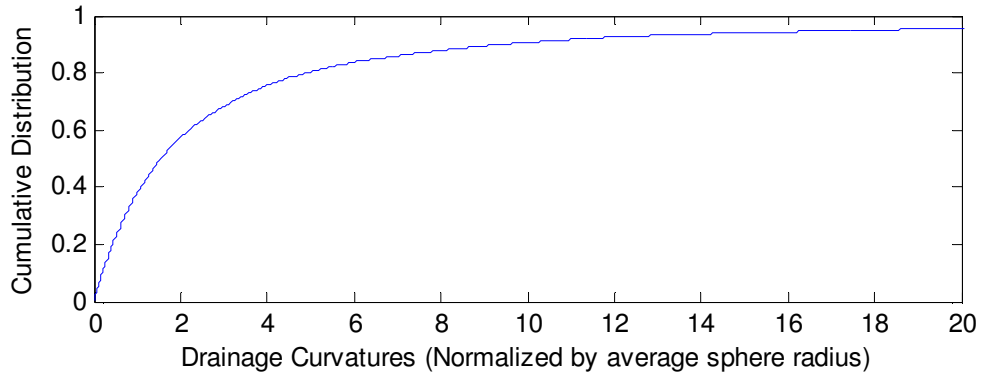
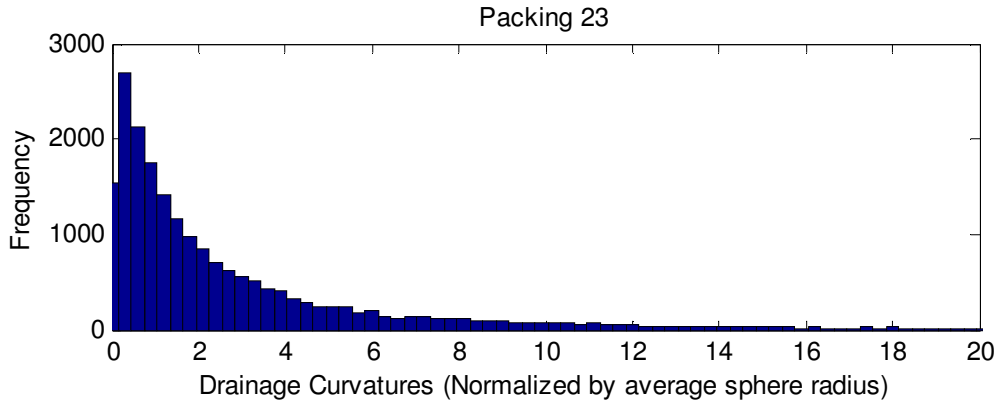


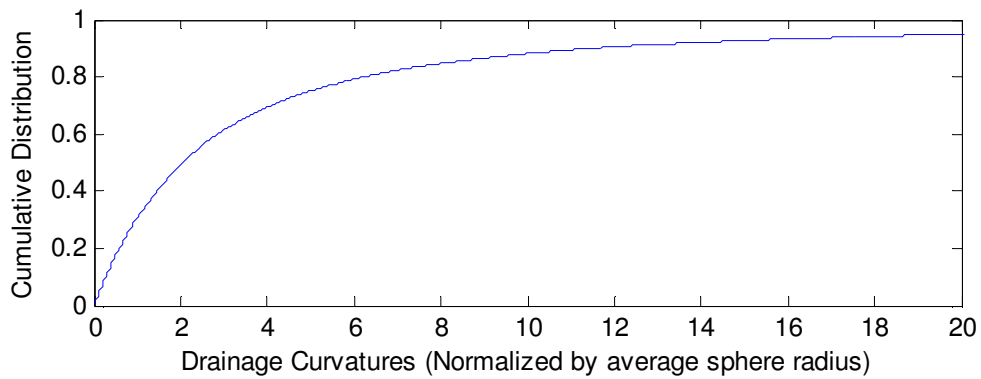
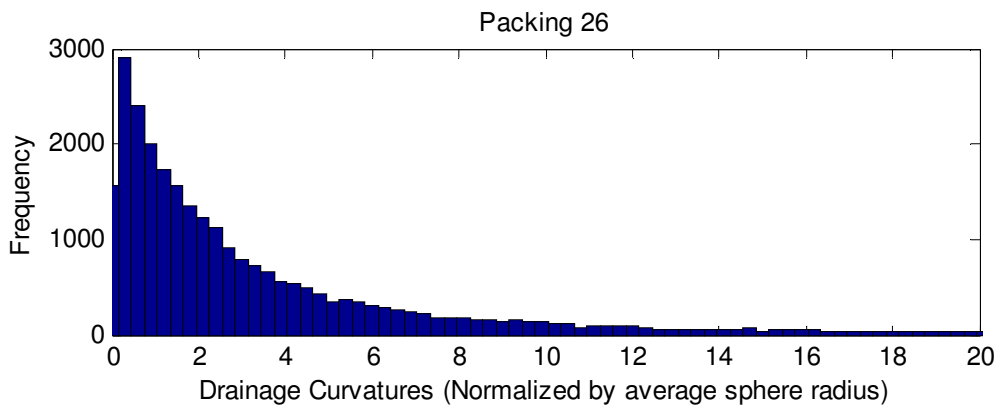
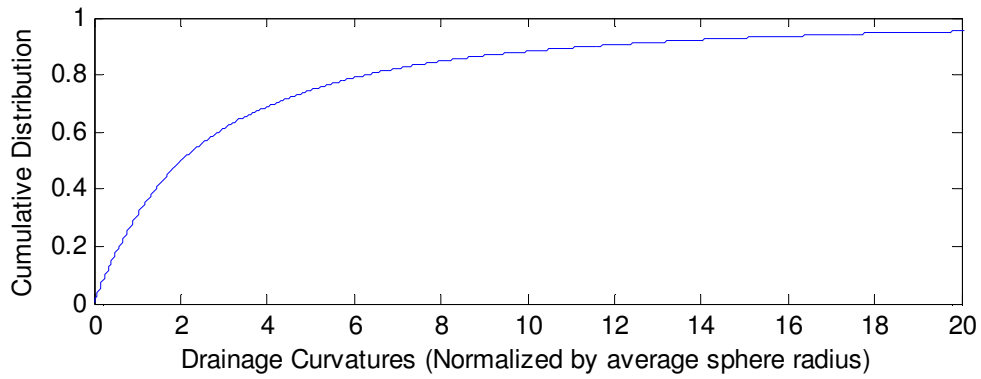
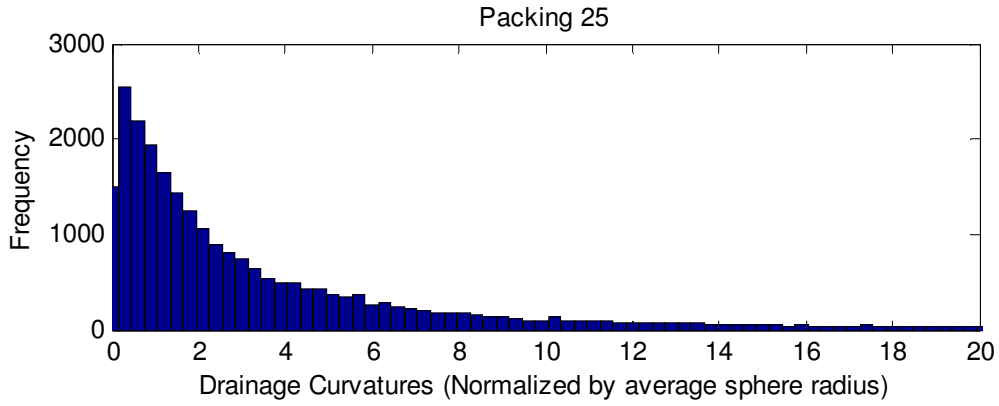


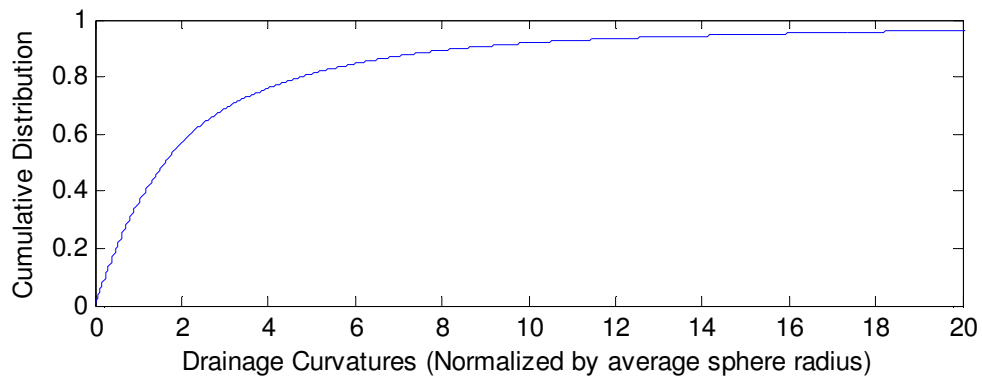
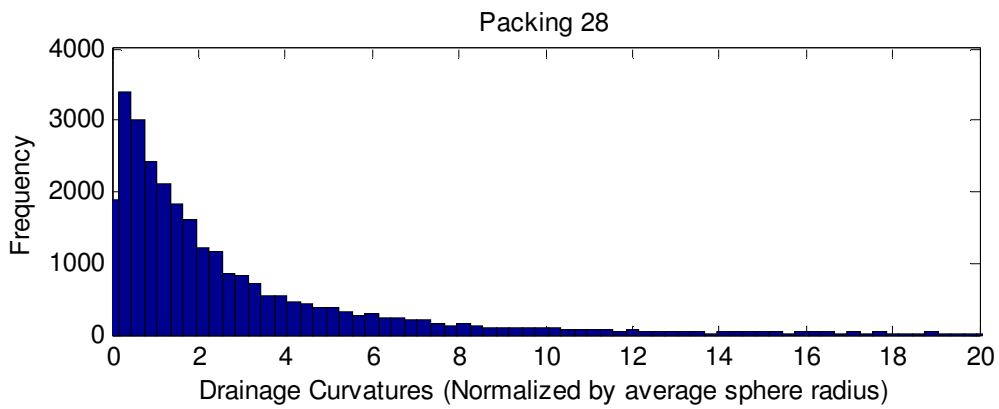
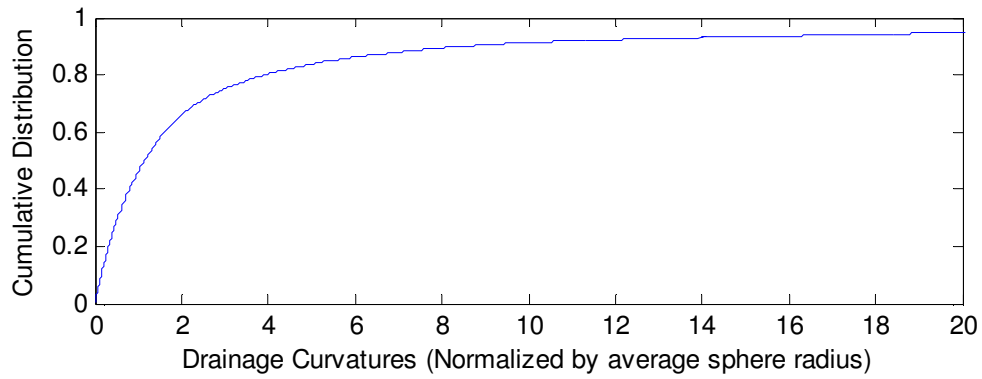
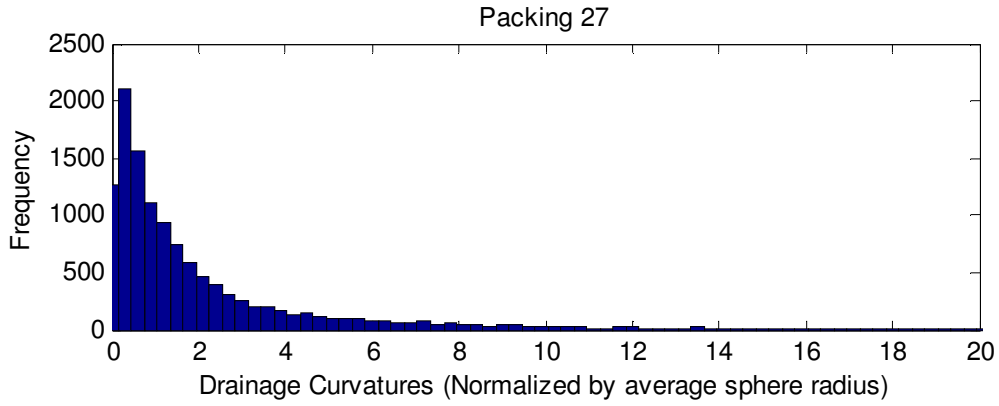


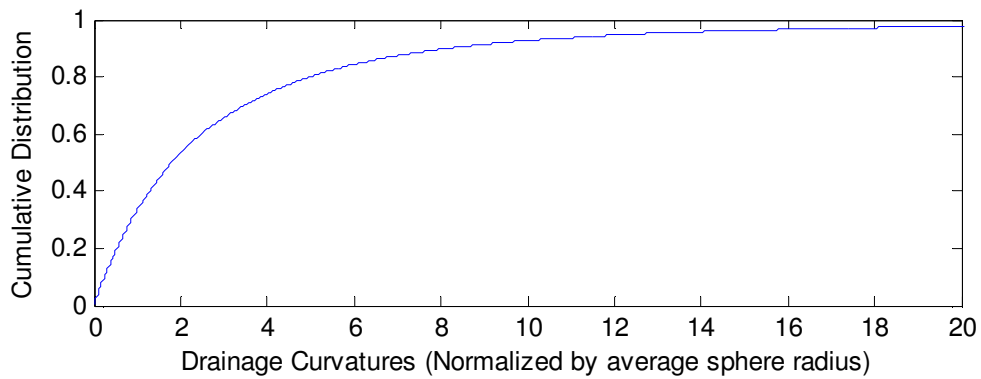
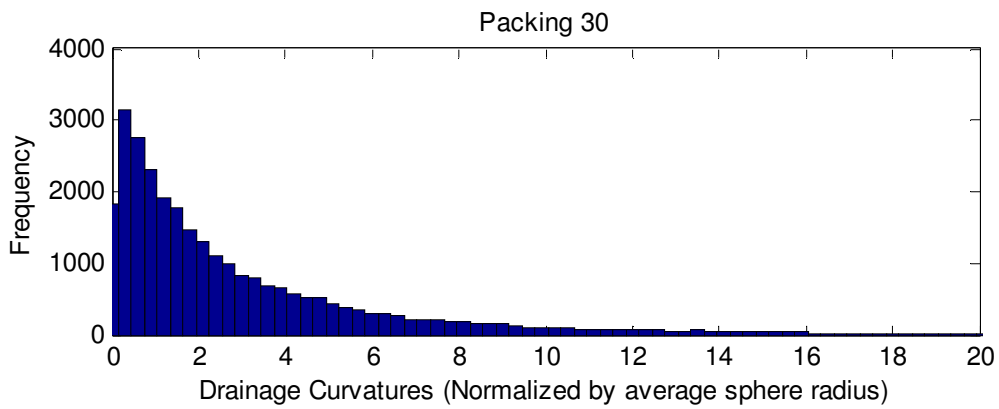
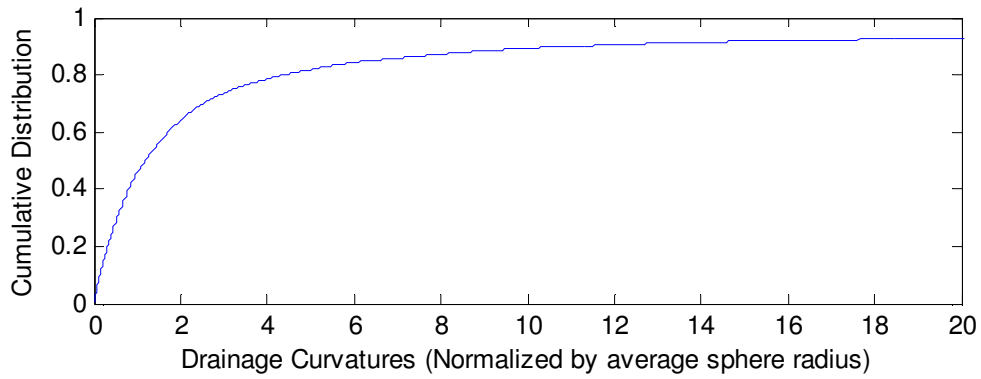
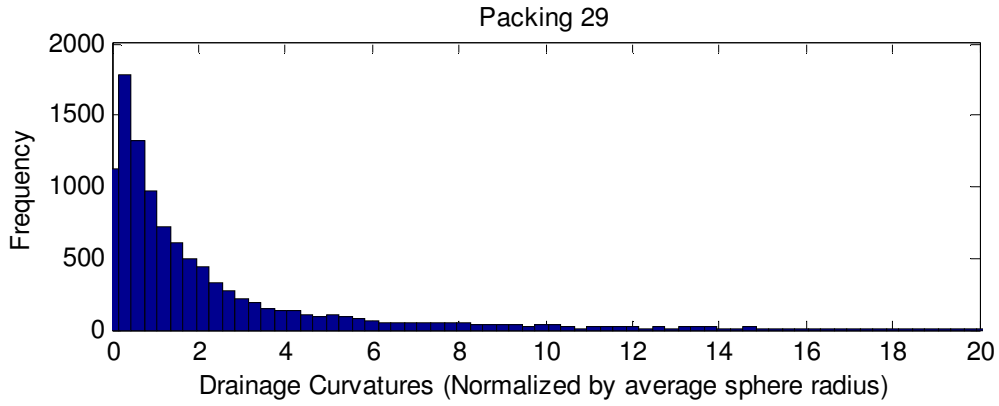


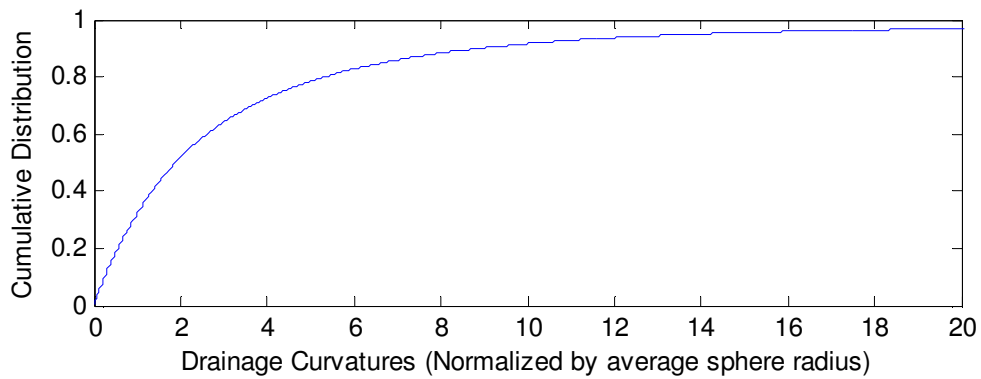
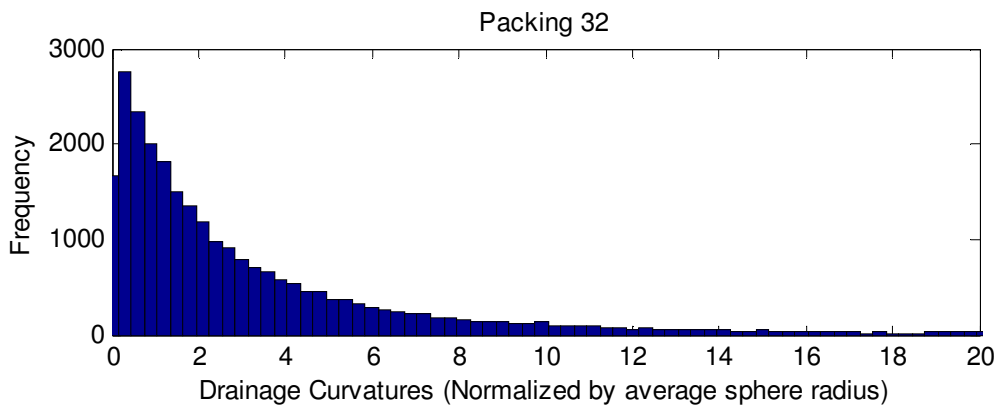
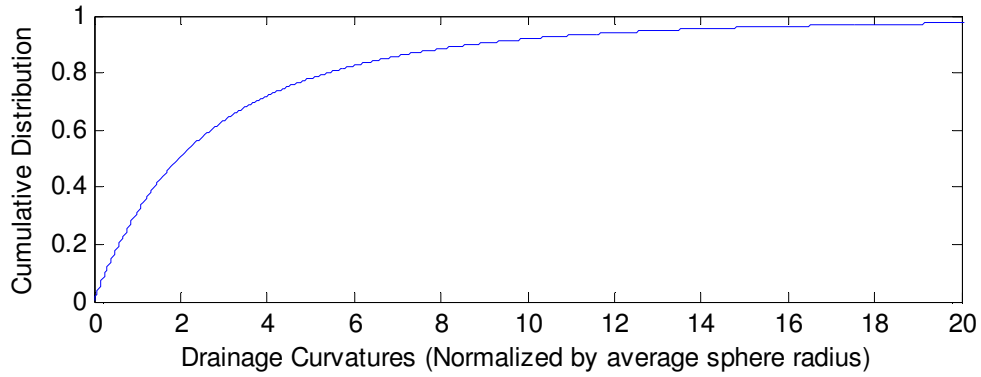
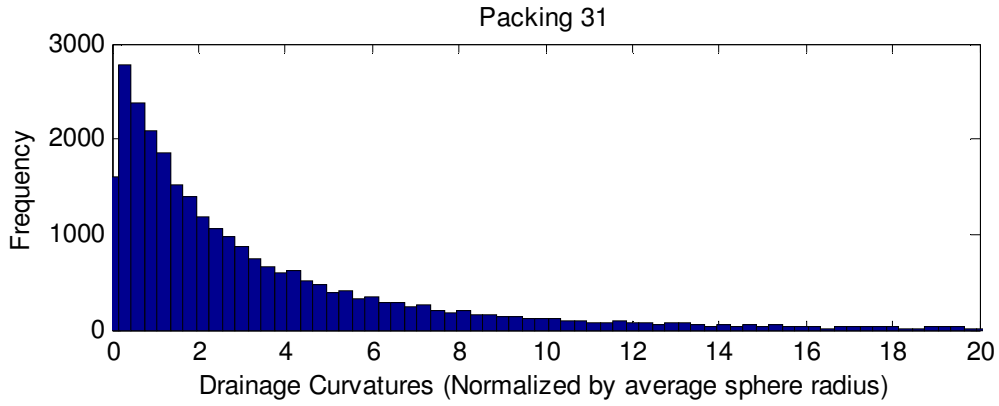


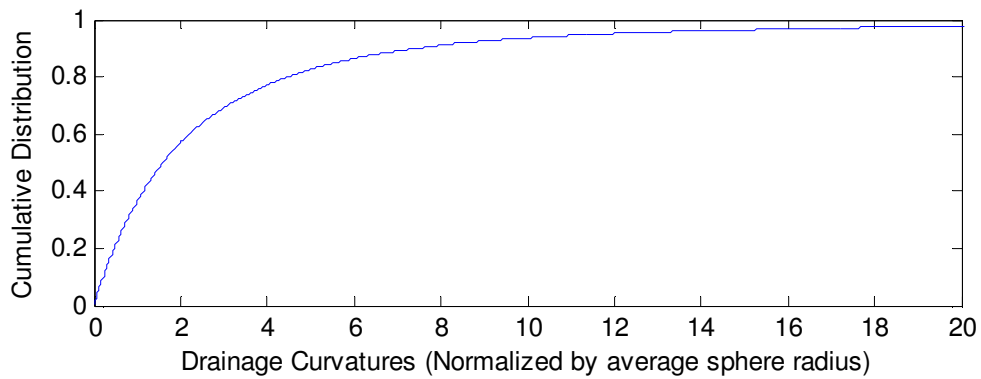
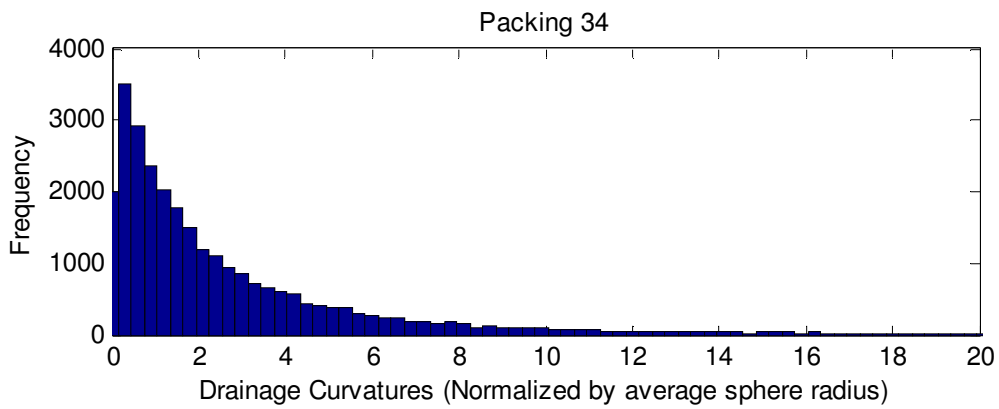
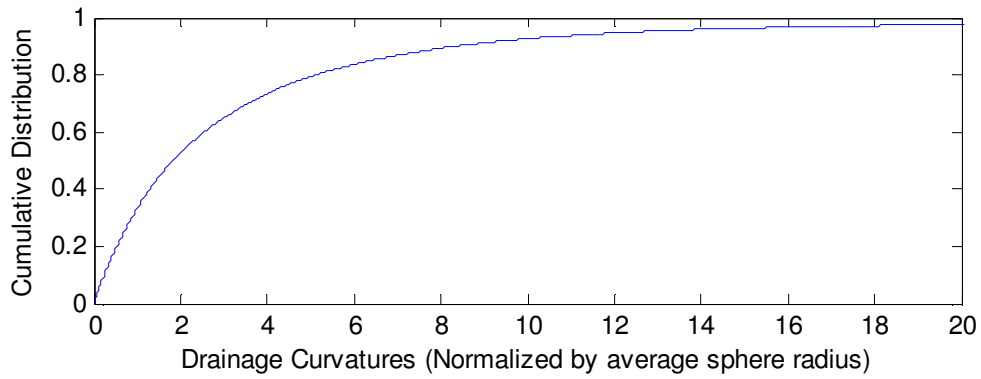
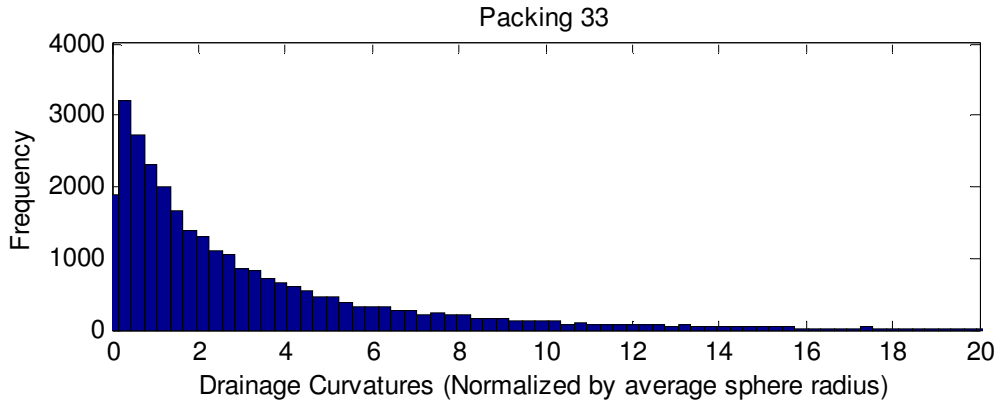


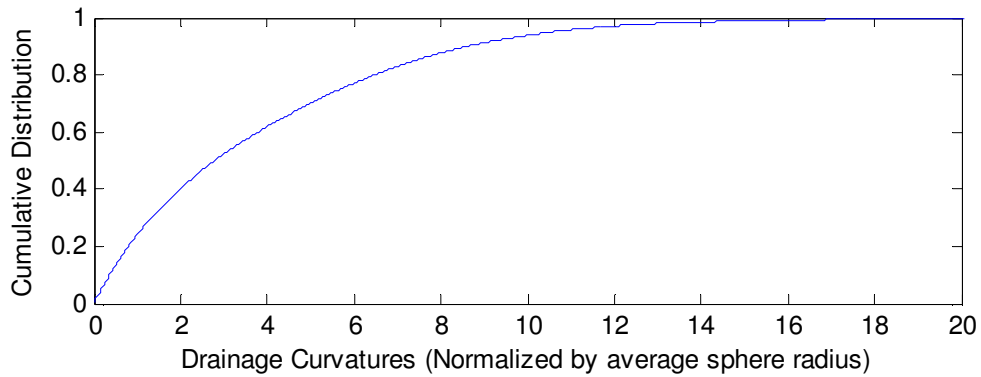
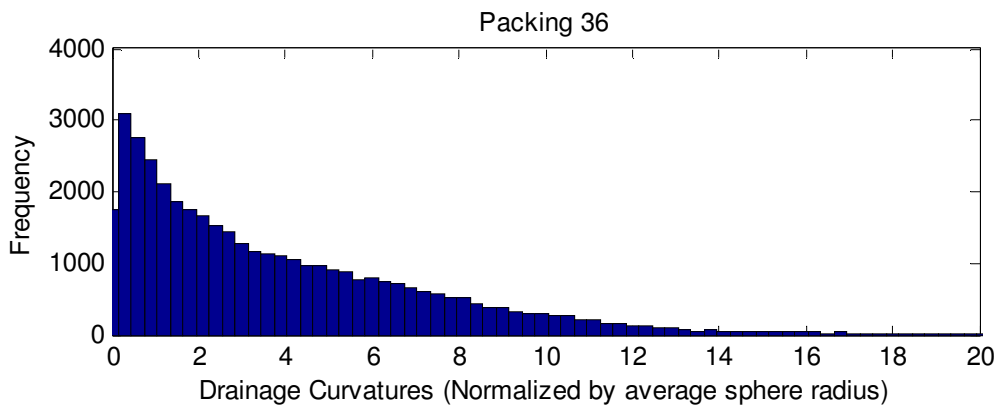
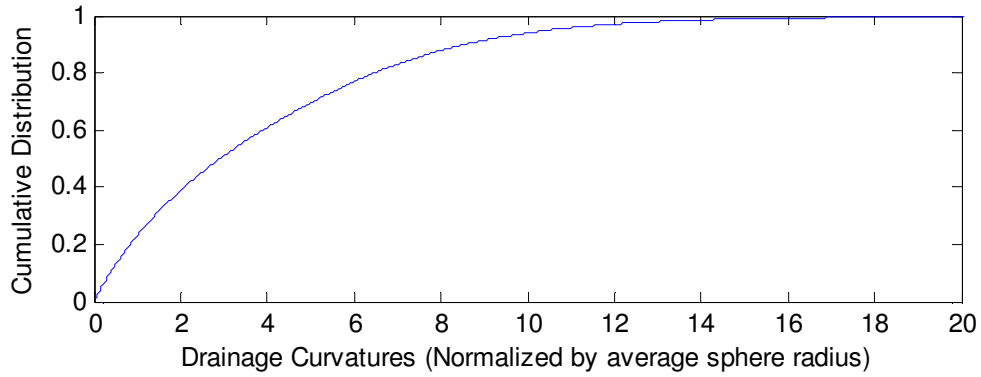
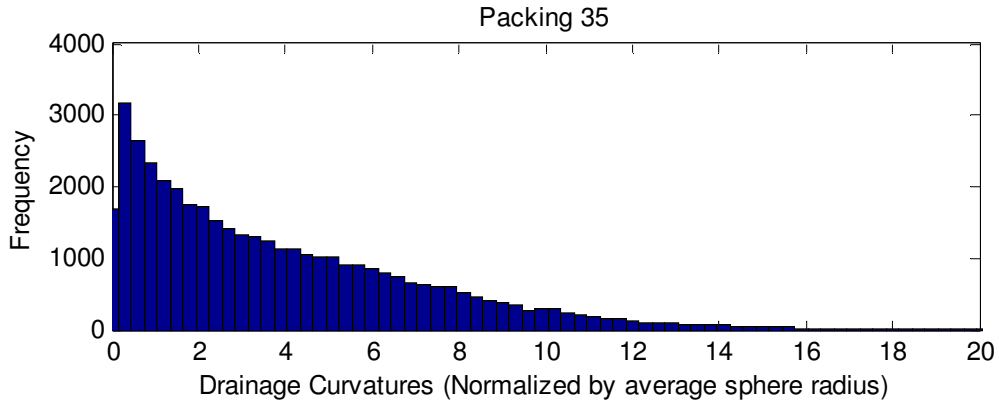


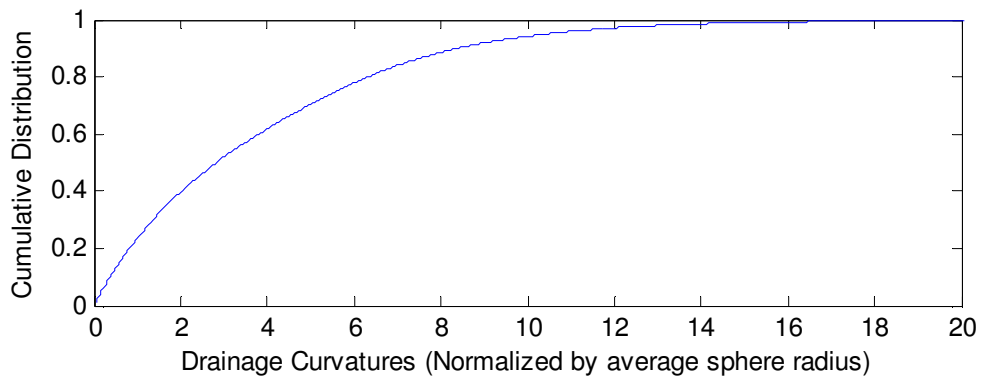
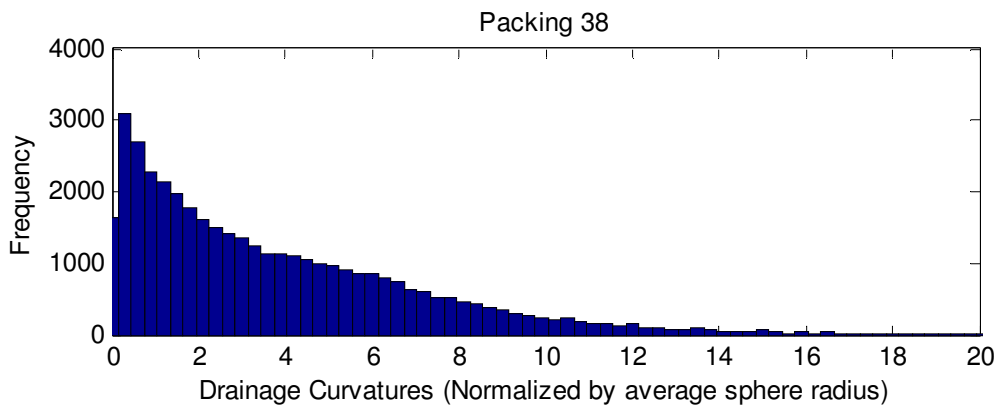
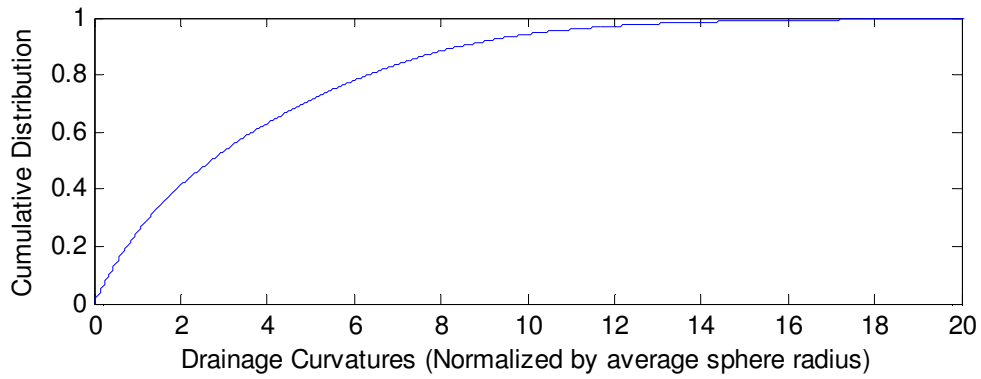
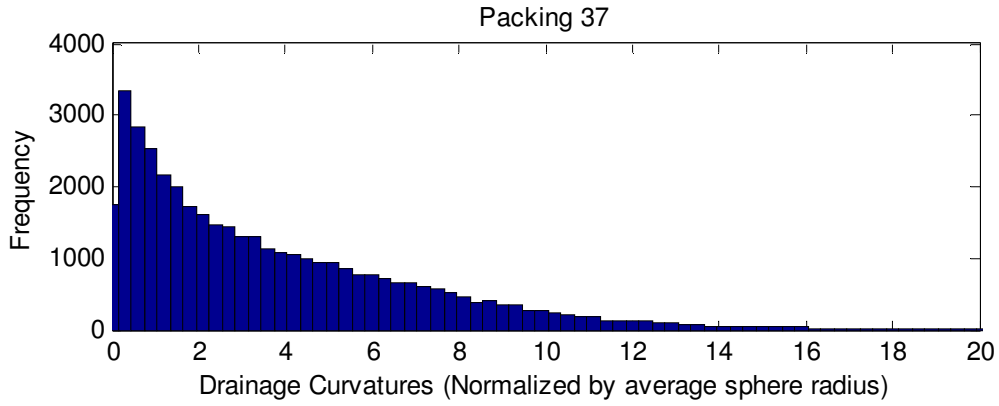


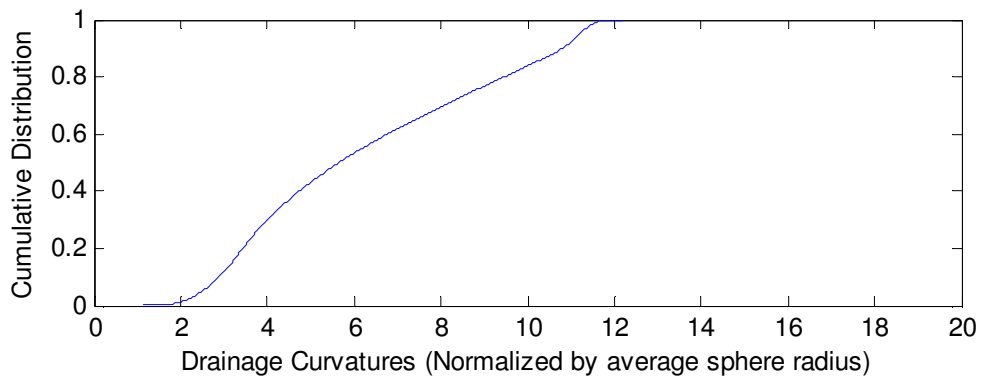
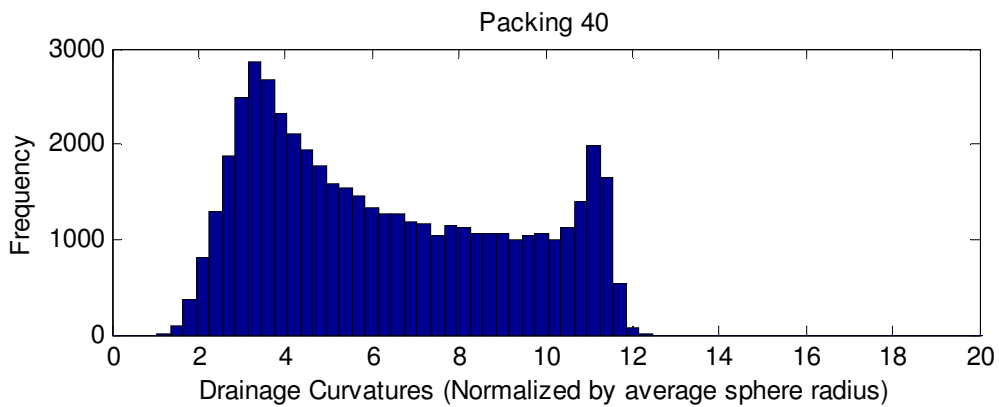
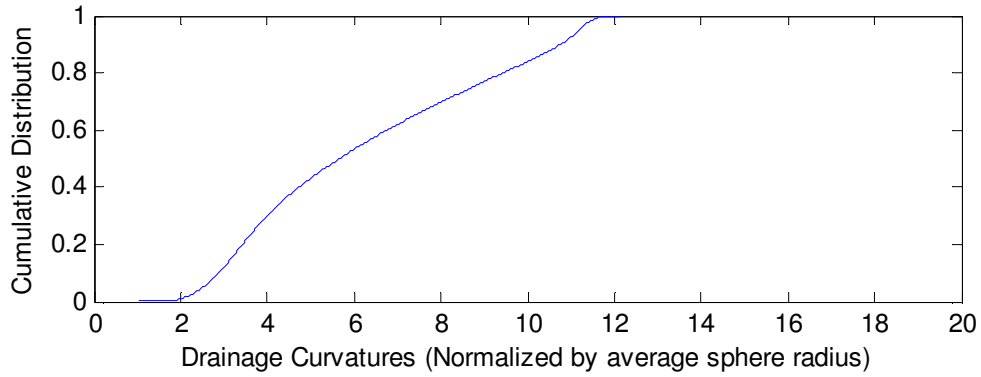
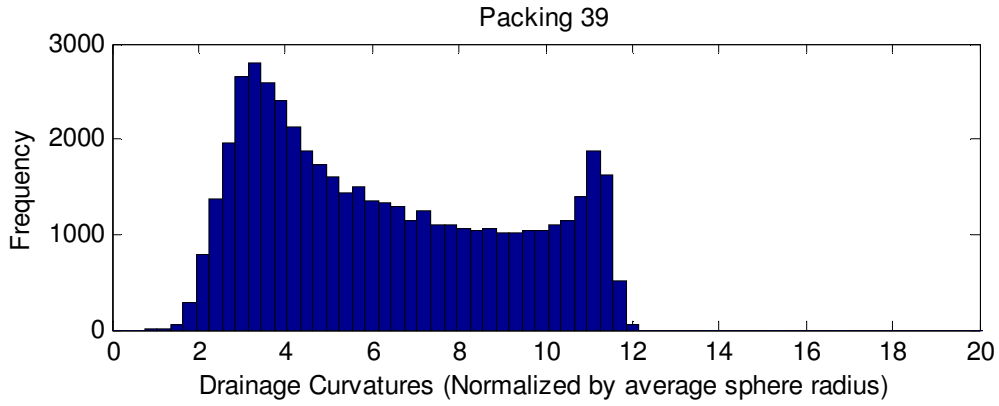


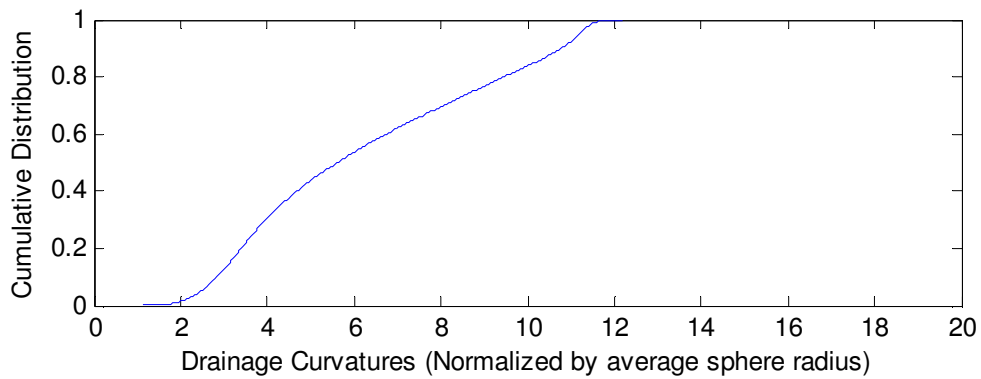
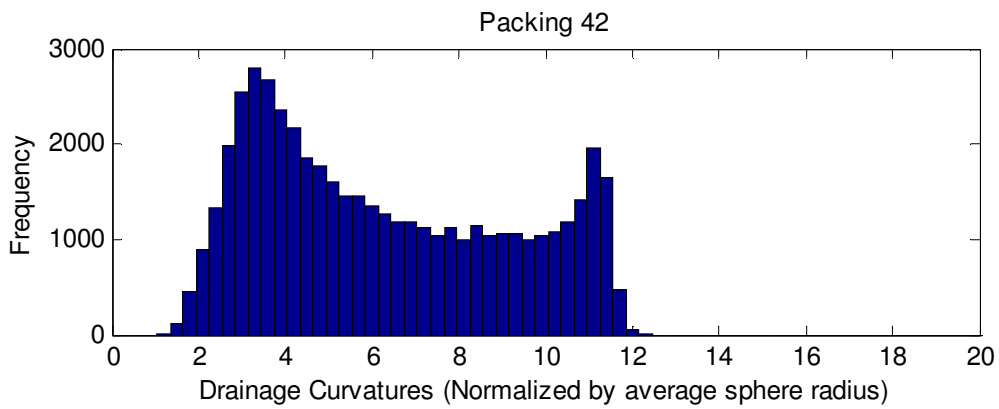
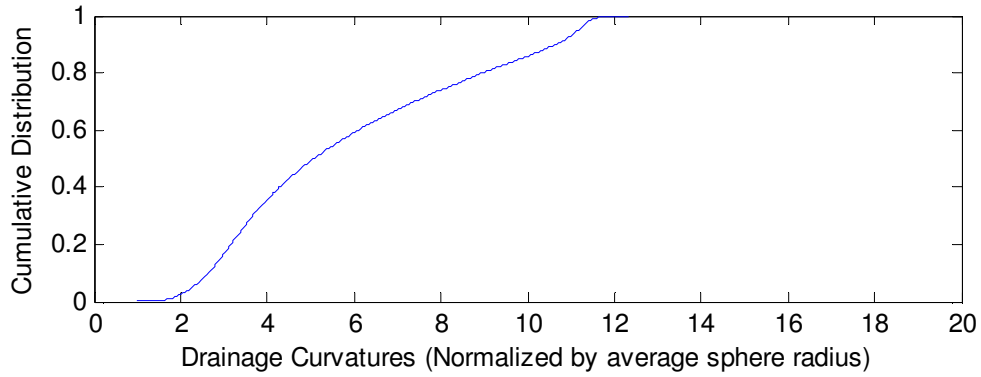
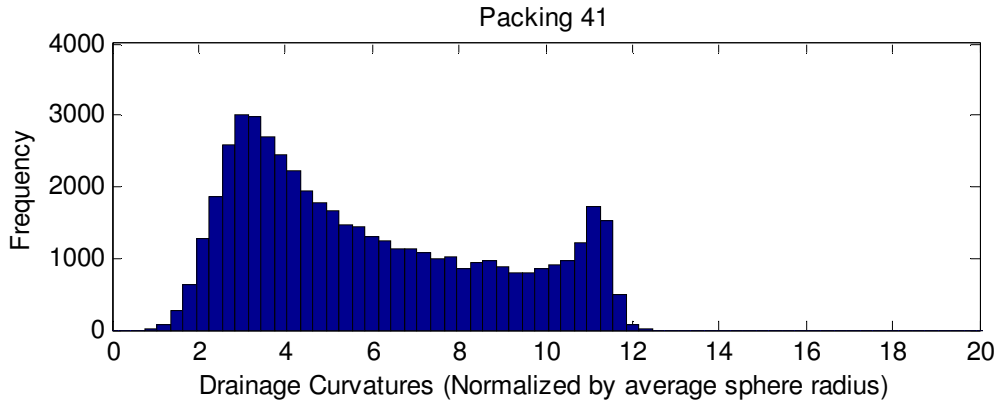


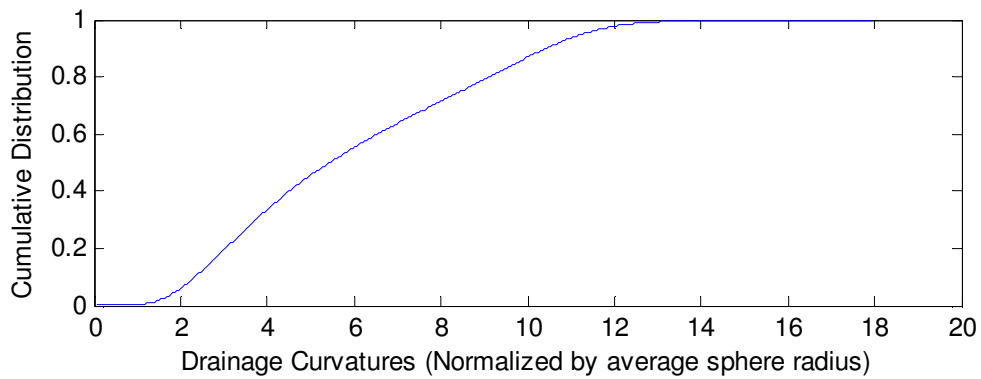
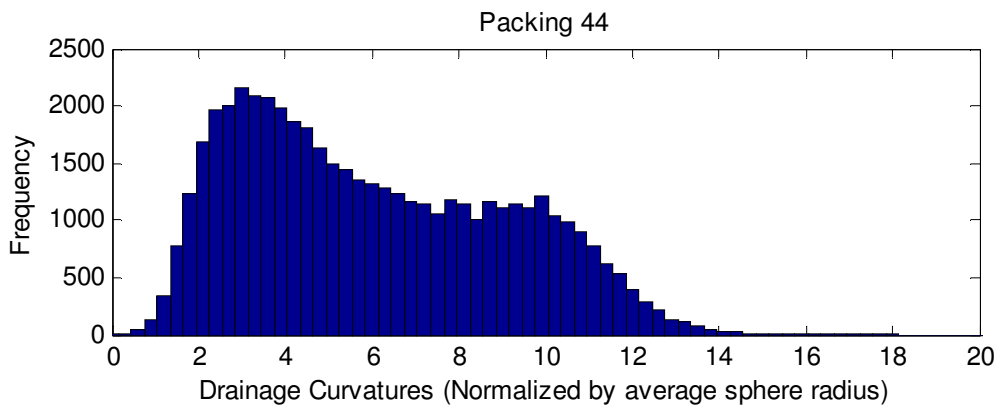
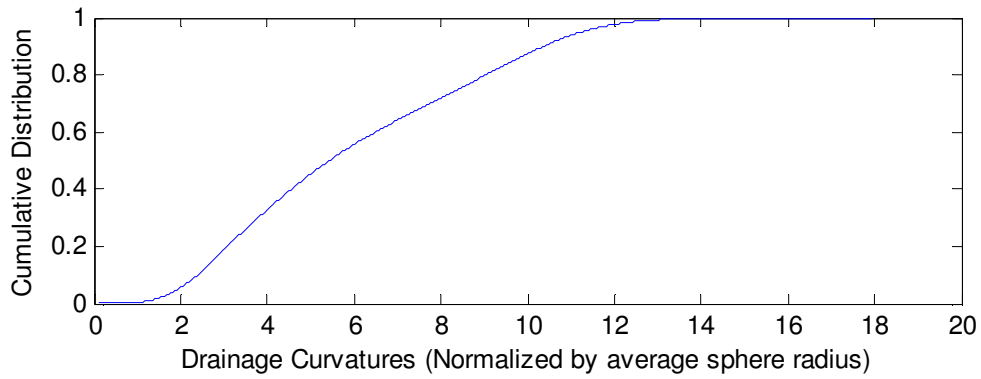
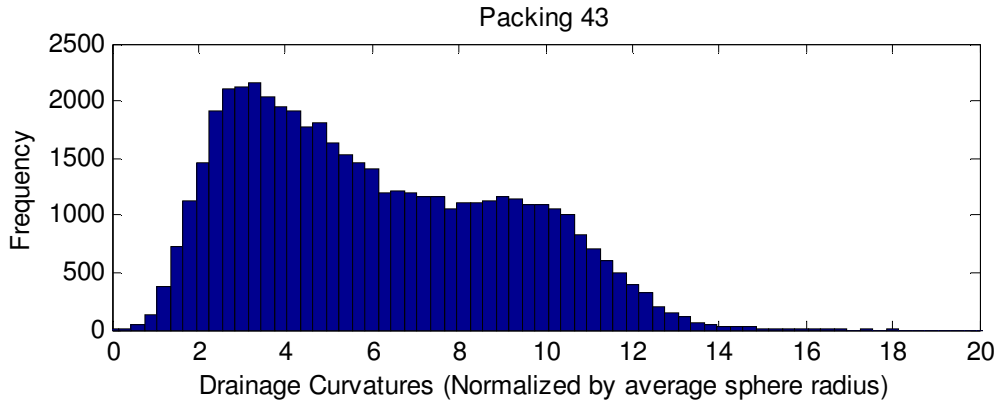


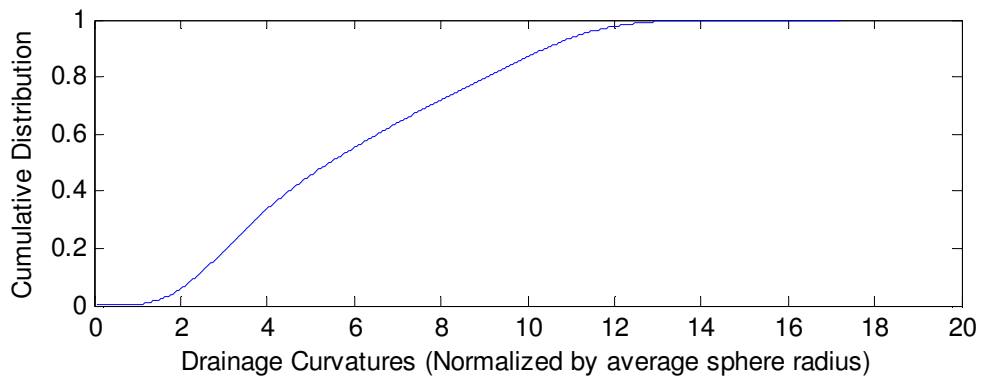
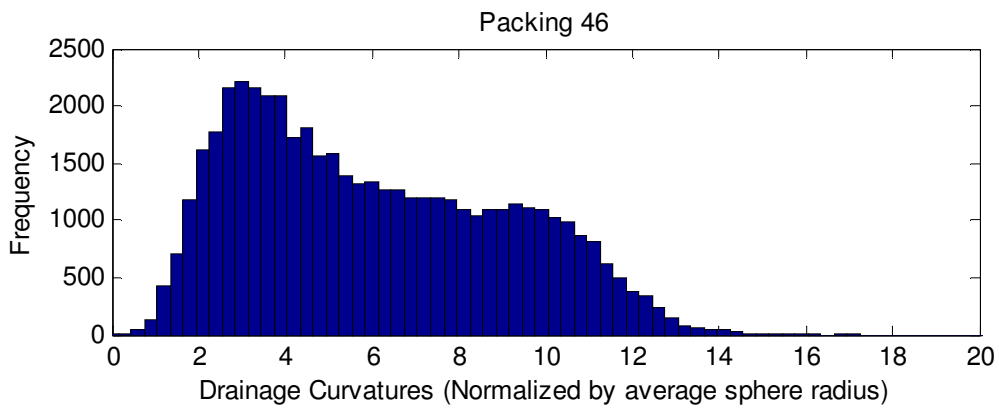
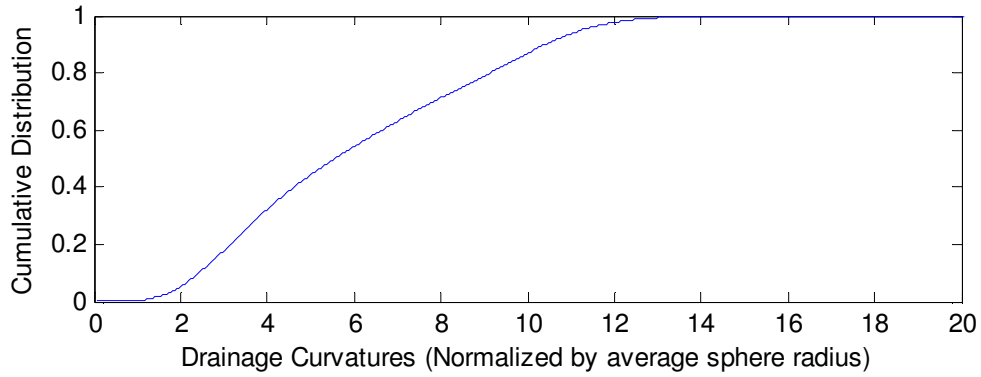
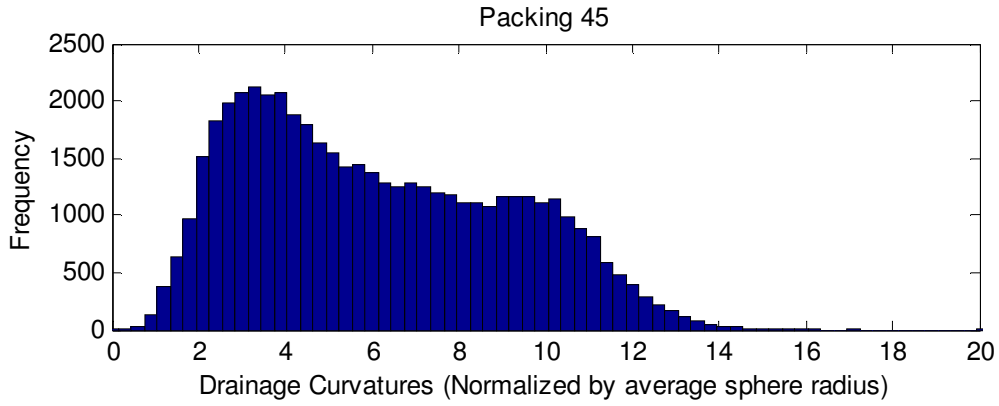


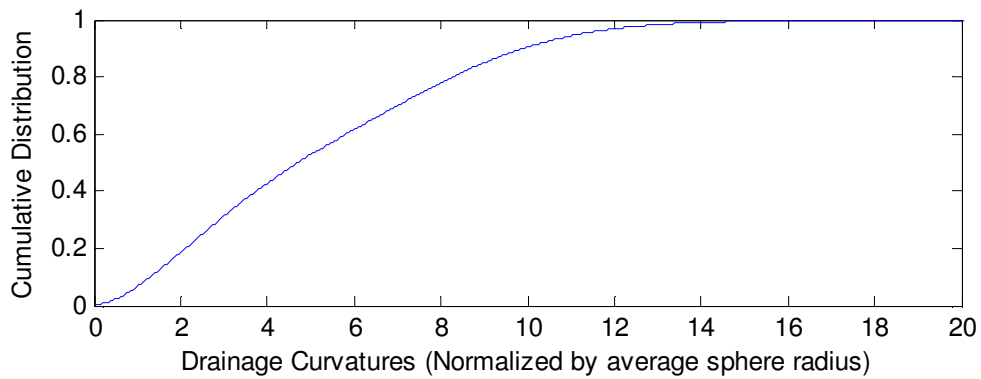
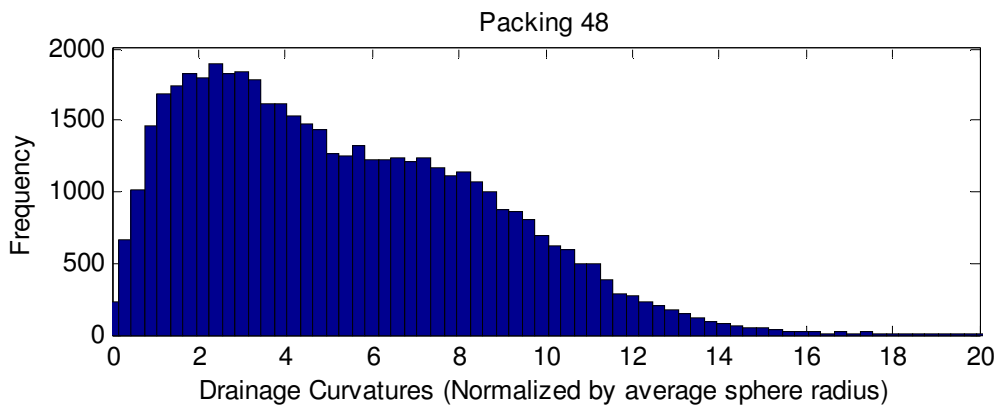
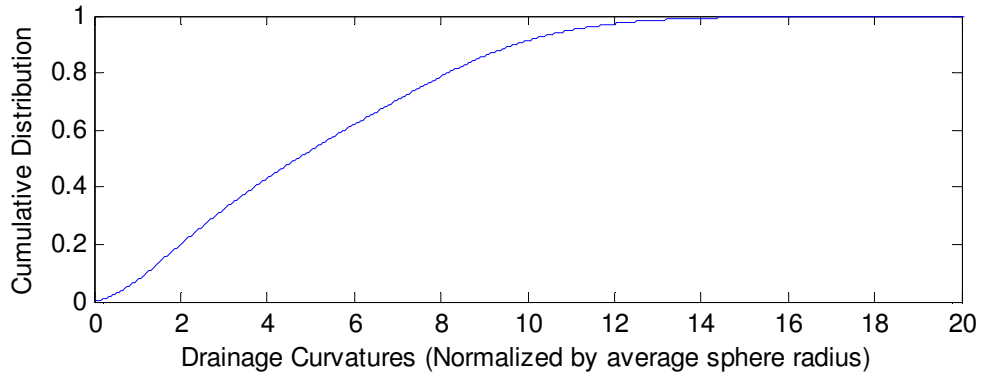
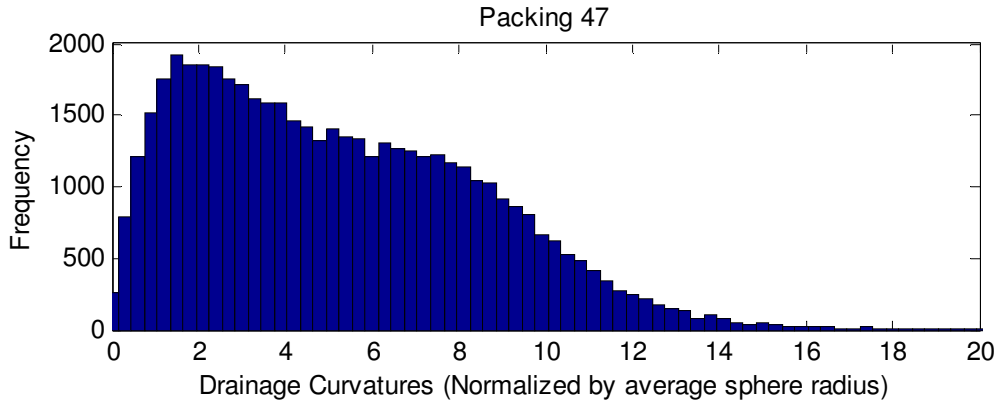


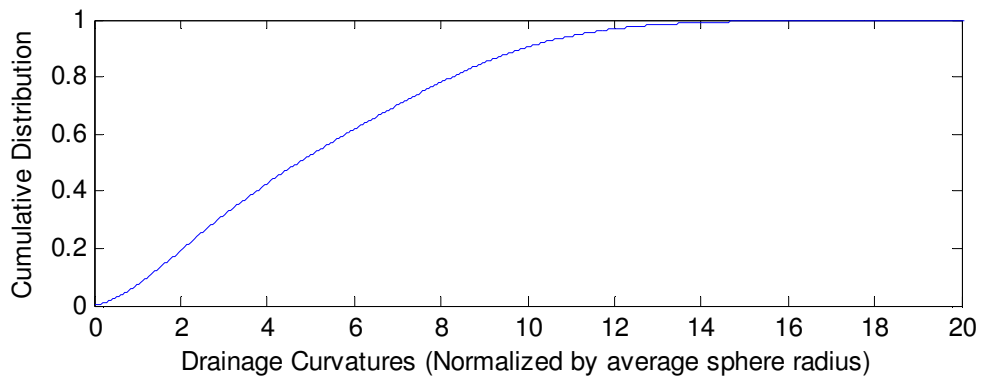
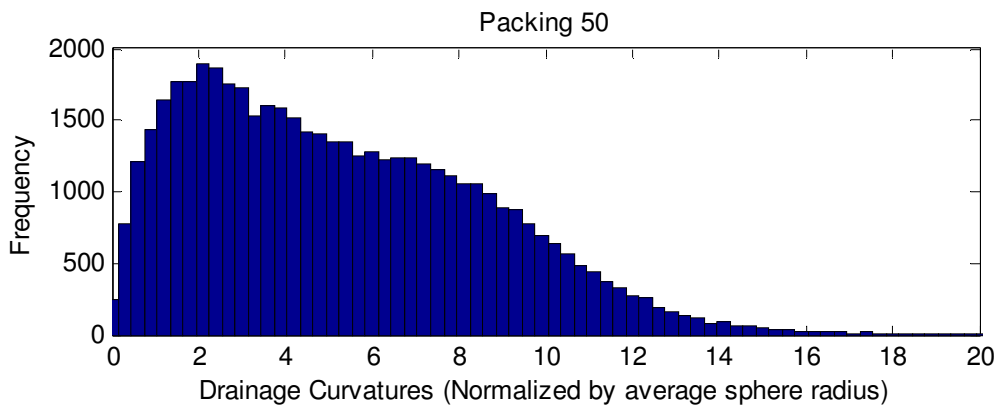
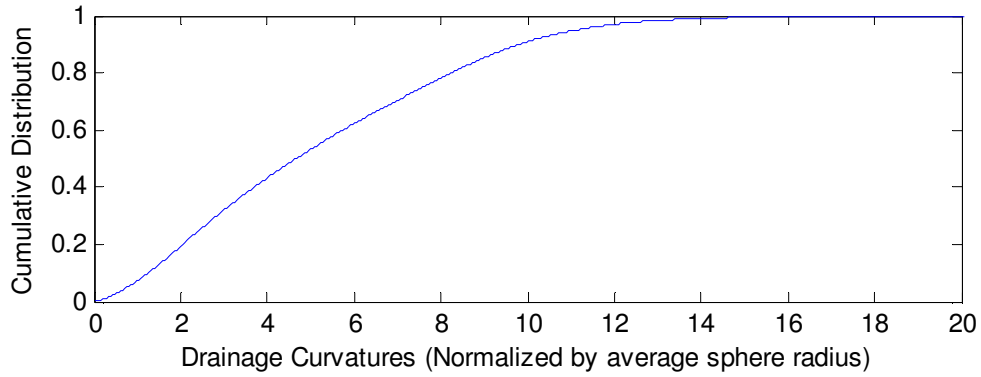
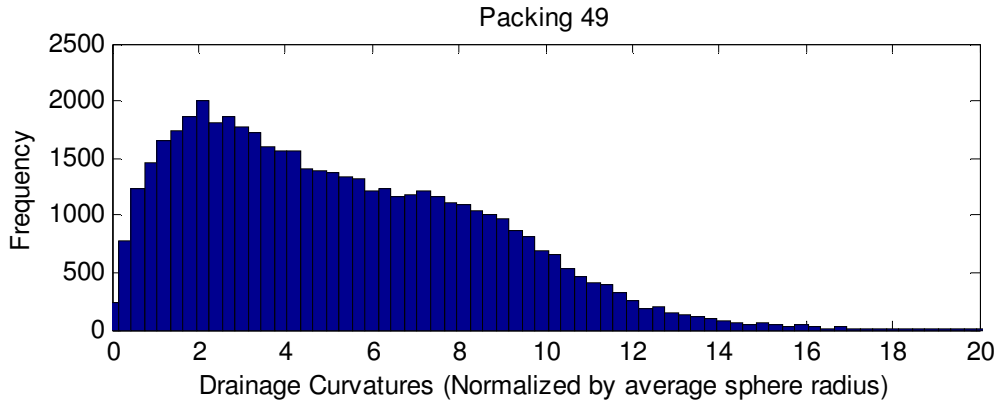


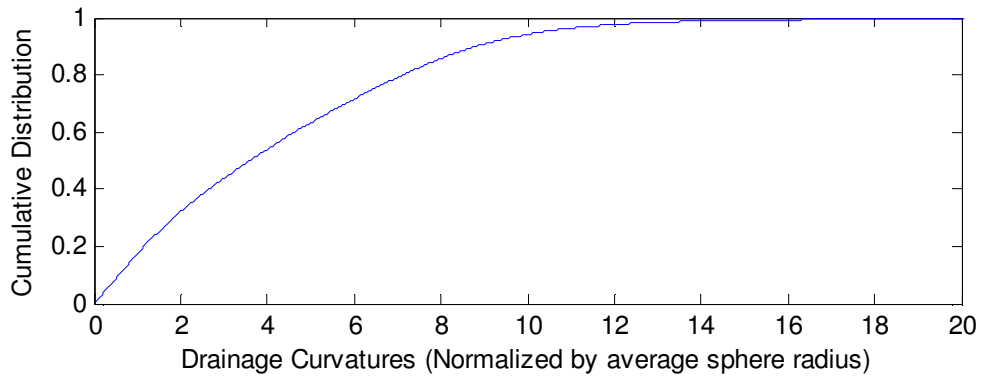
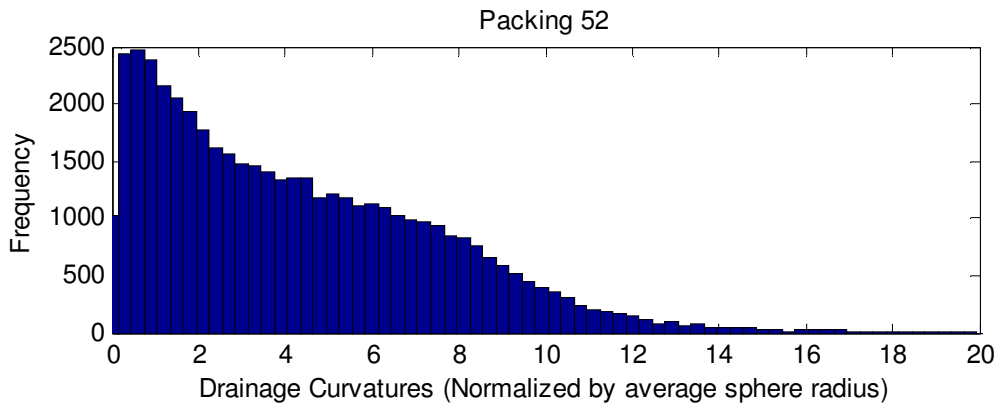
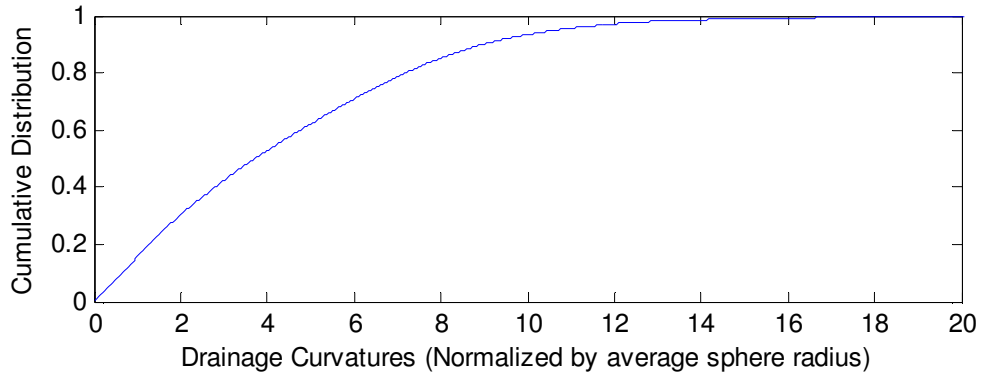
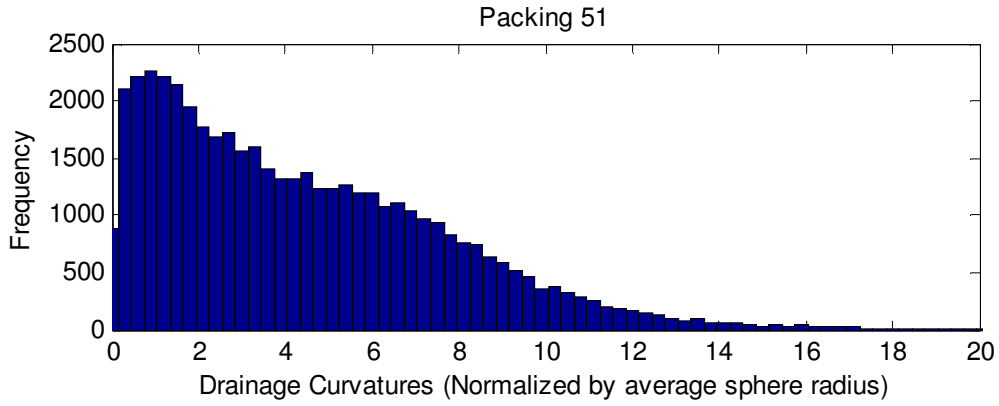


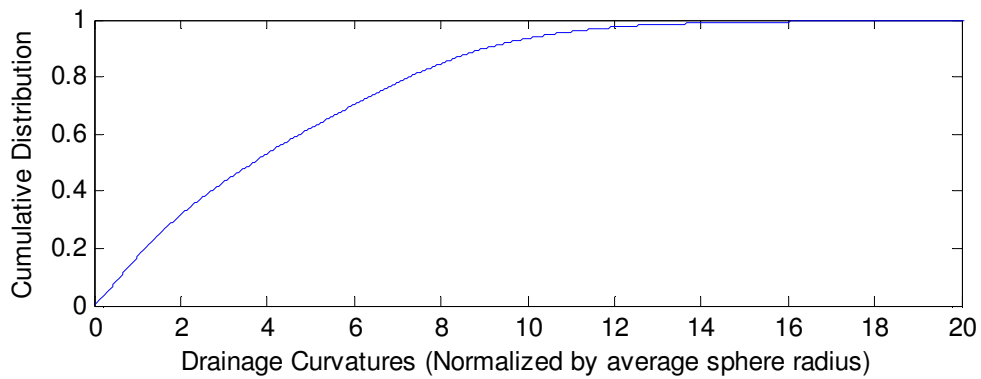
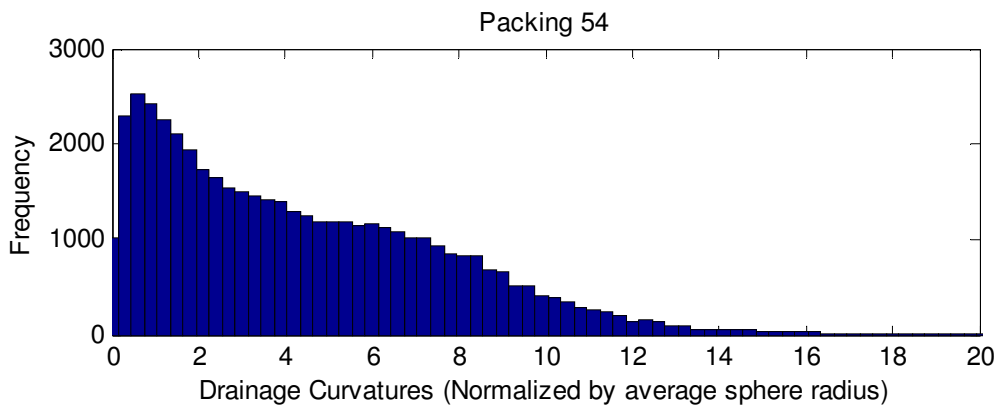
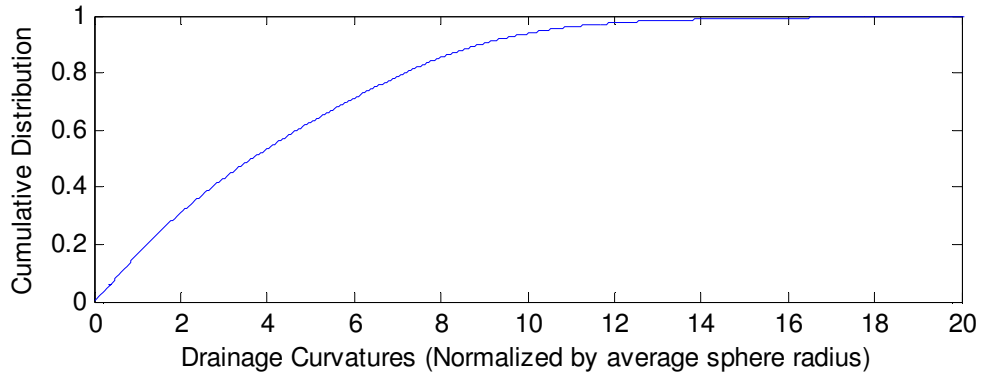
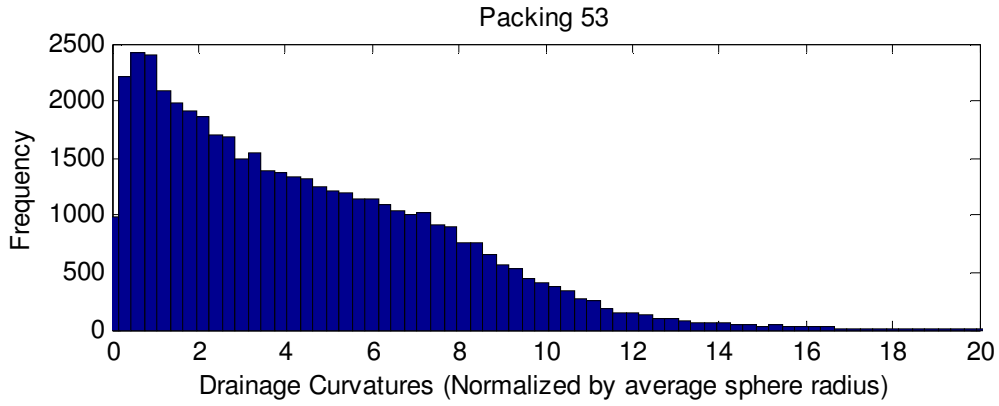


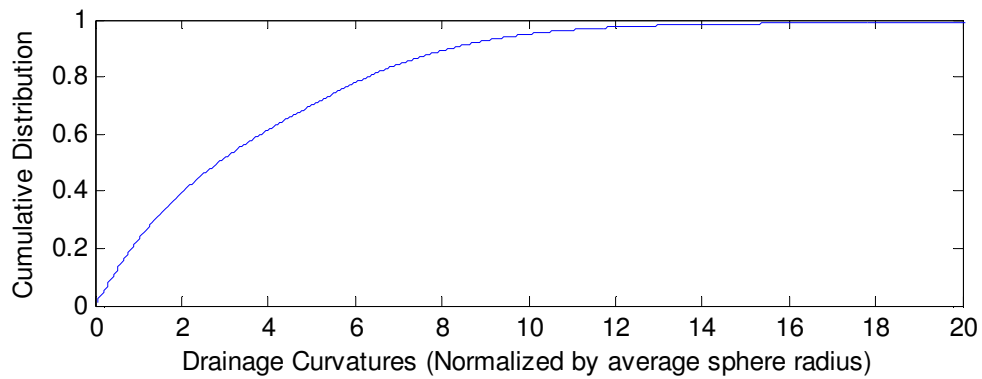
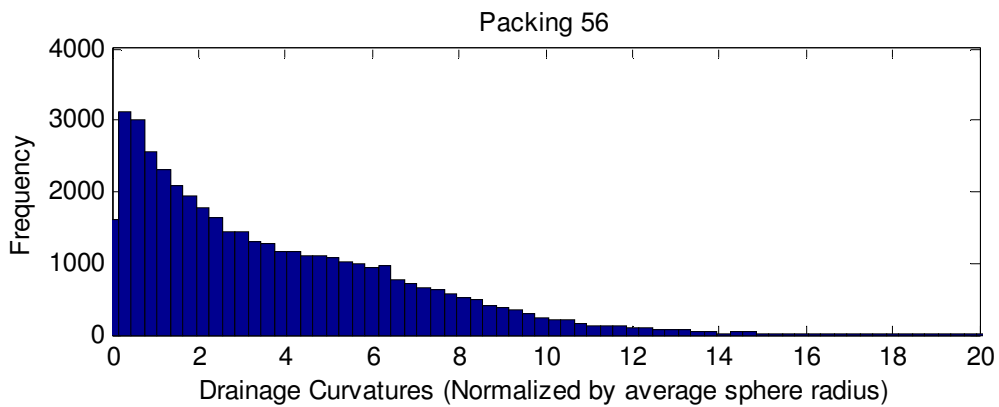
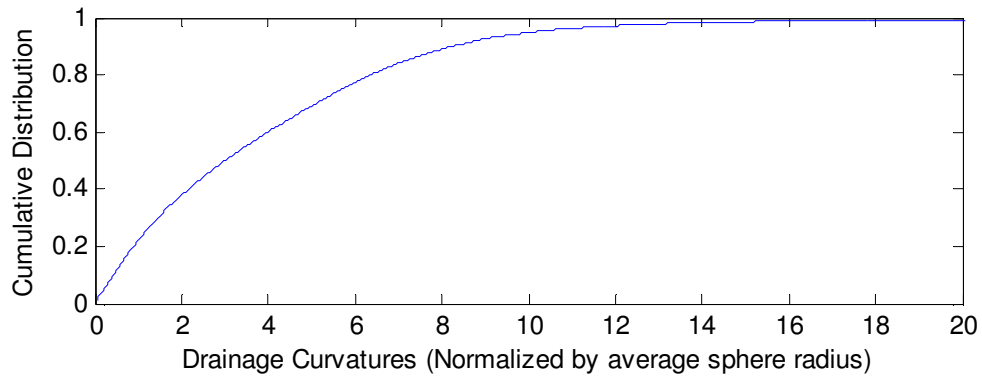
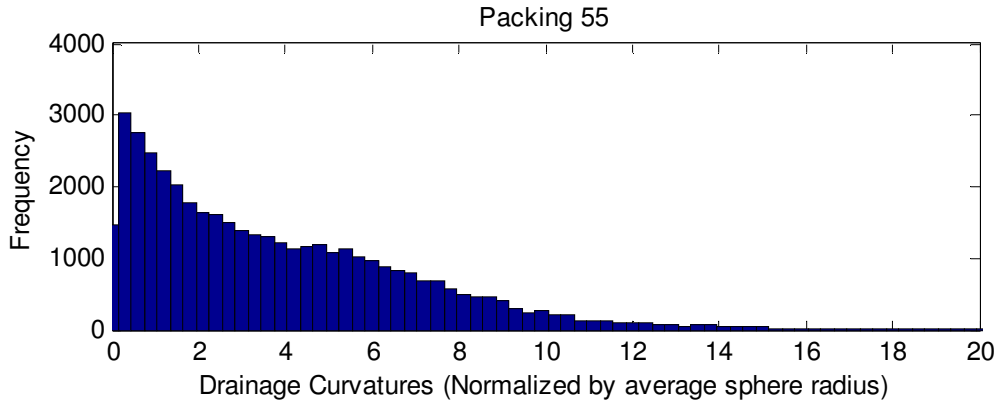


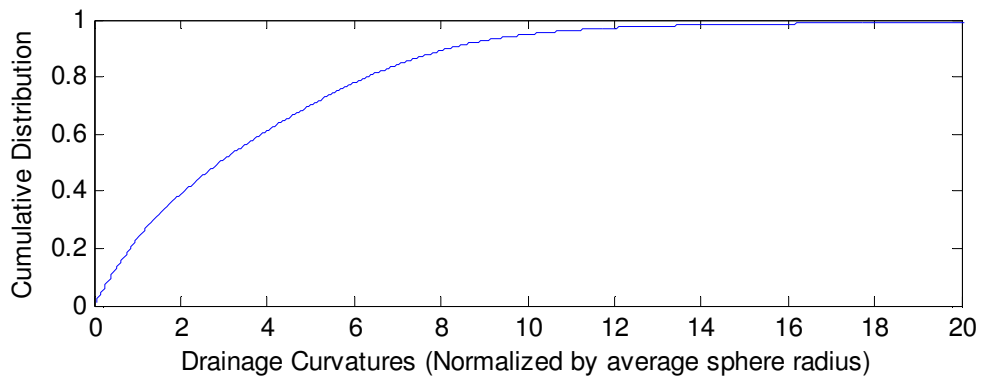
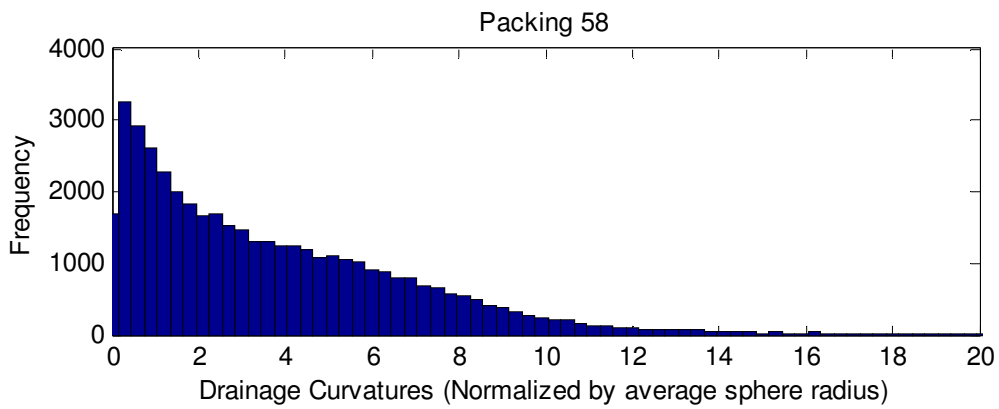
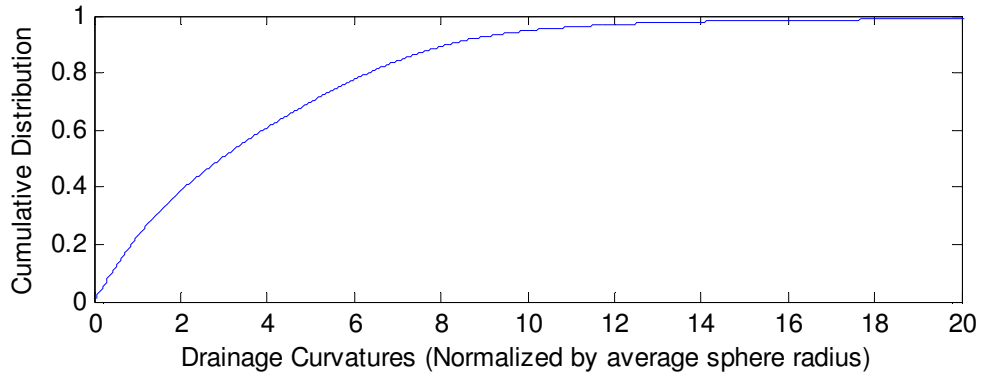
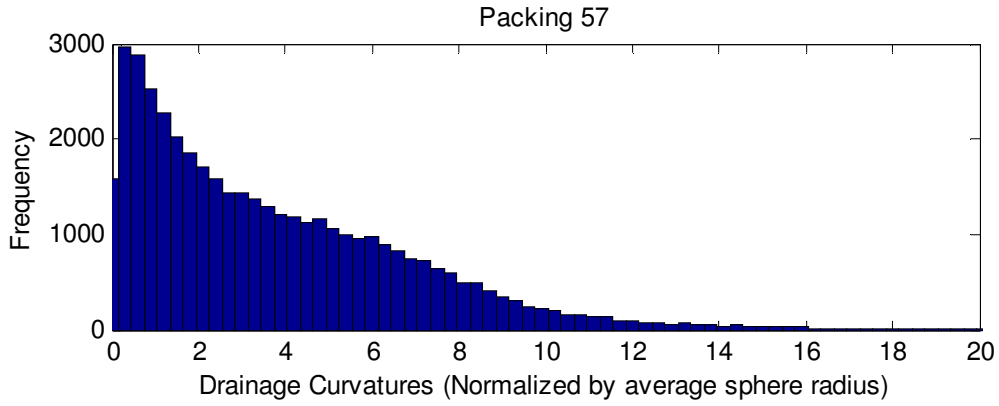


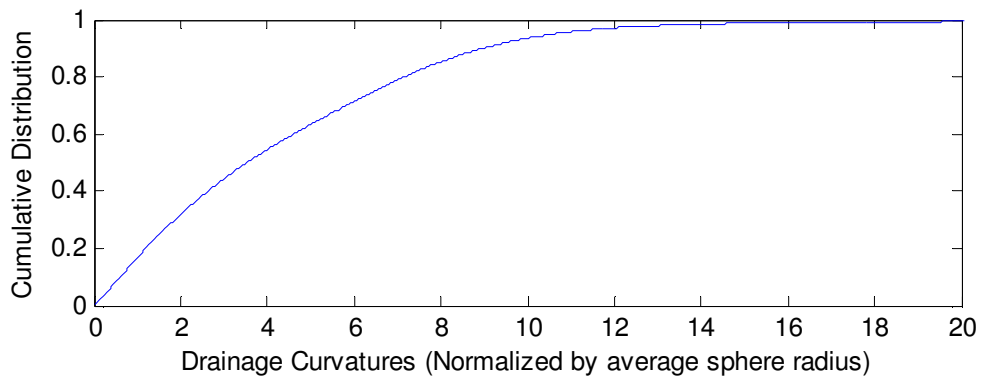
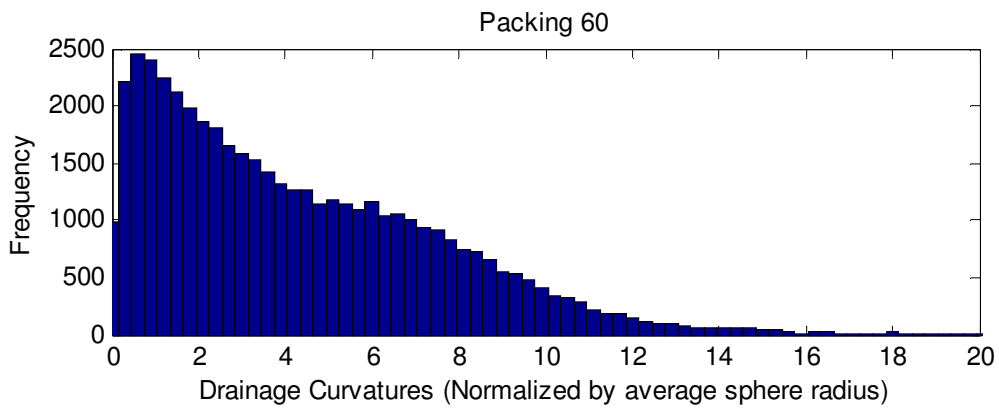
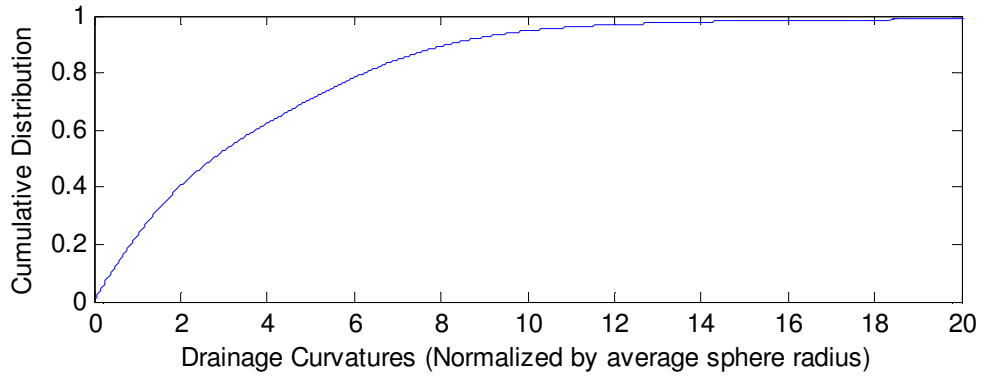
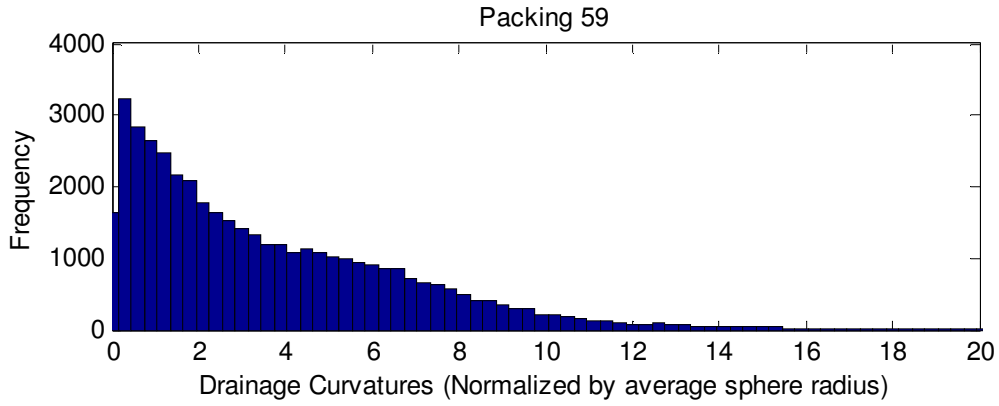


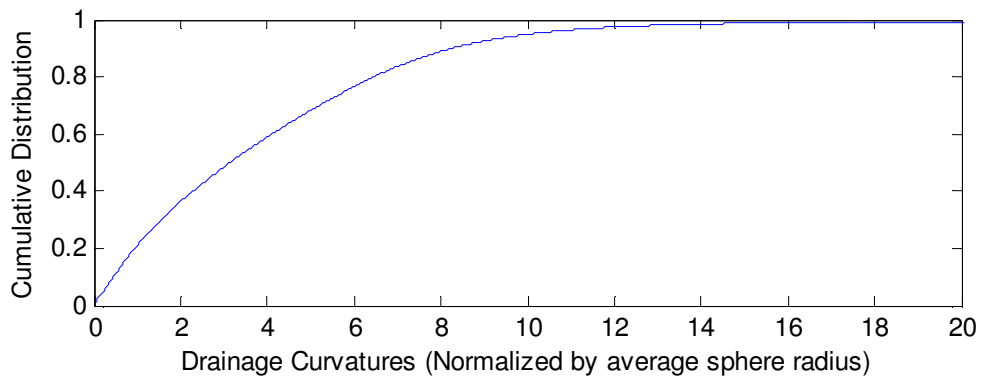
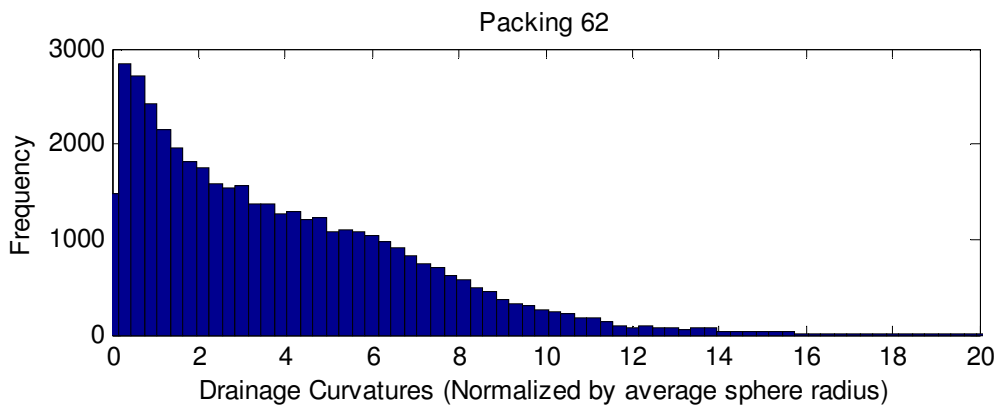
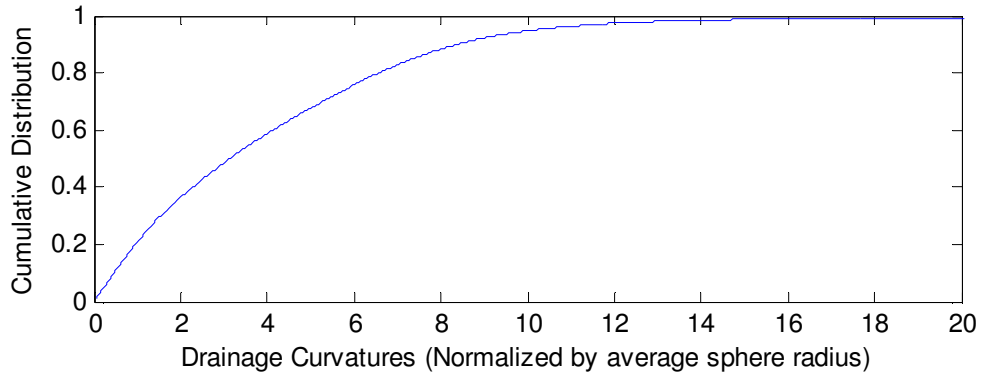
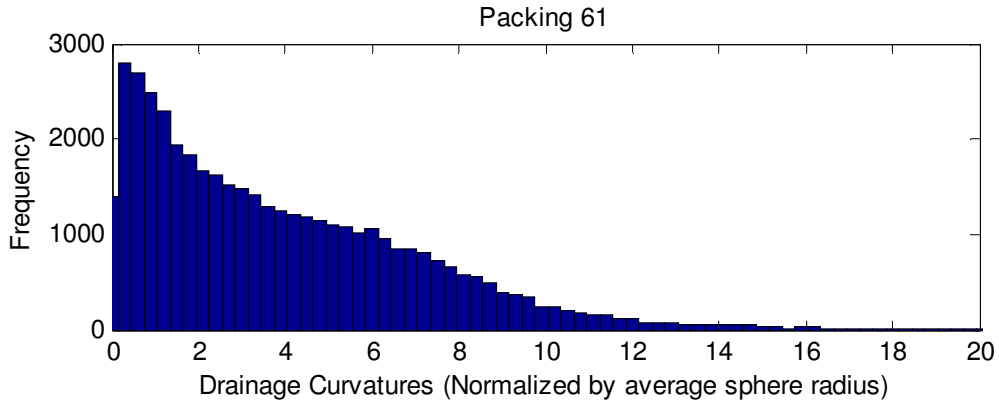


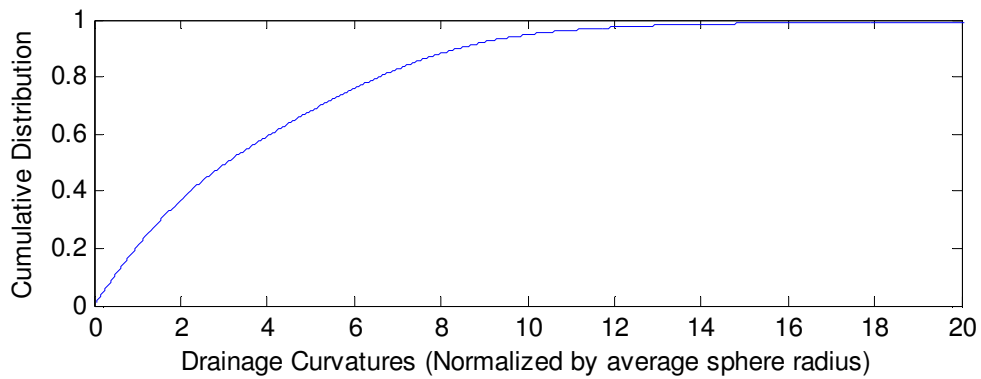
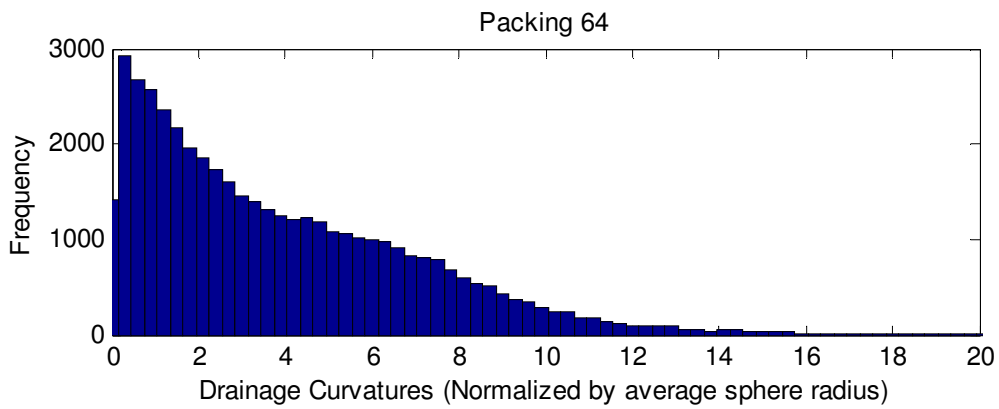
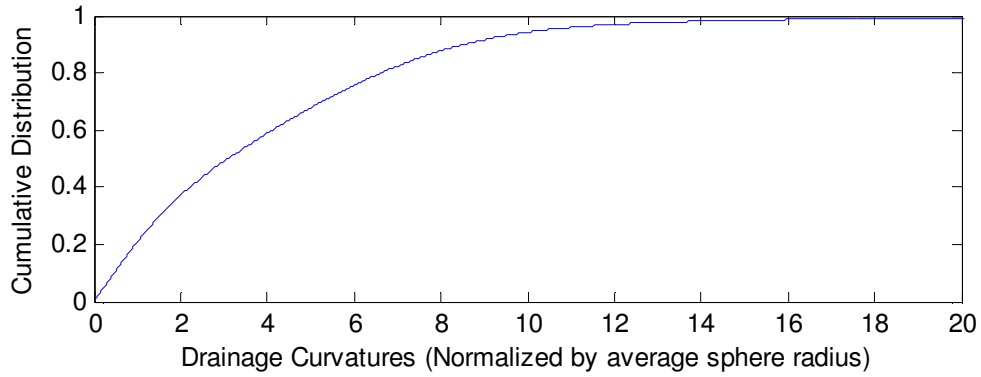
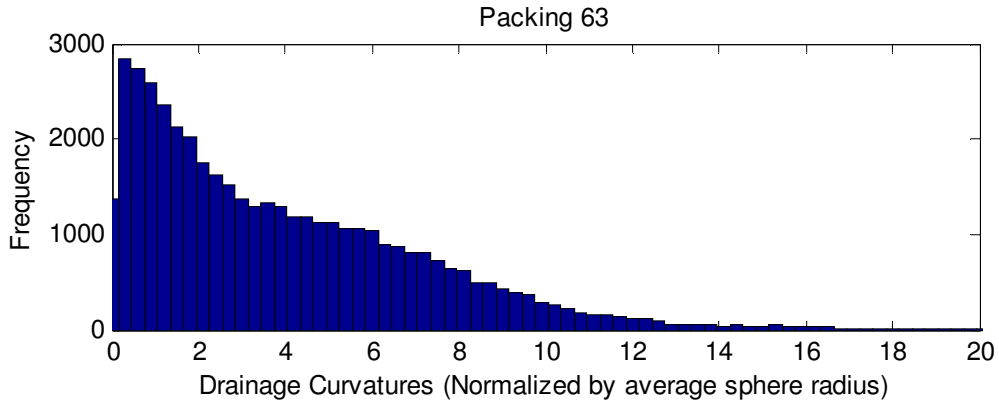


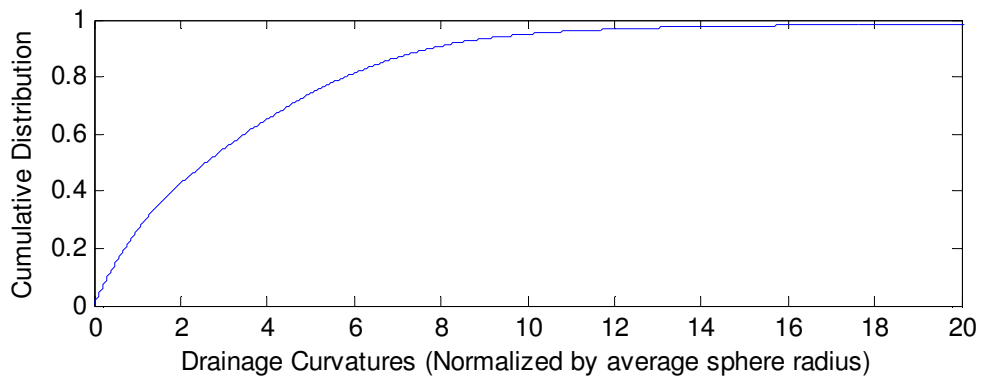
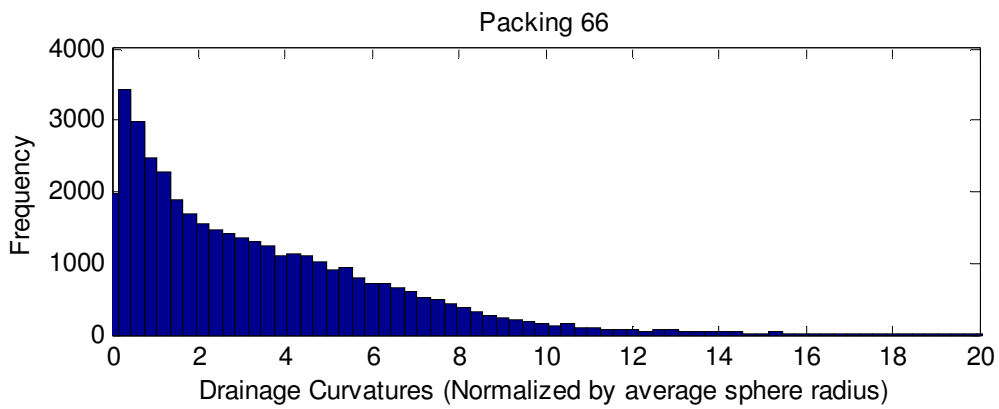
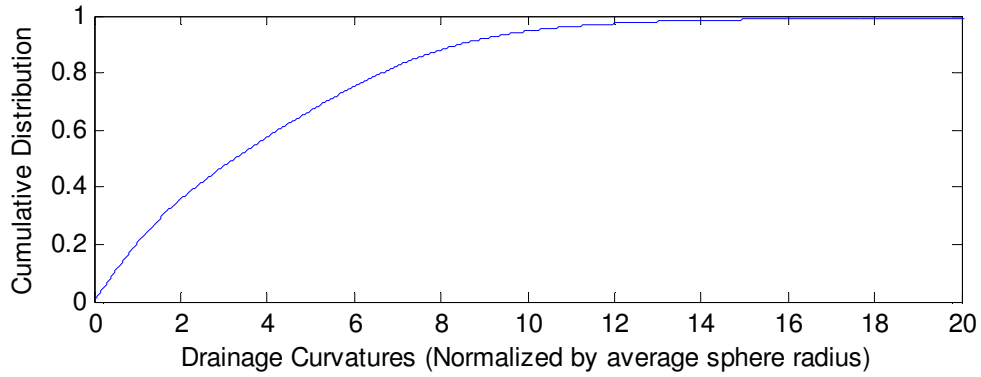
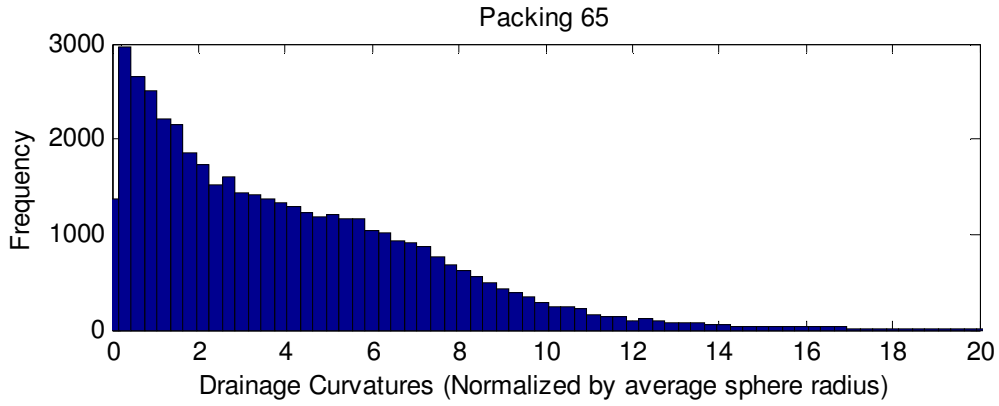


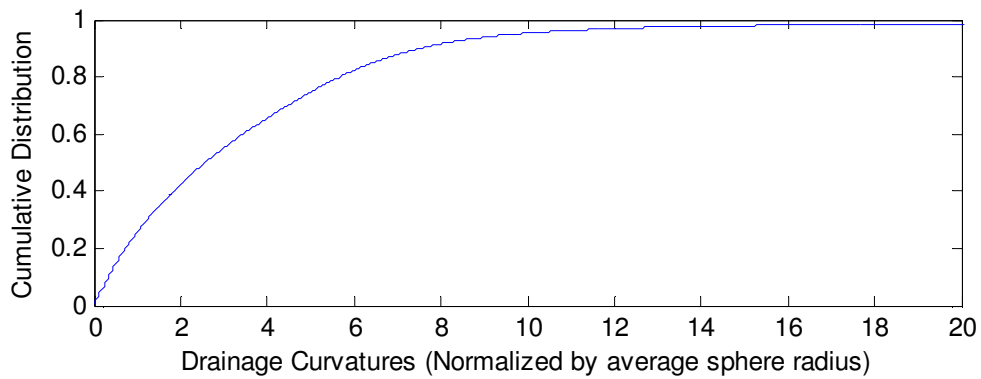
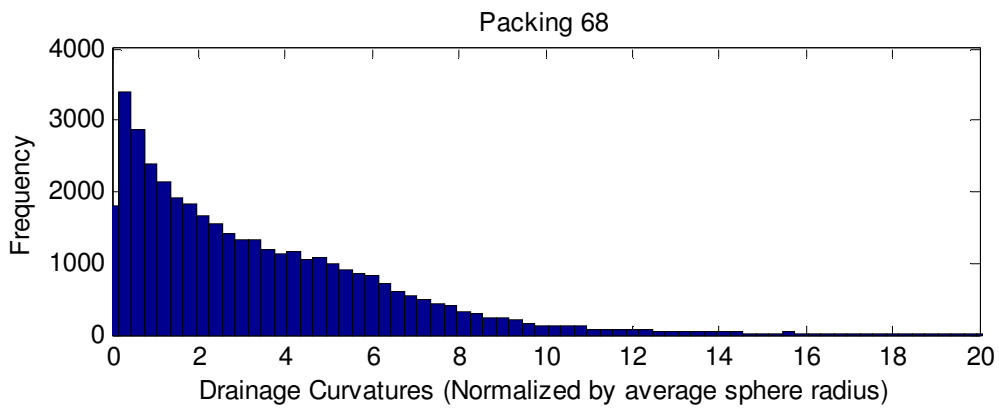
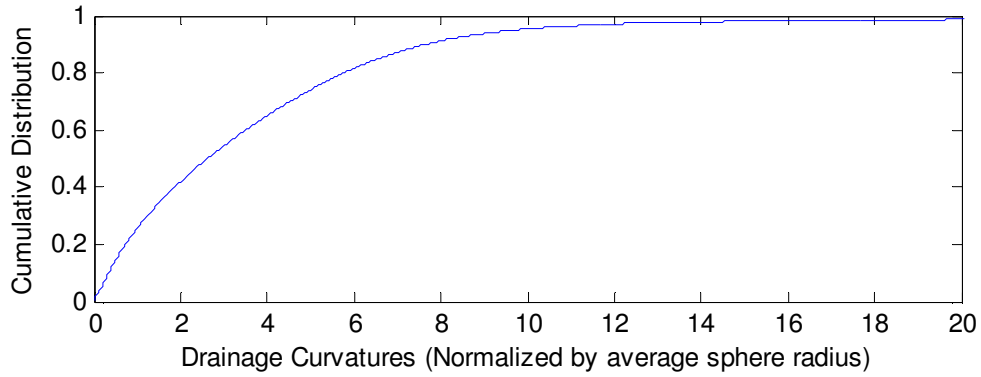
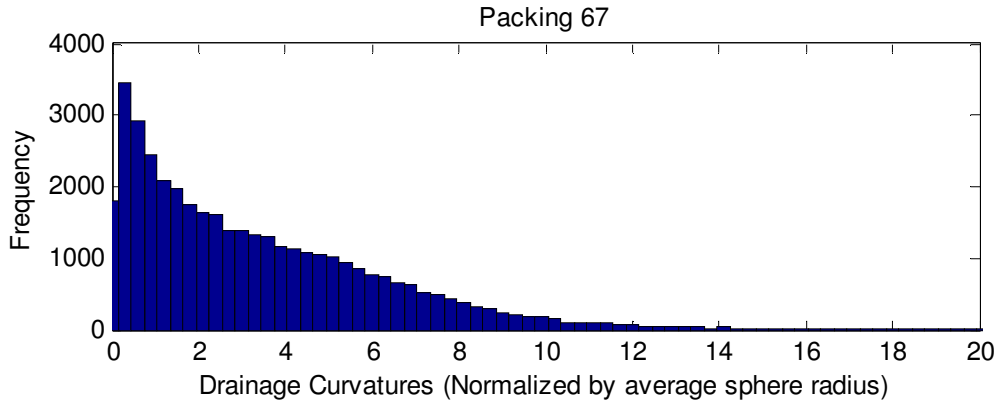


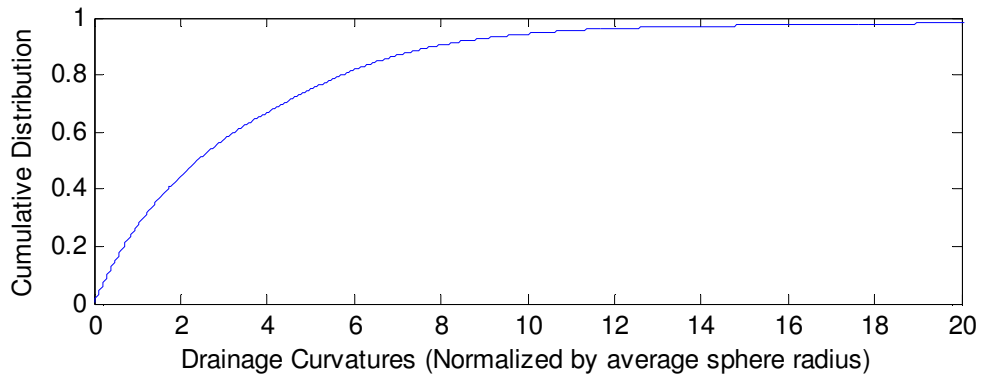
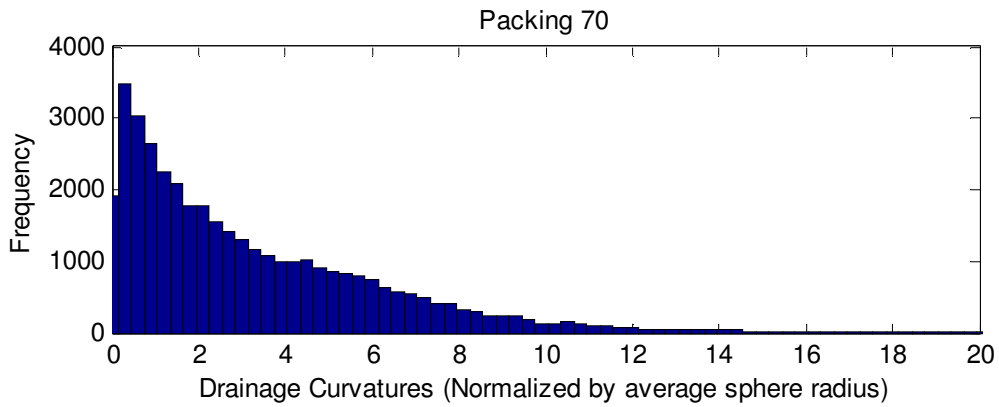
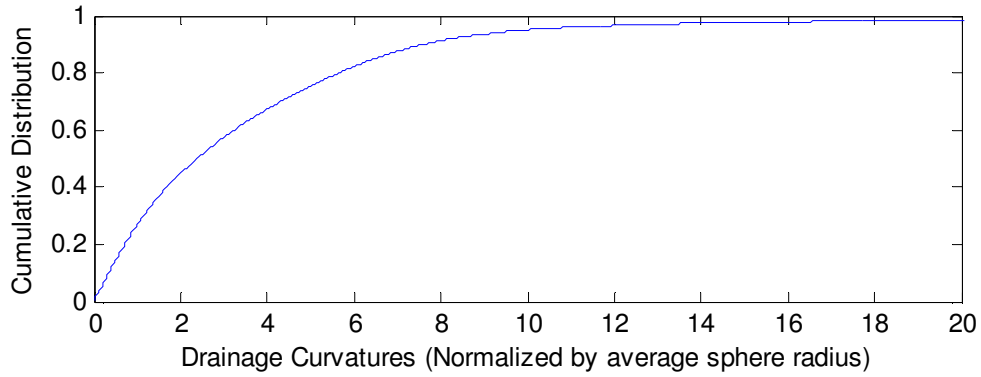
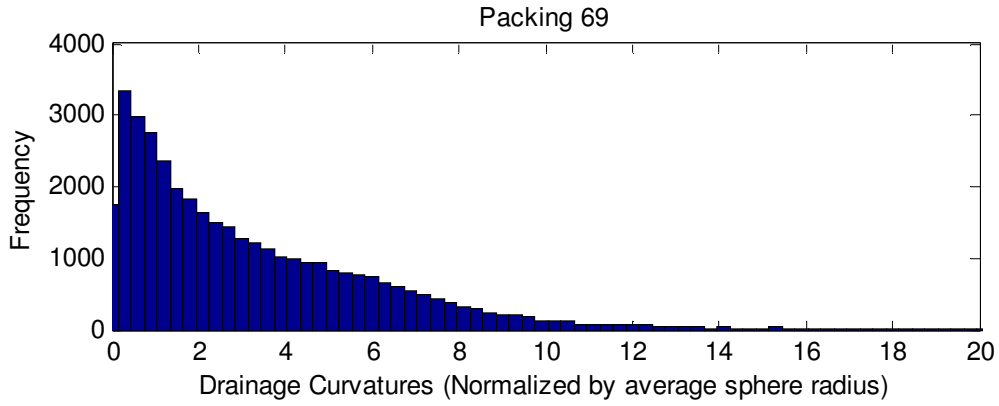


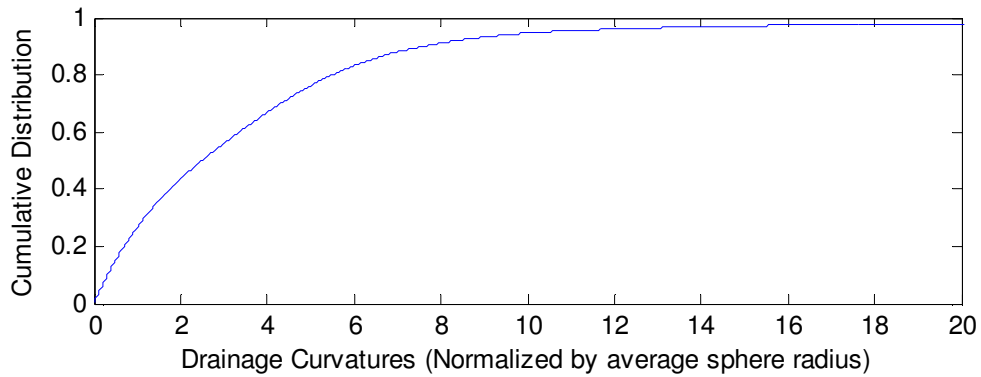
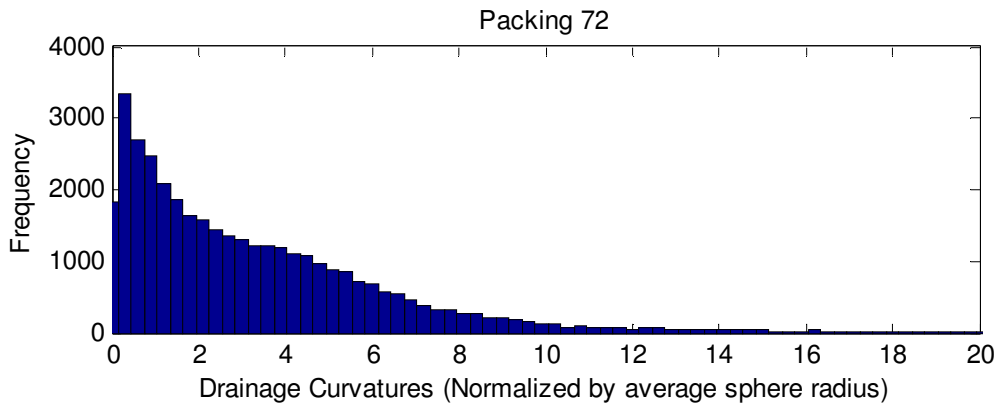
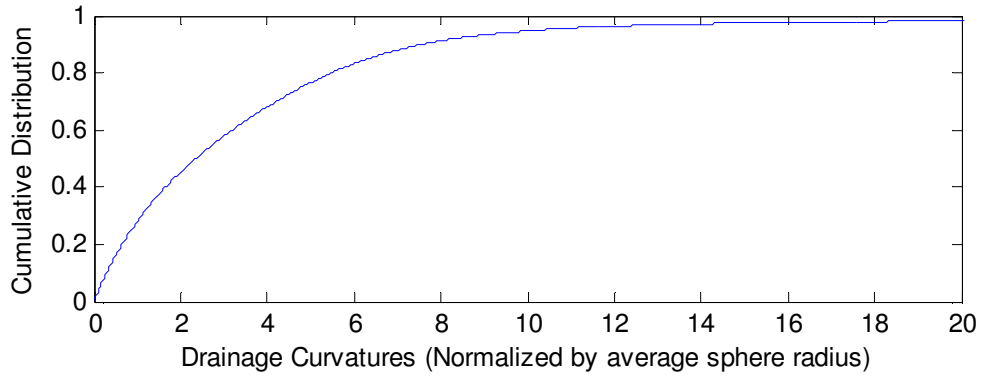
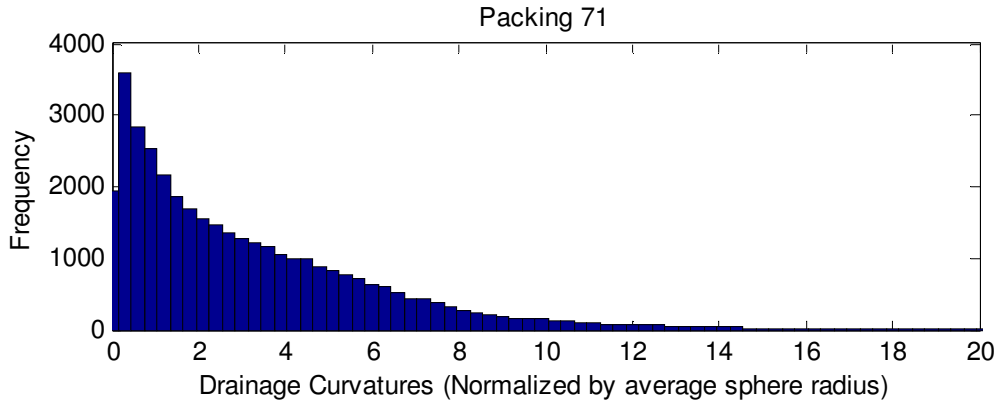


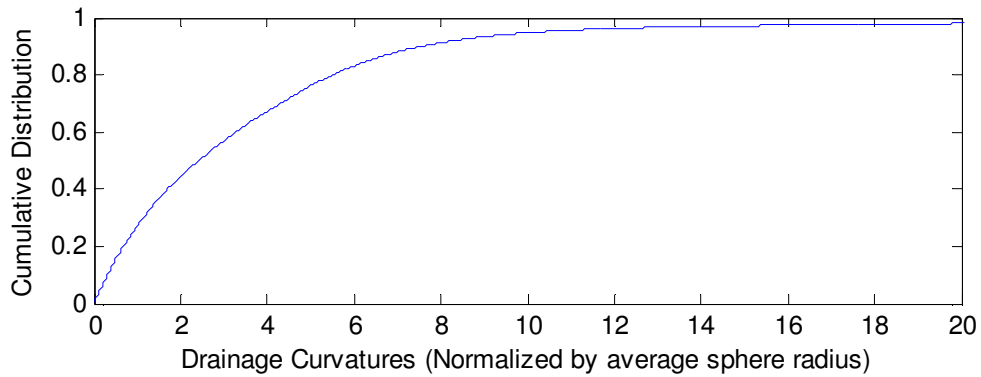
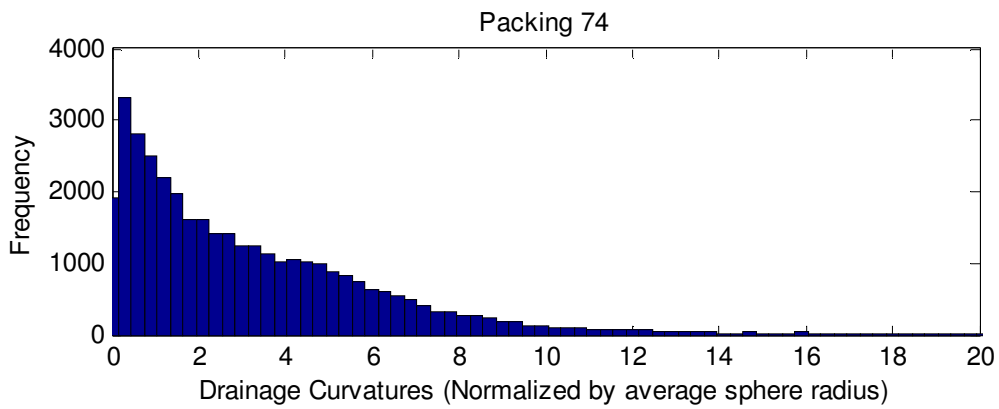
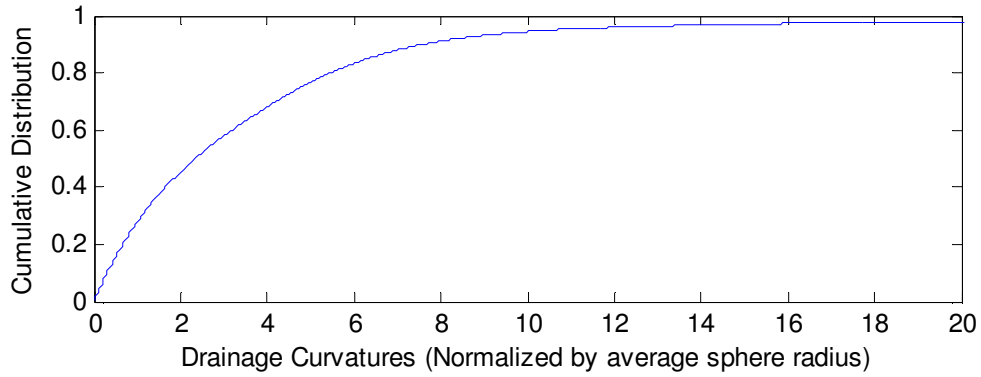
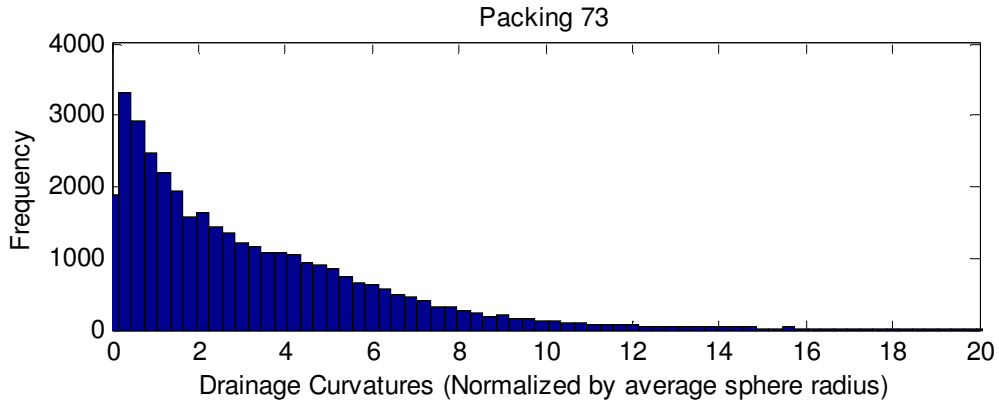


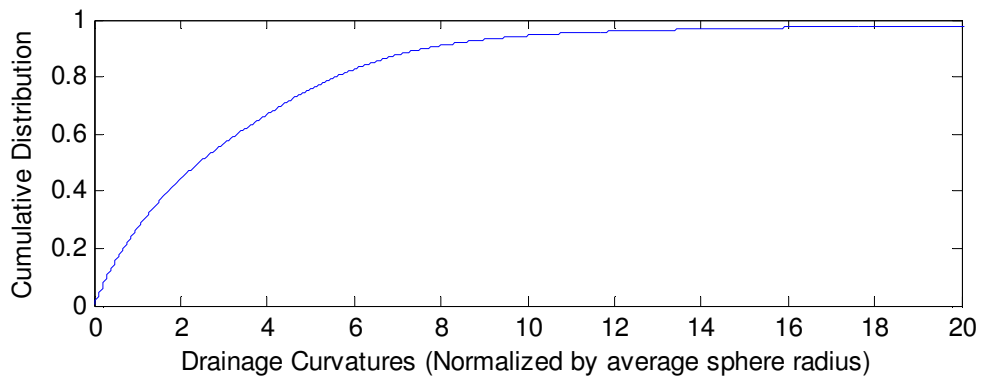
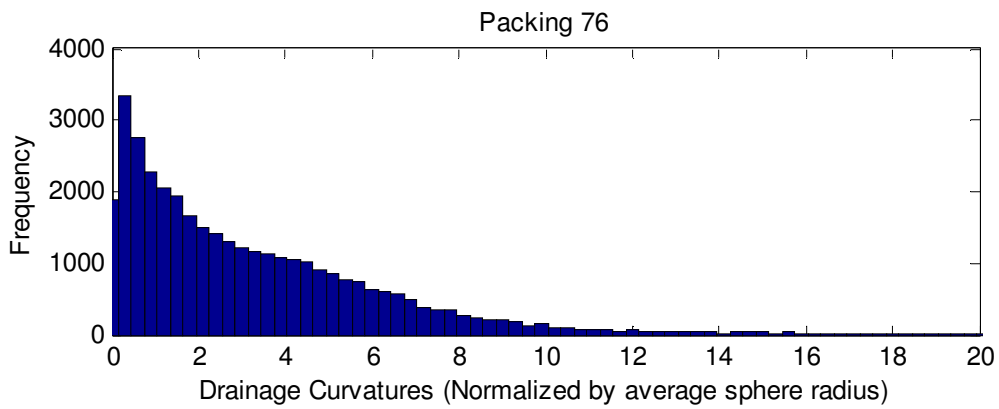
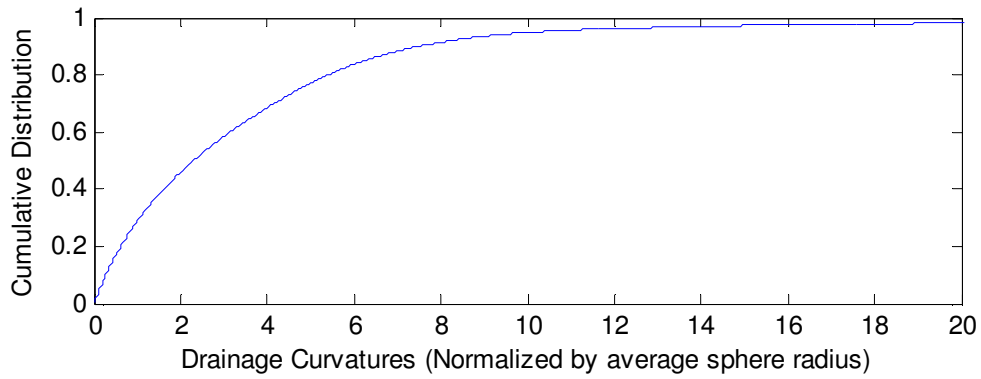
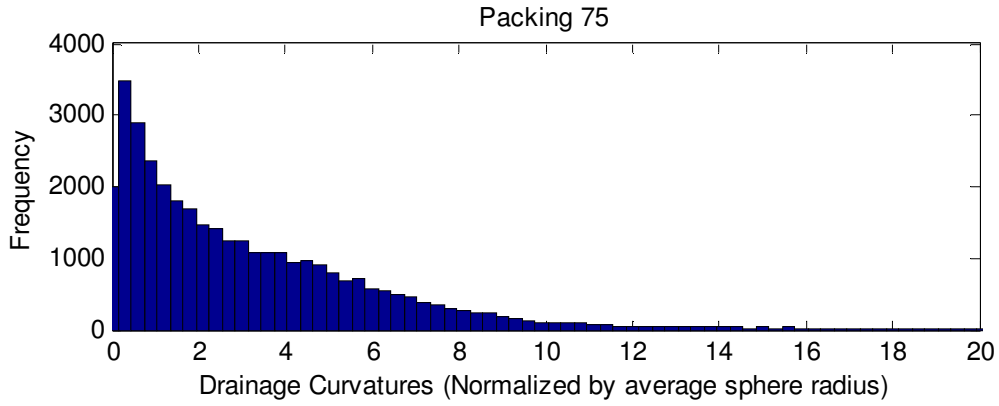






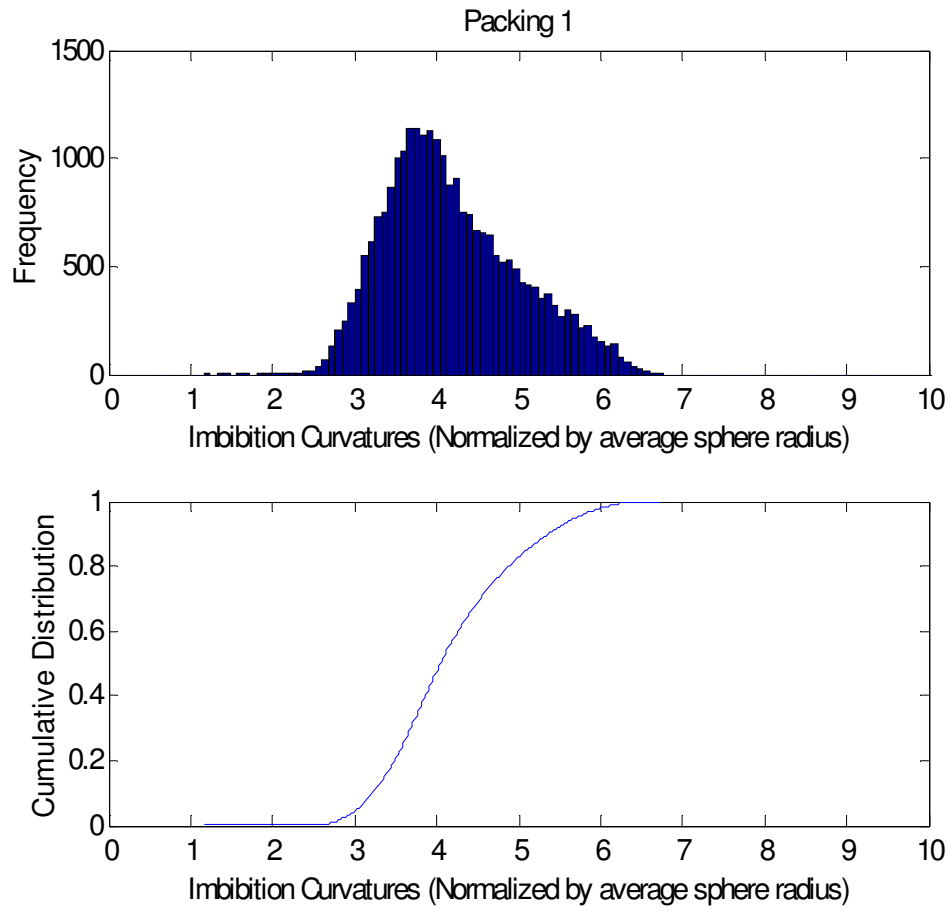


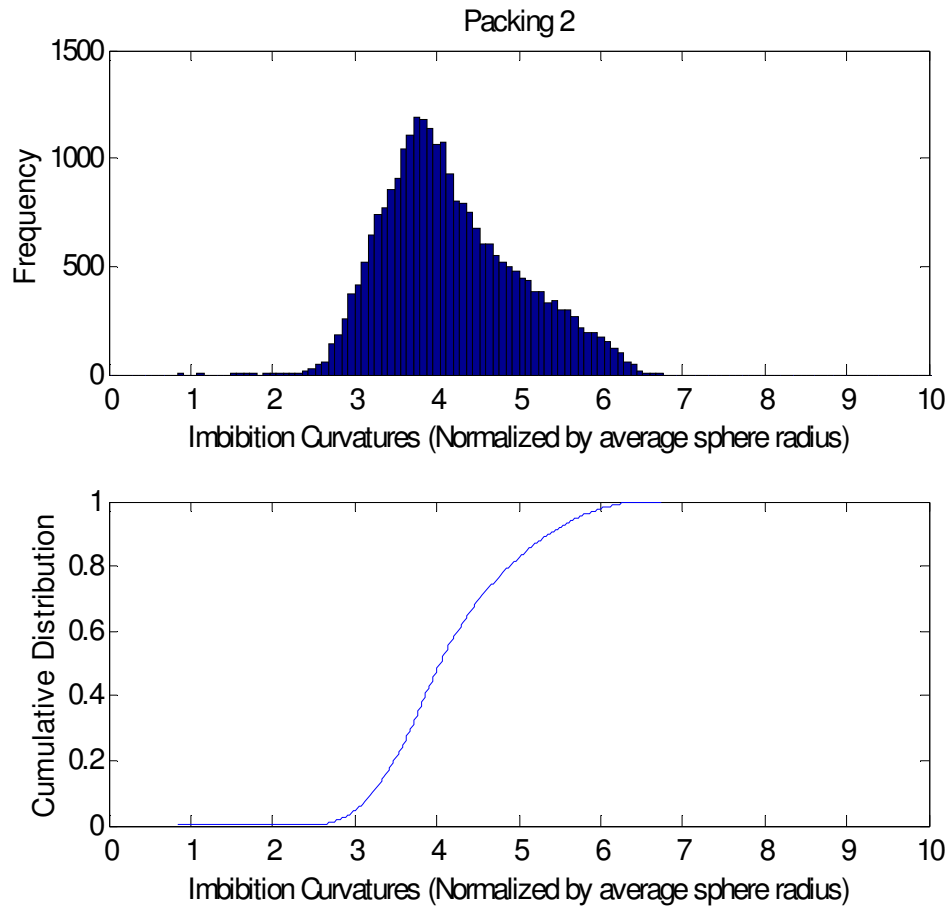


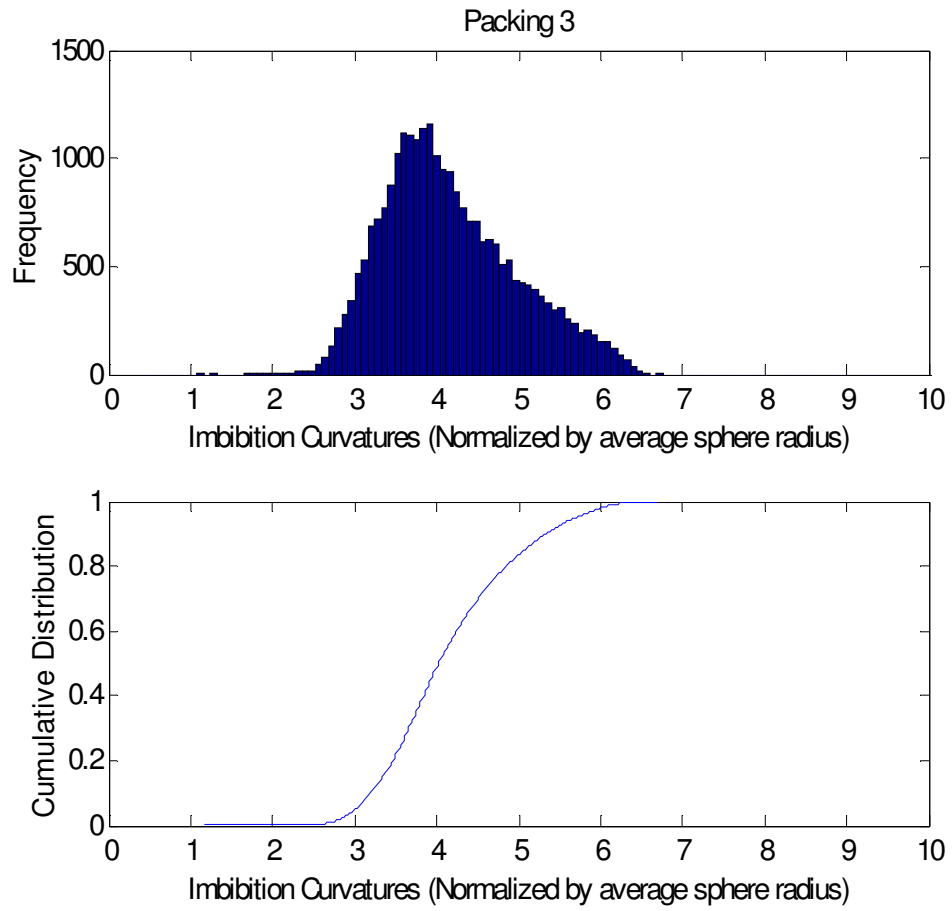


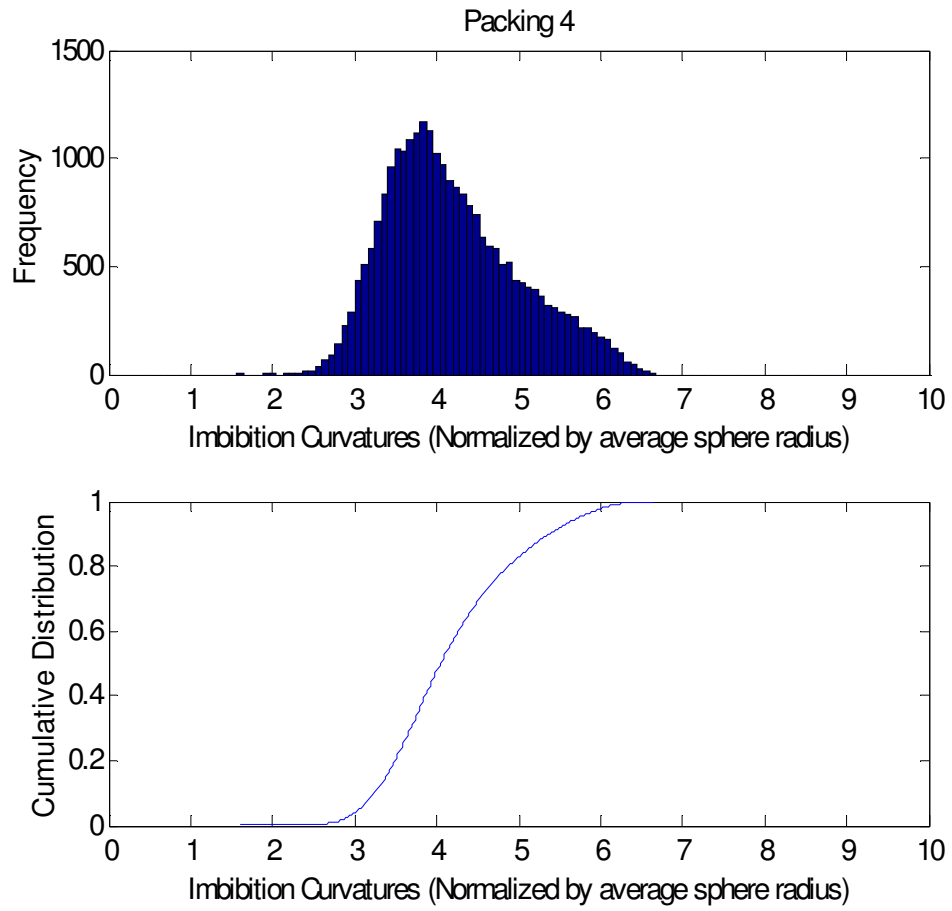
APPENDIX B

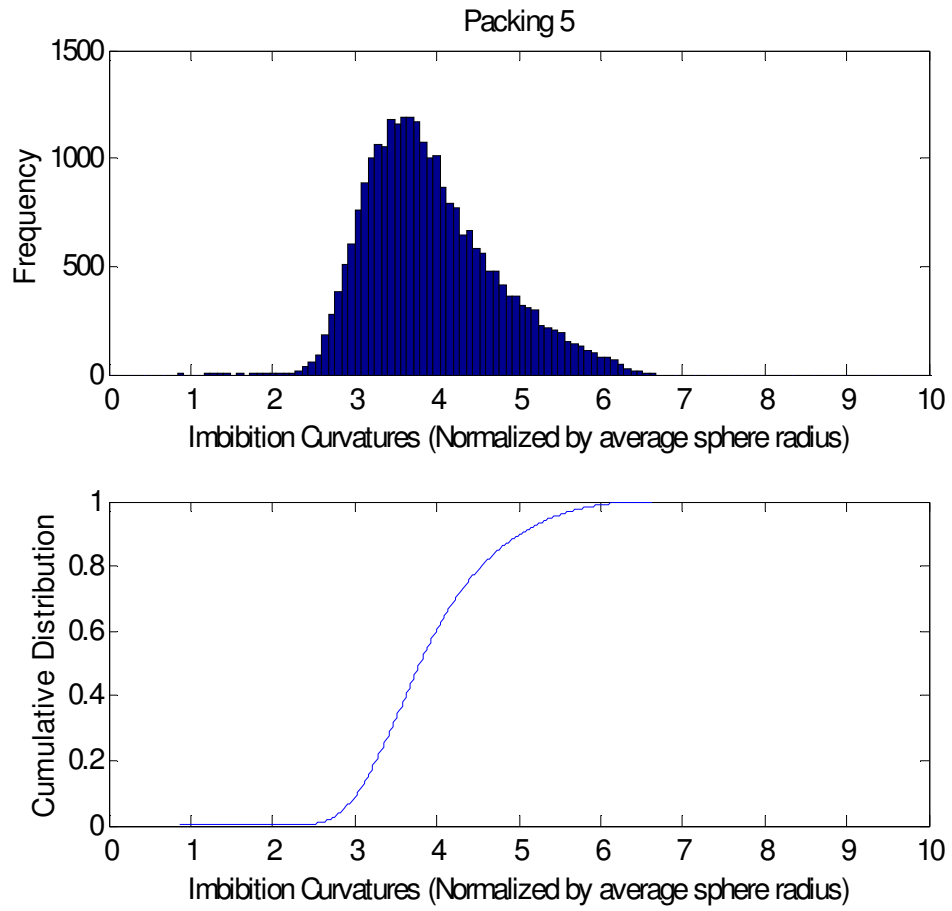
Statistical Information on Imbibition Curvatures

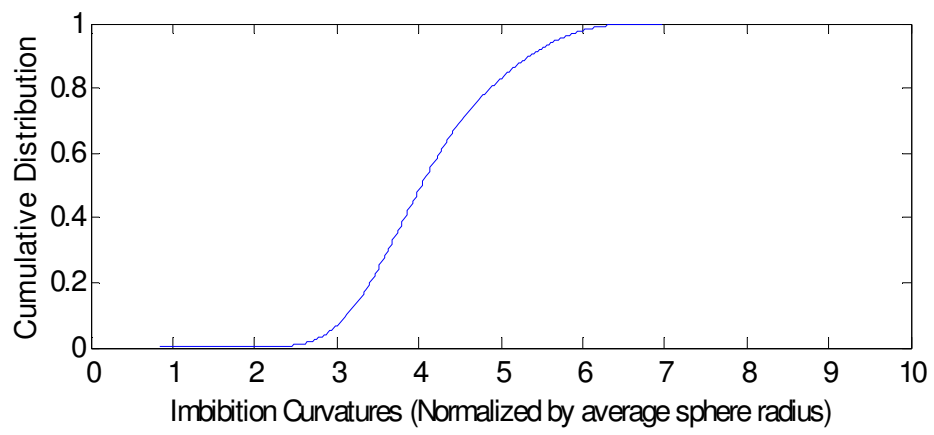
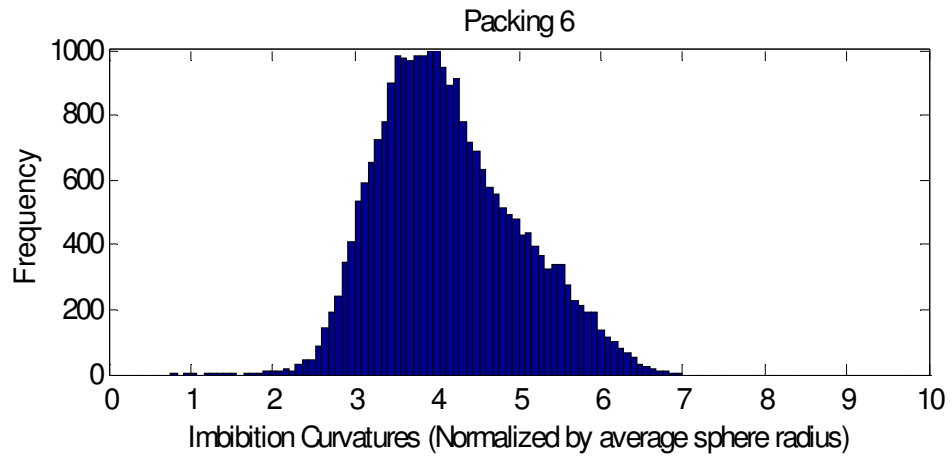


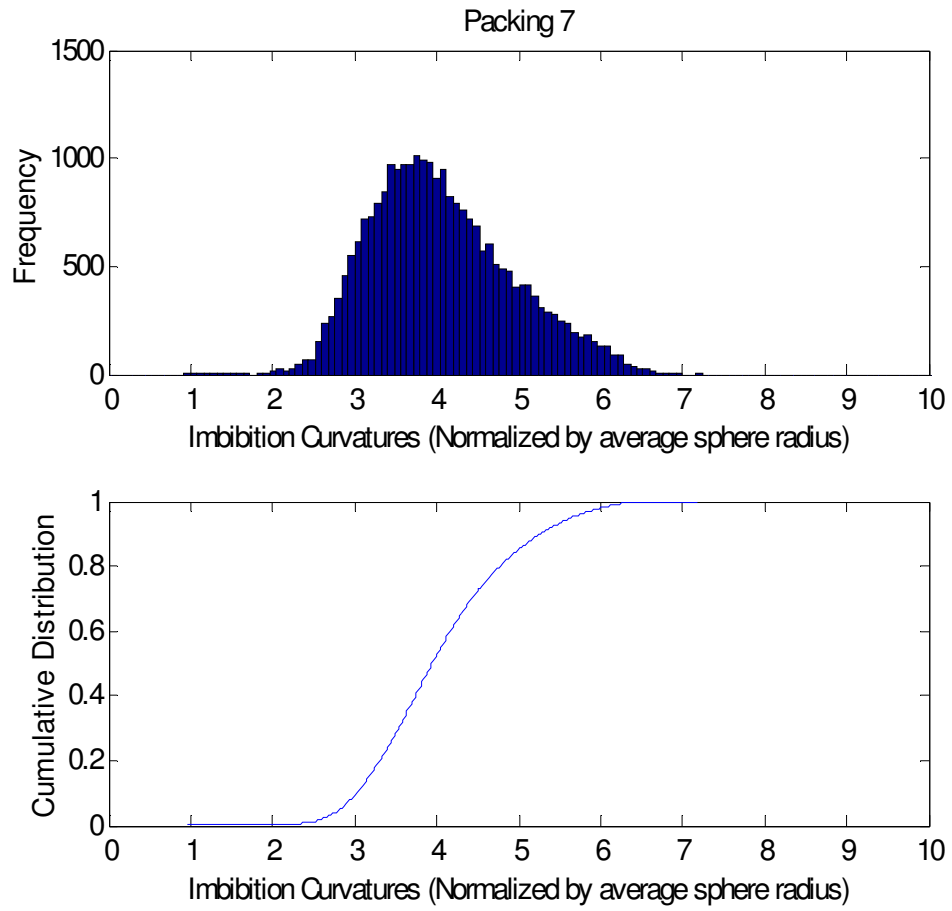


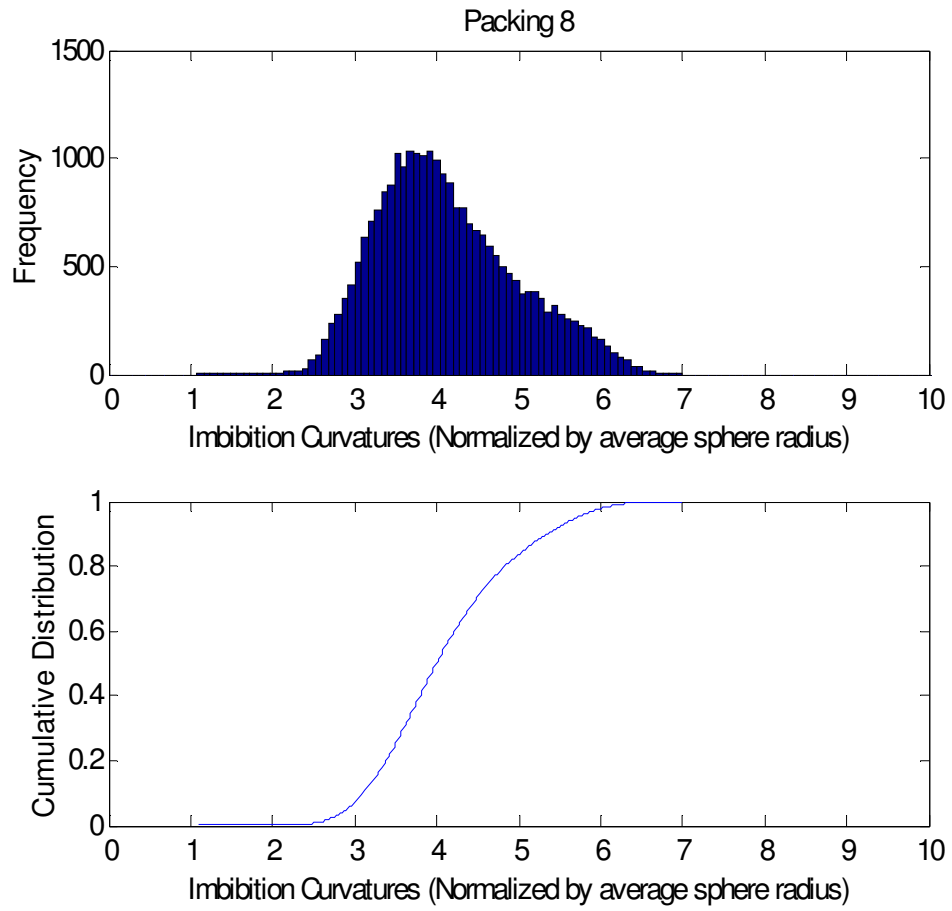


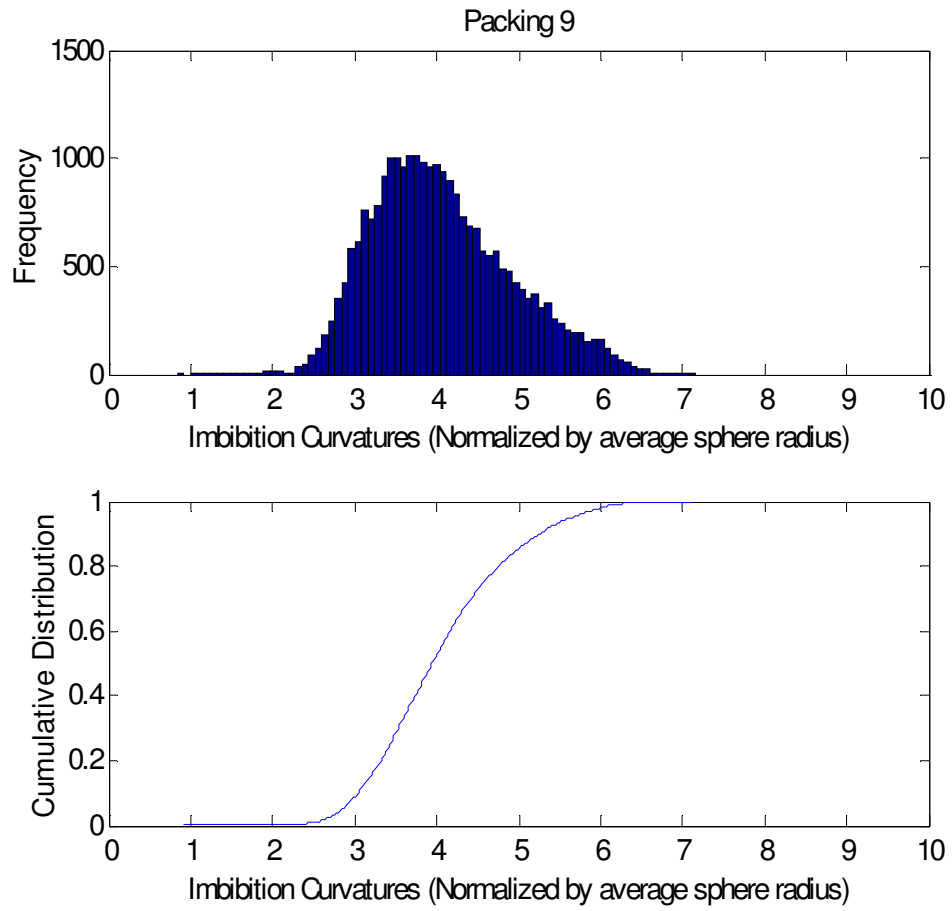


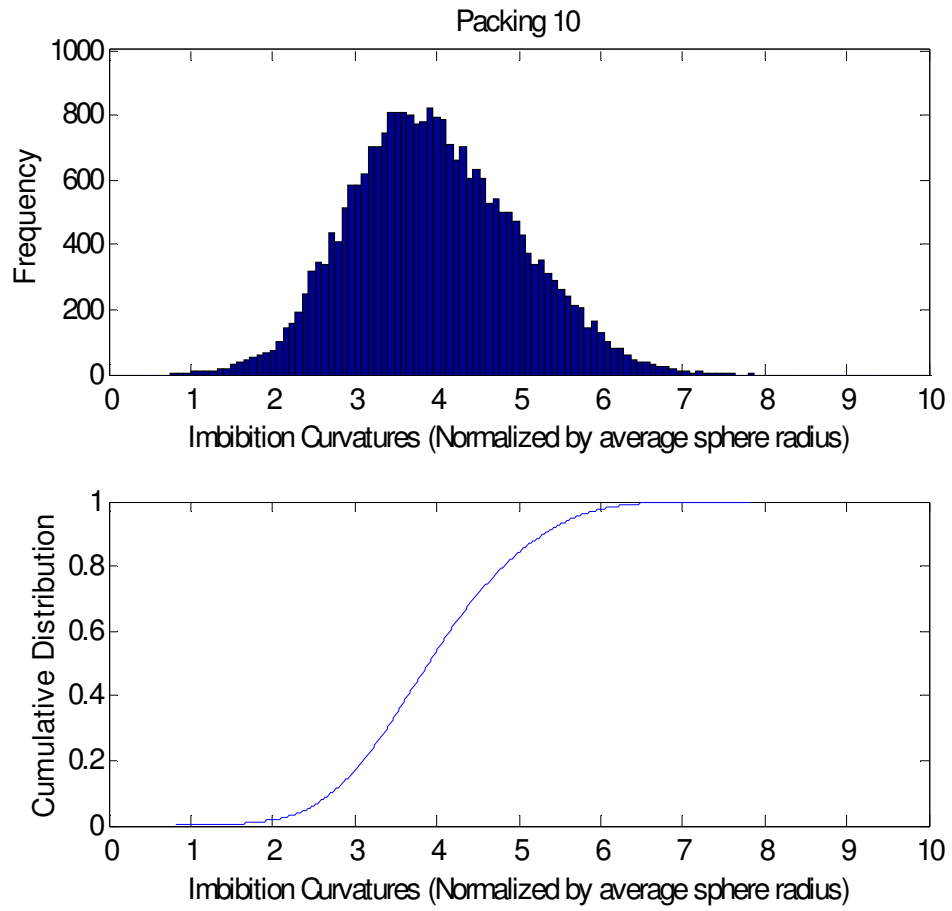


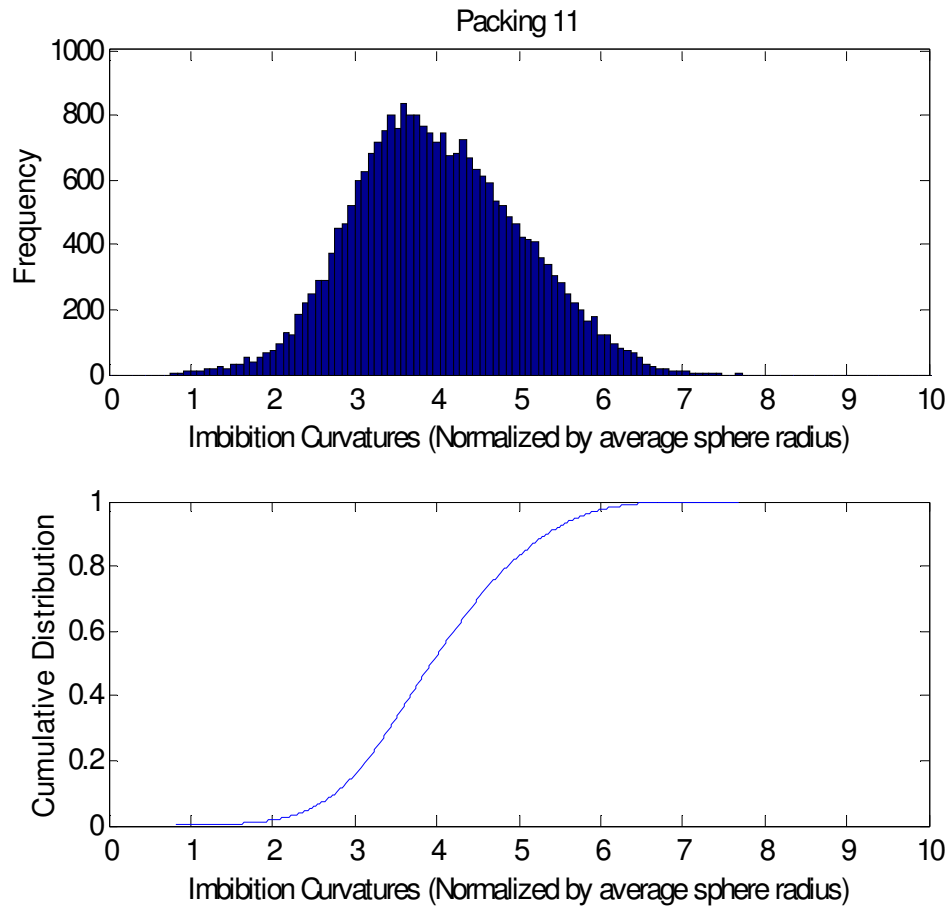


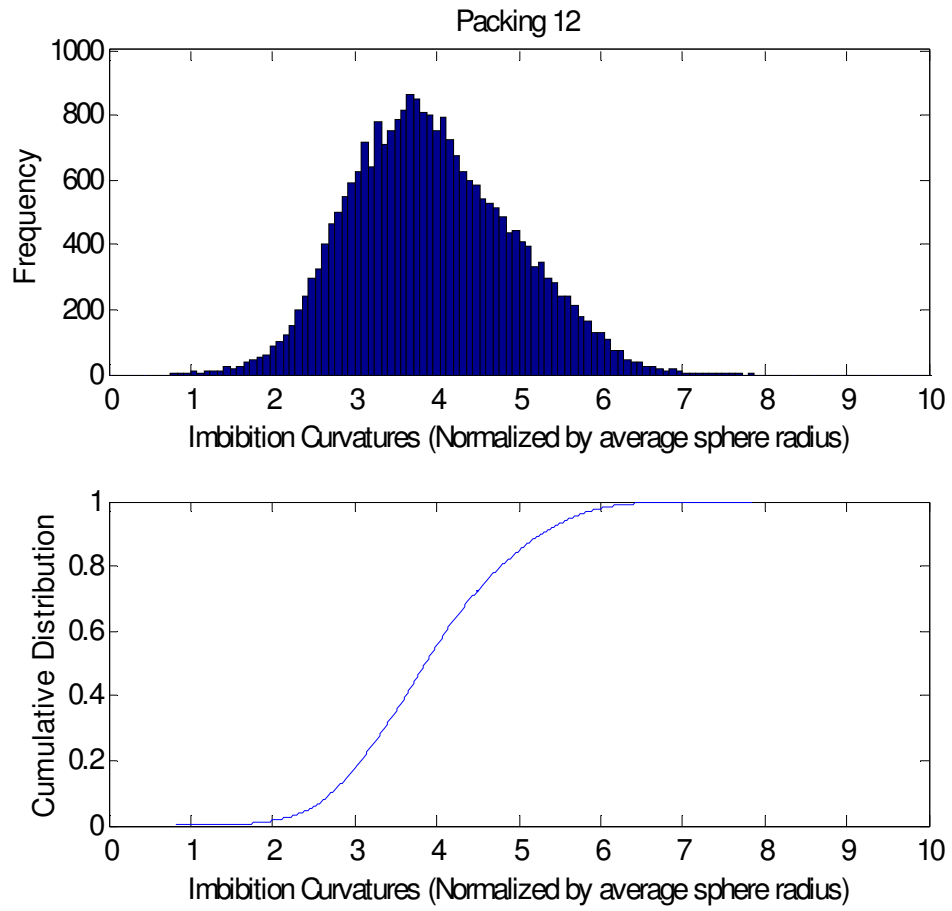


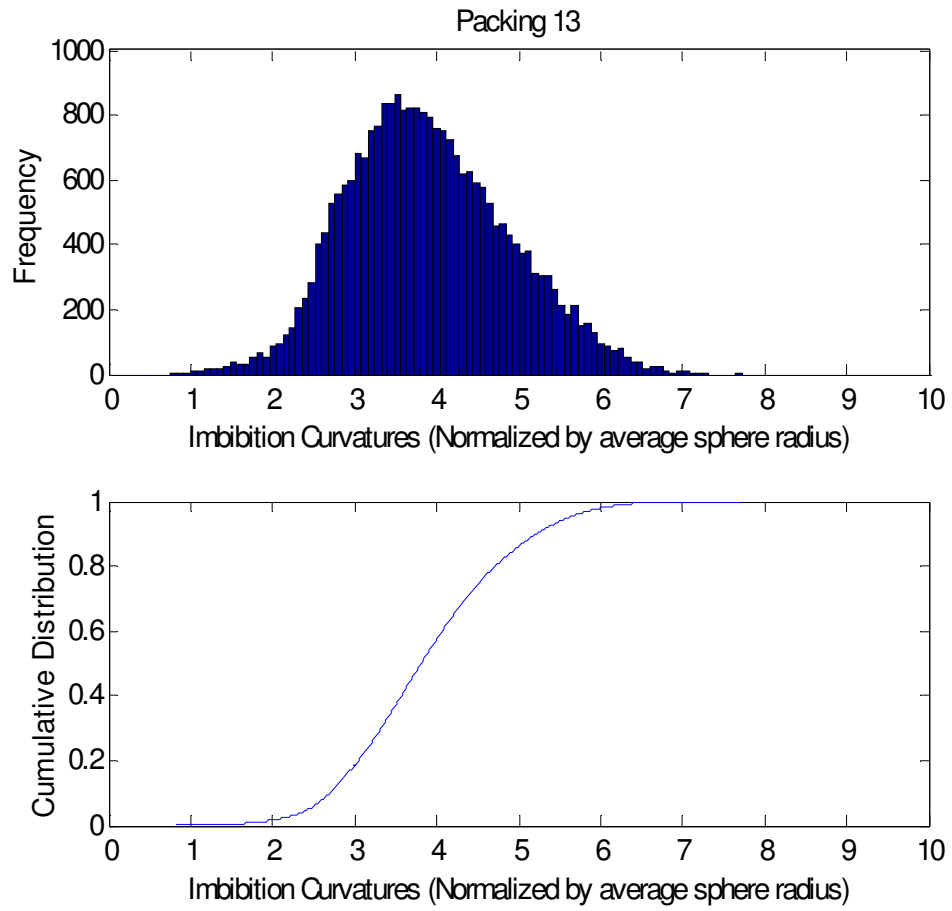


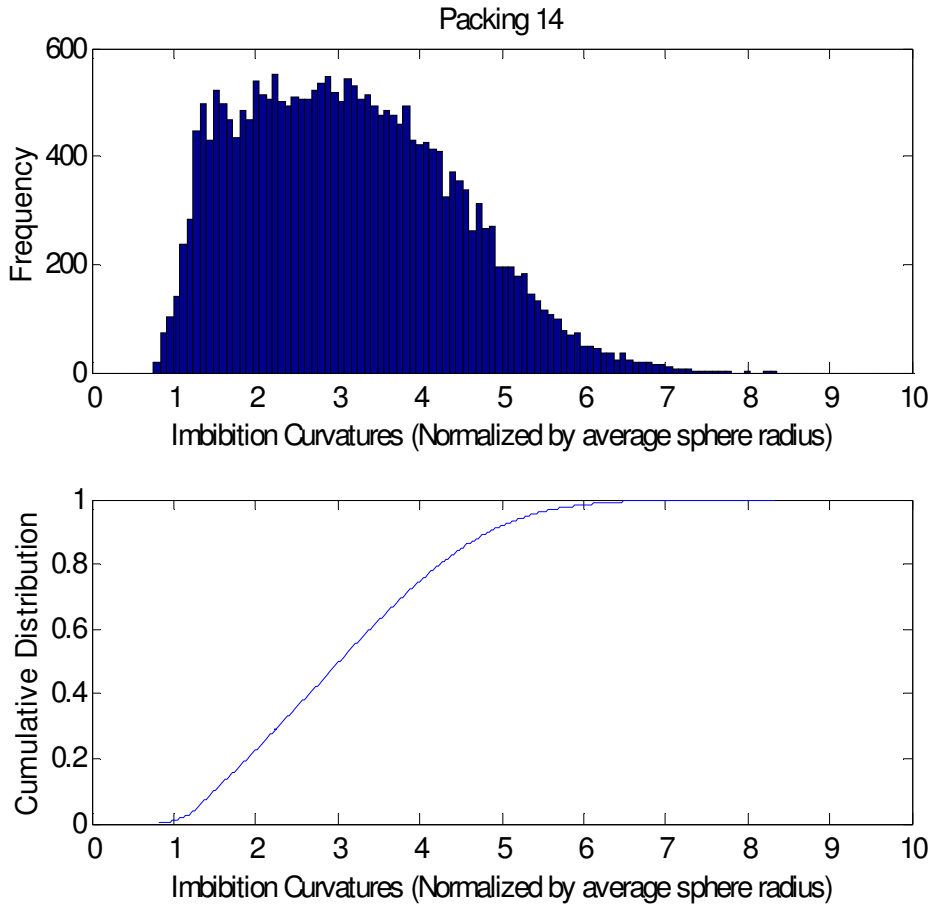


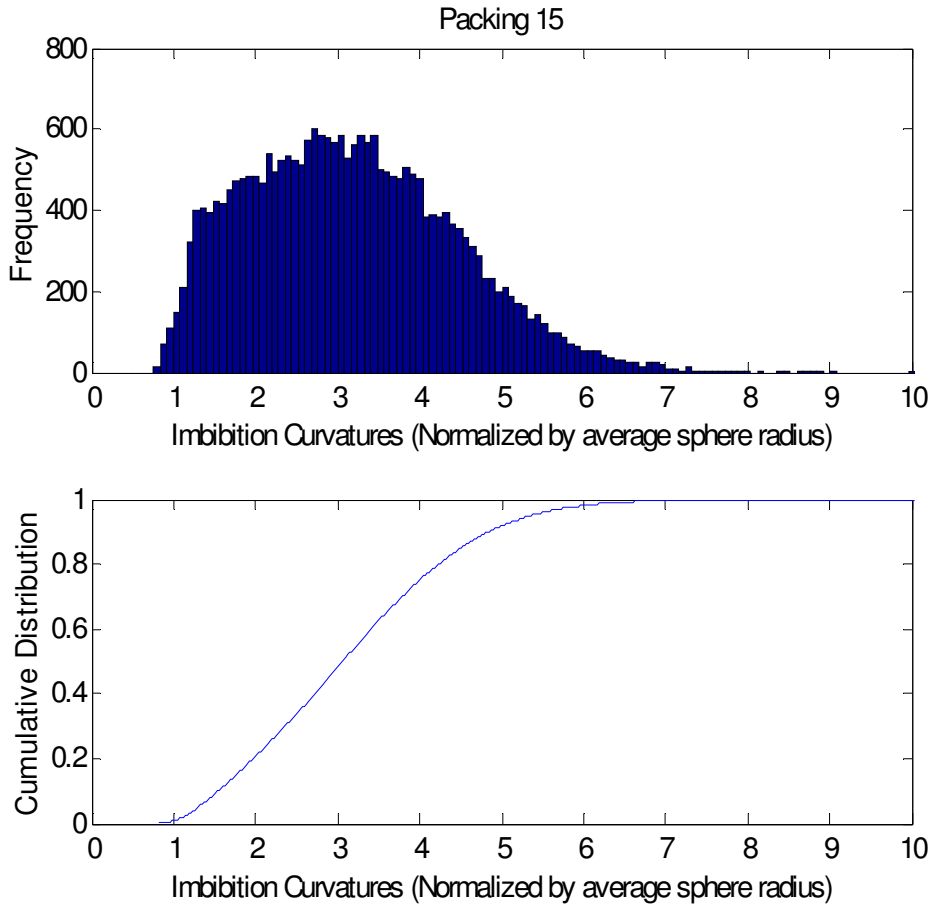


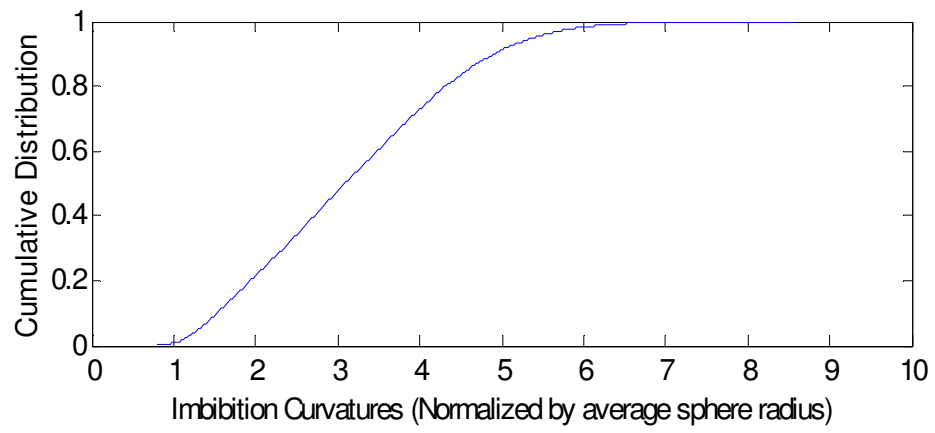
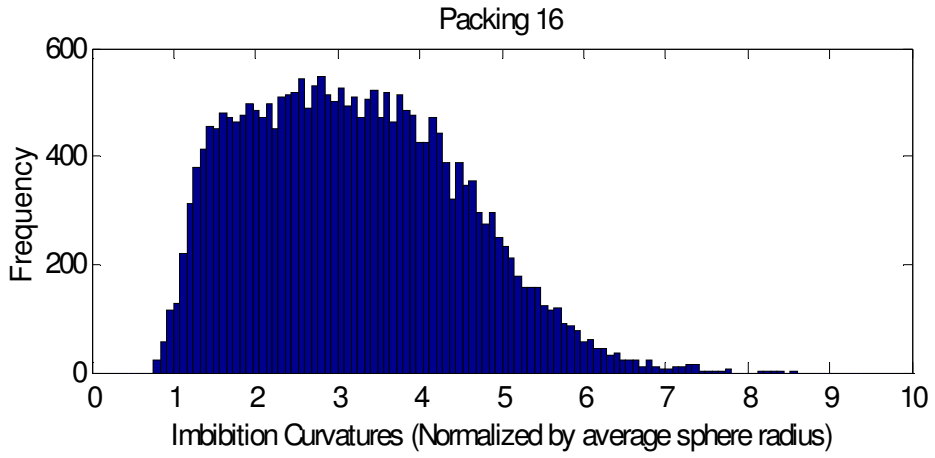


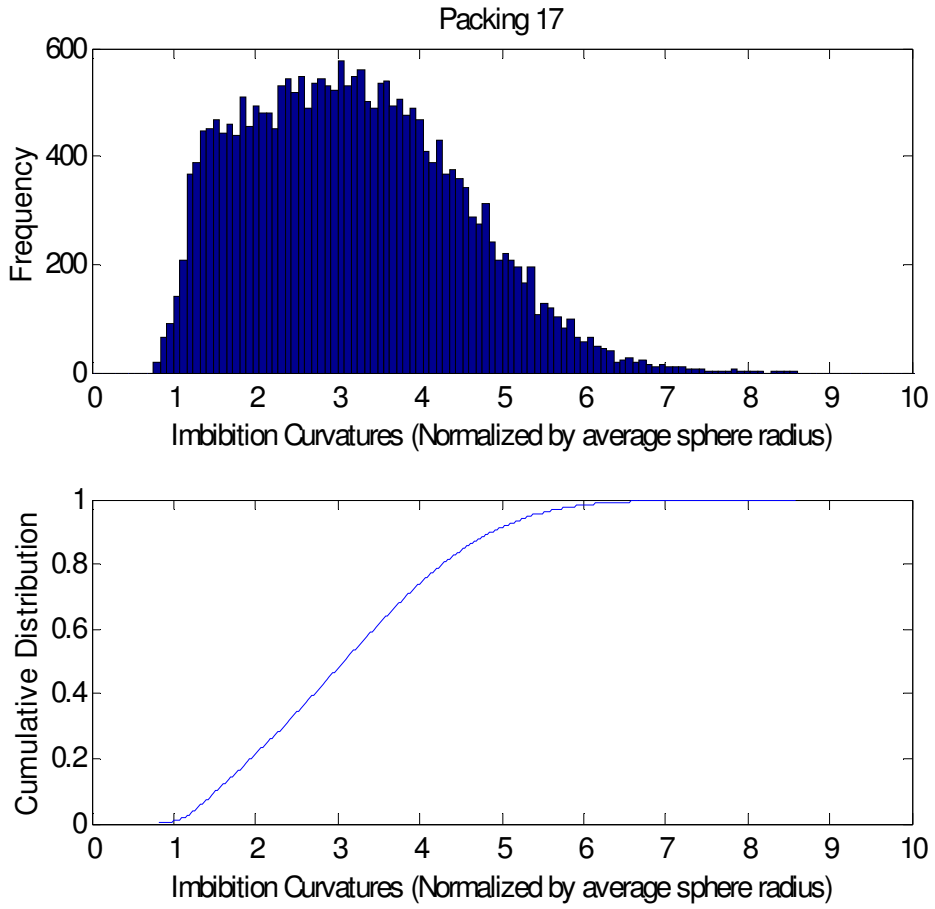


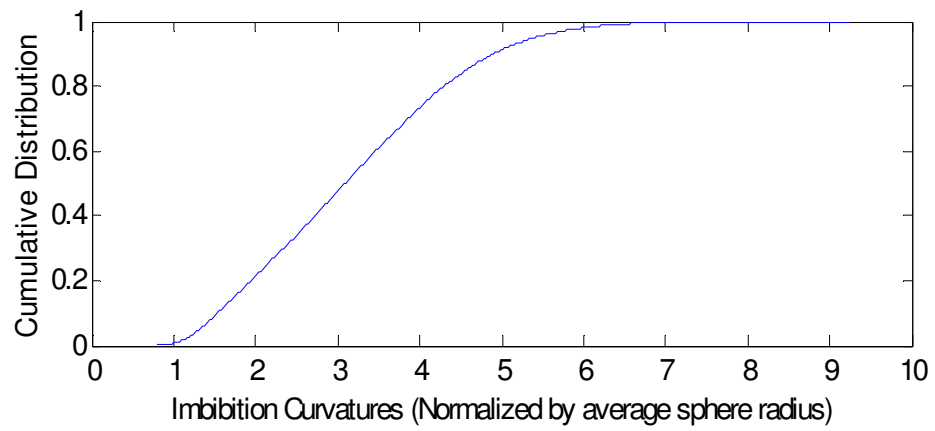
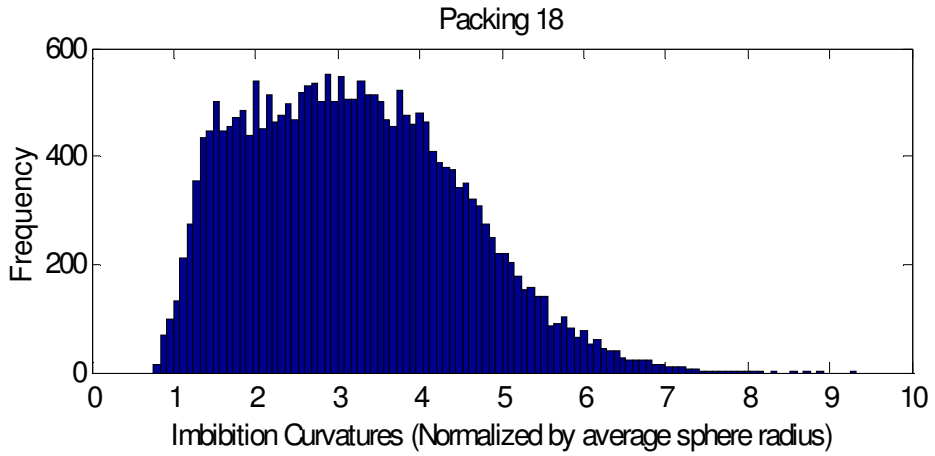


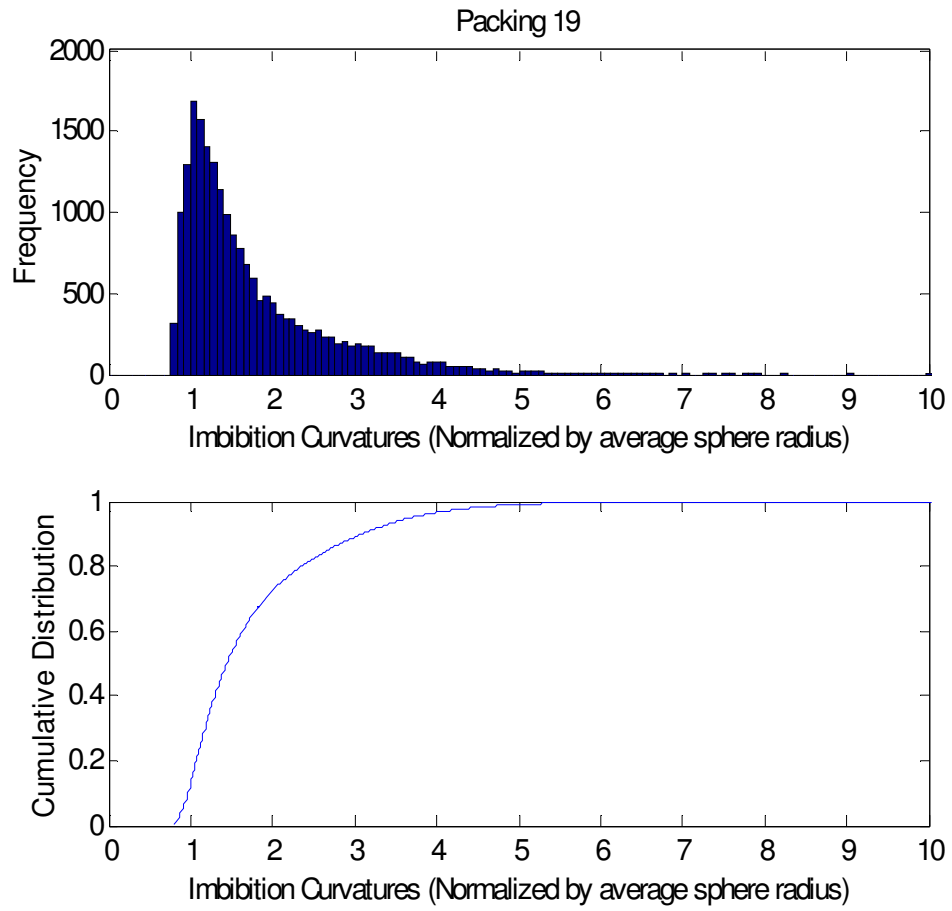


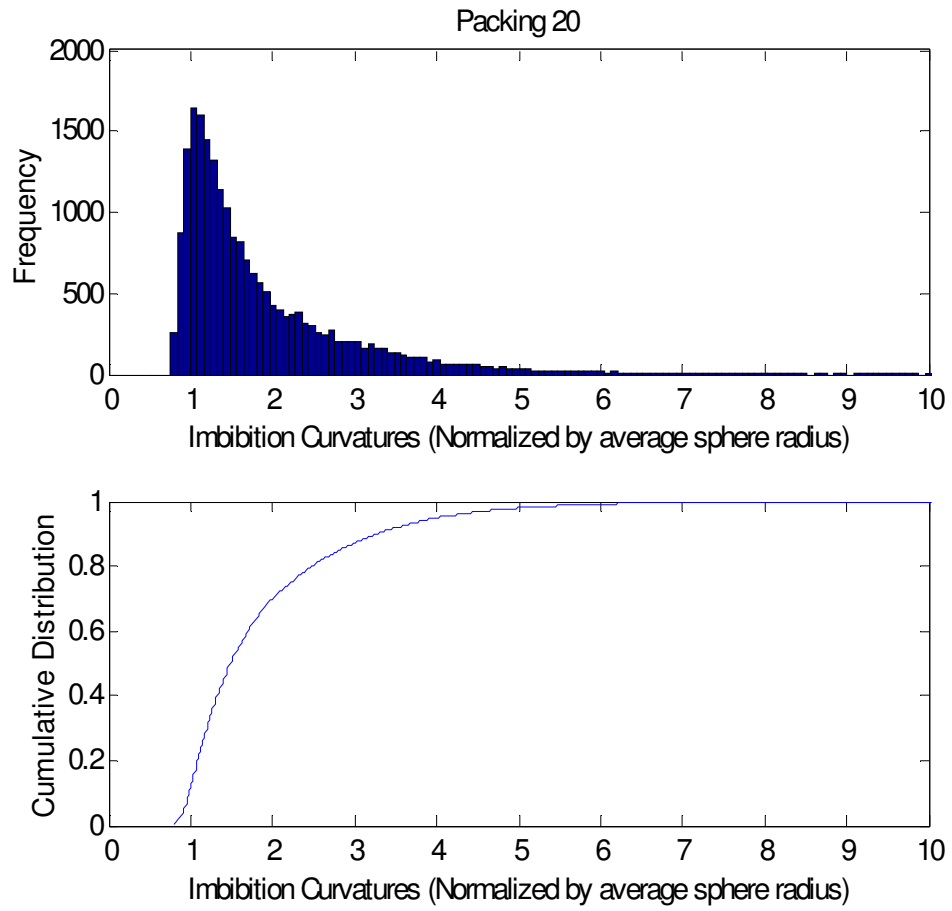


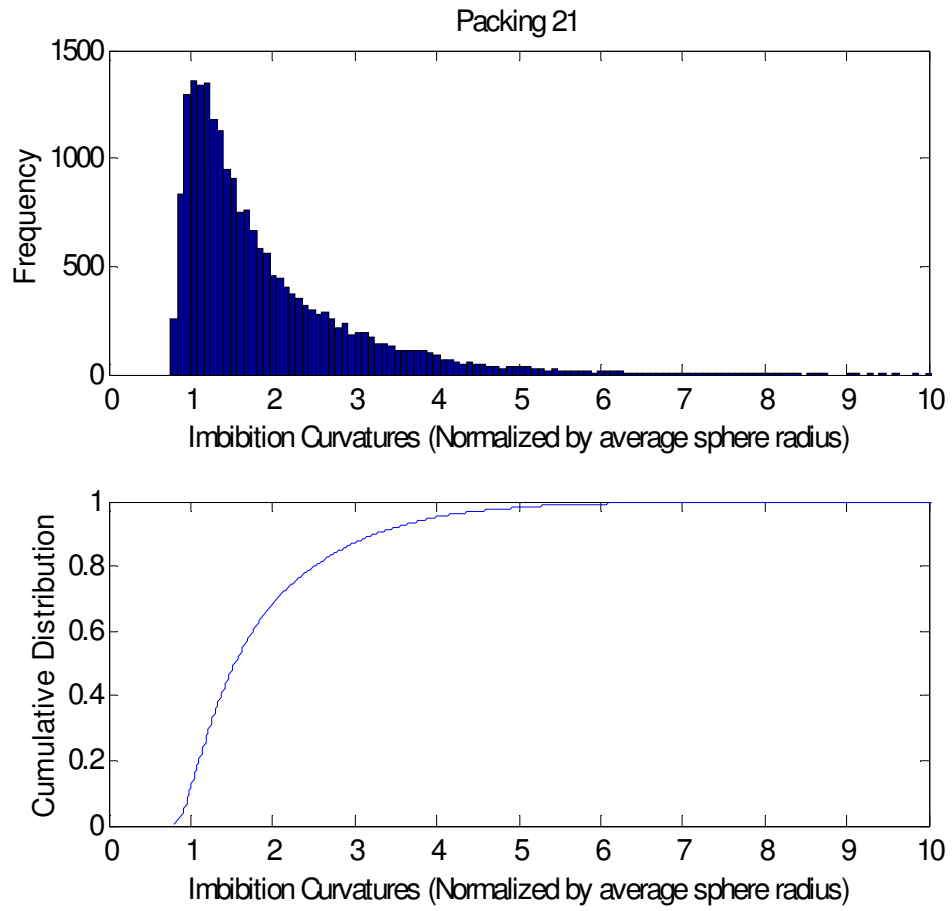


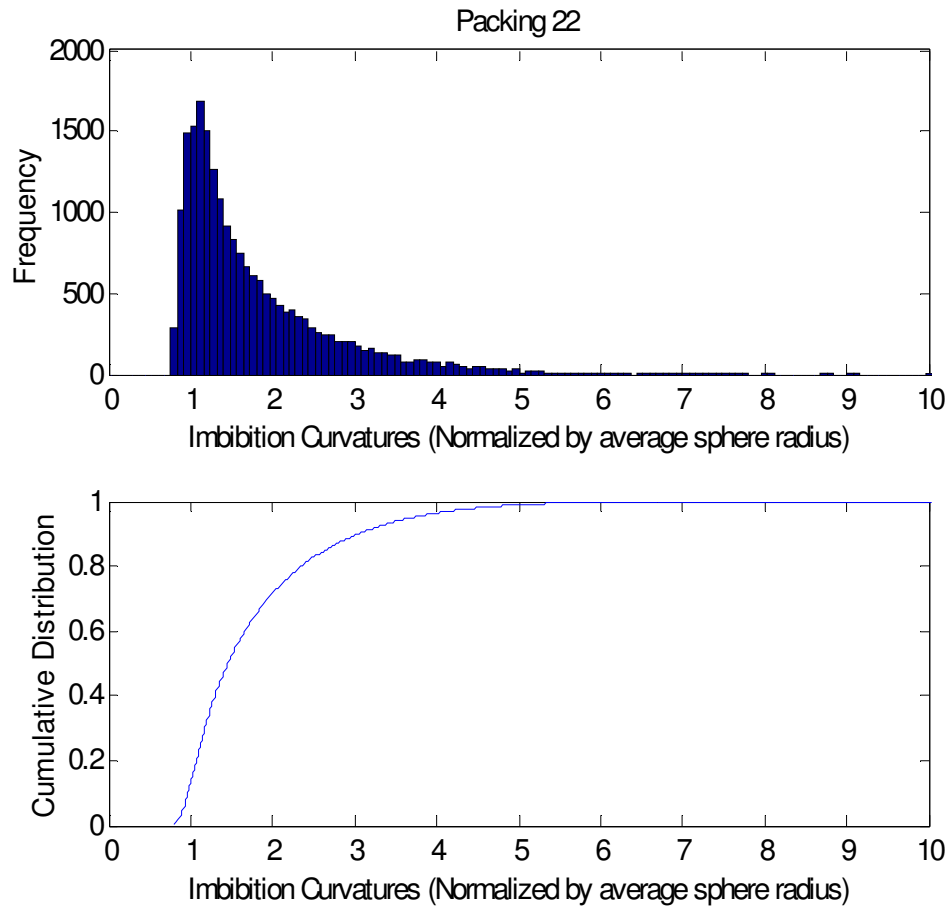


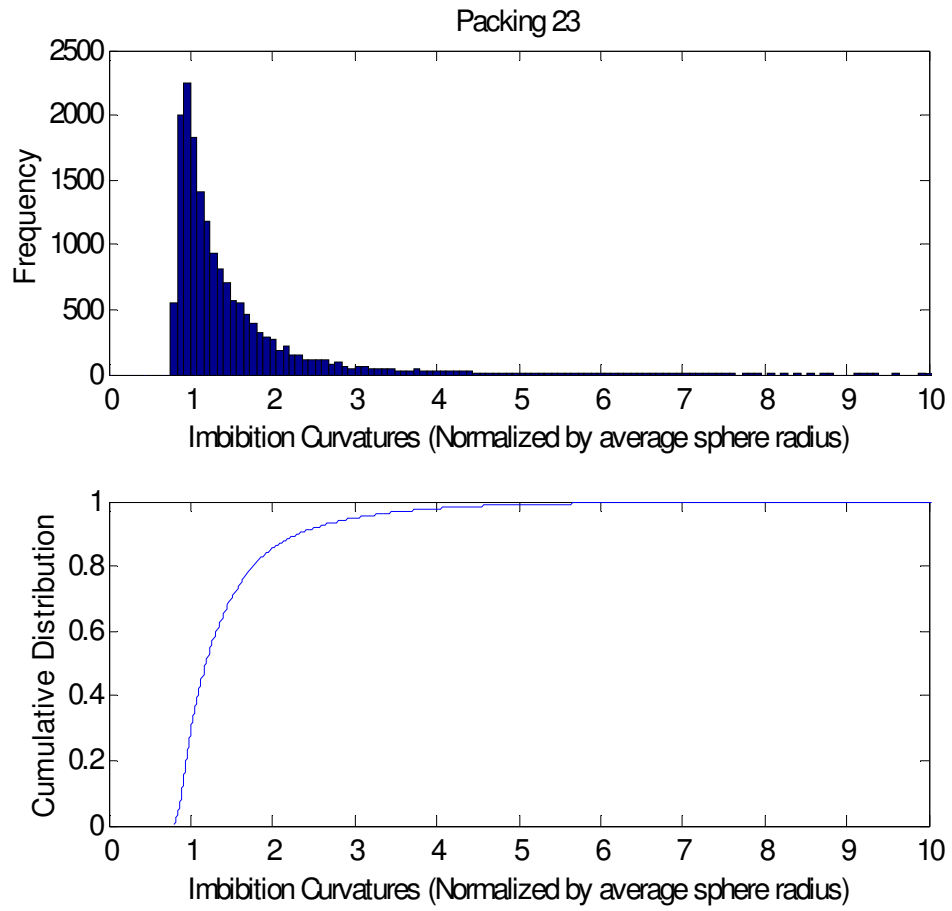


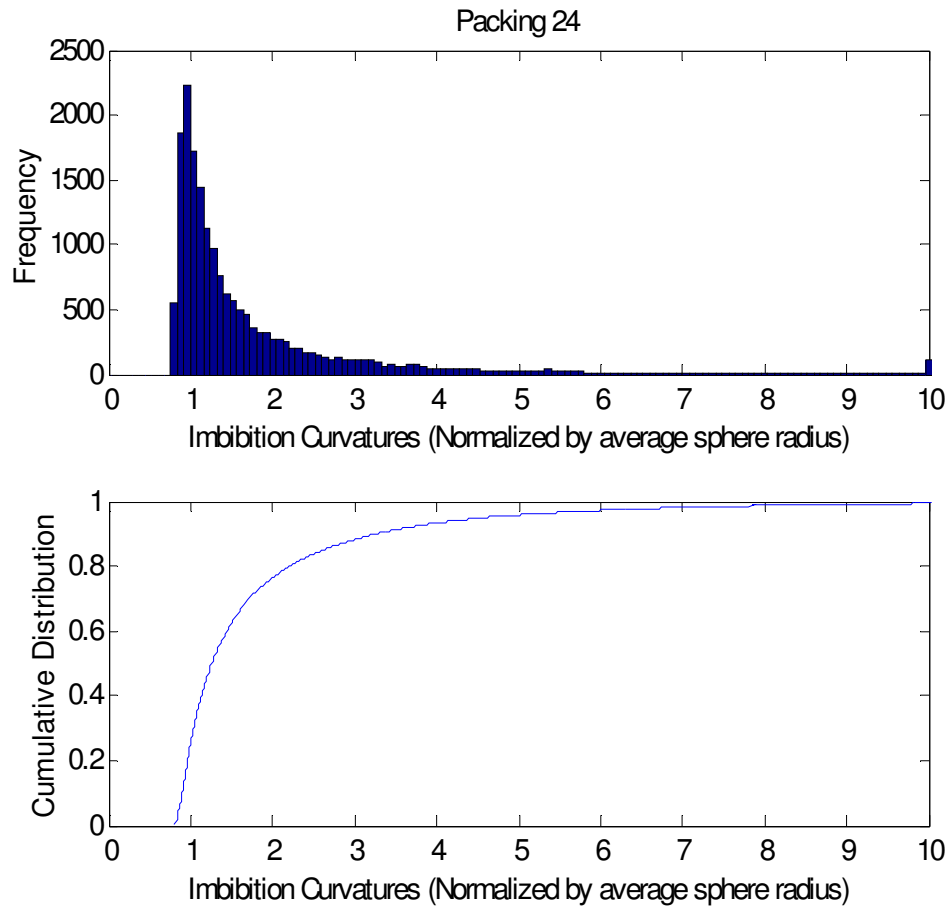


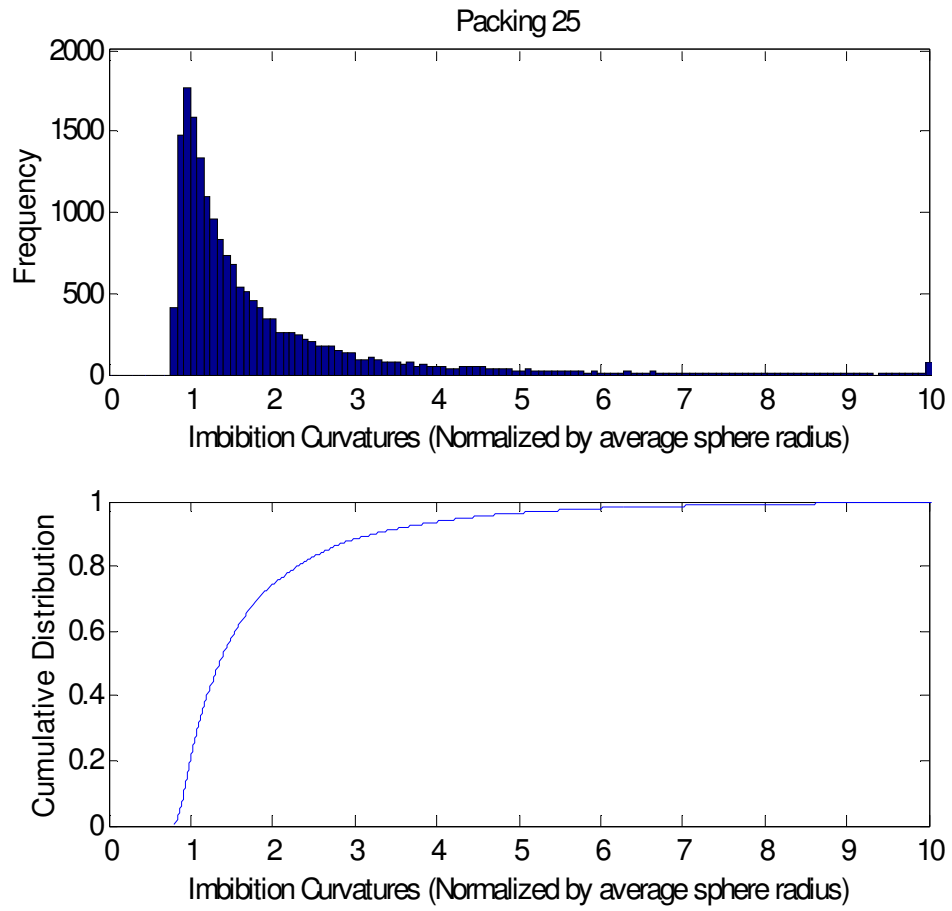


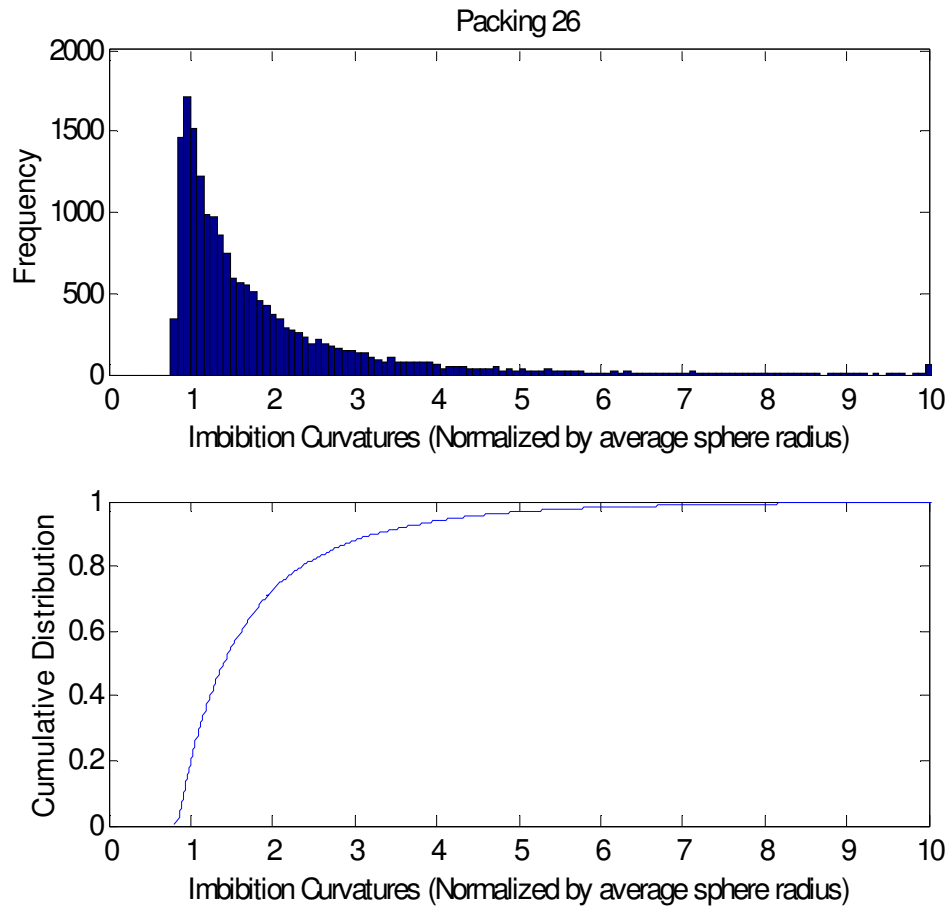


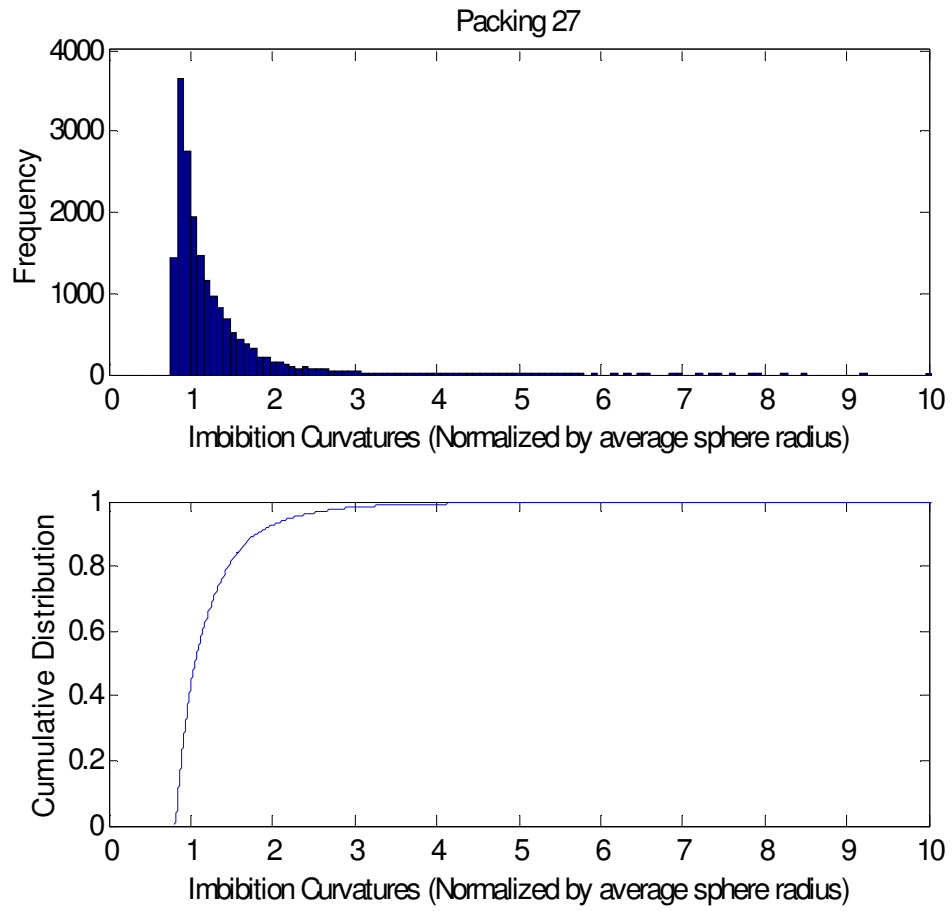


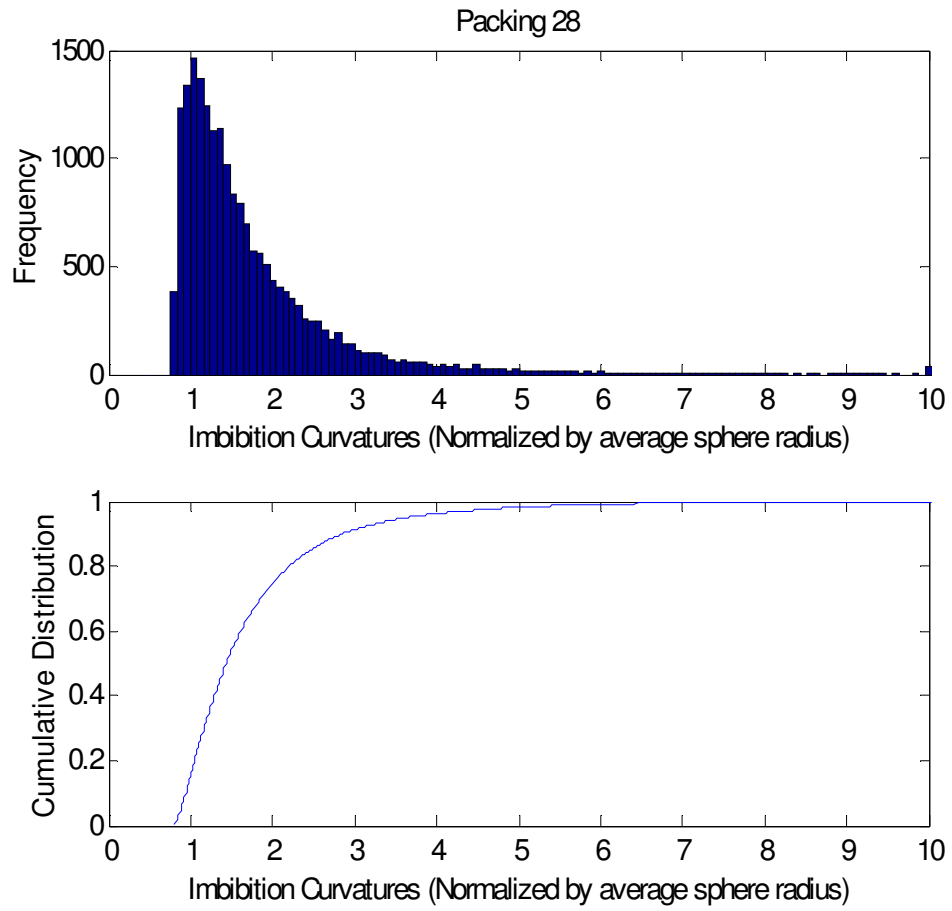


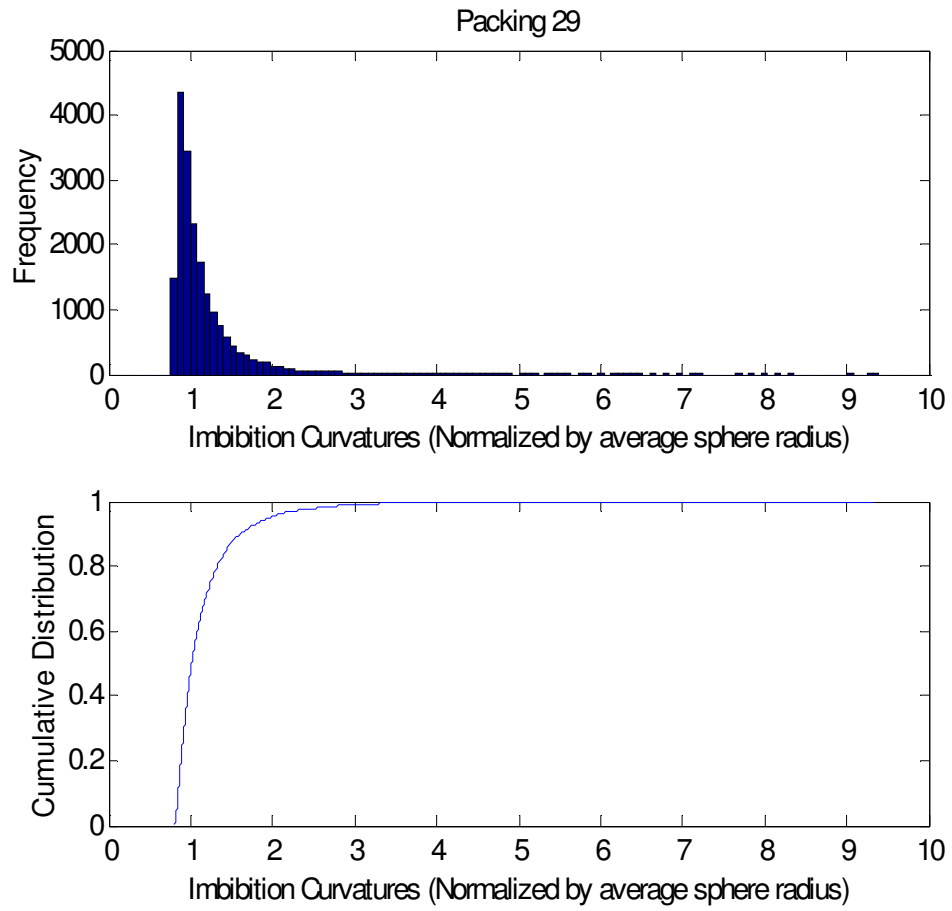


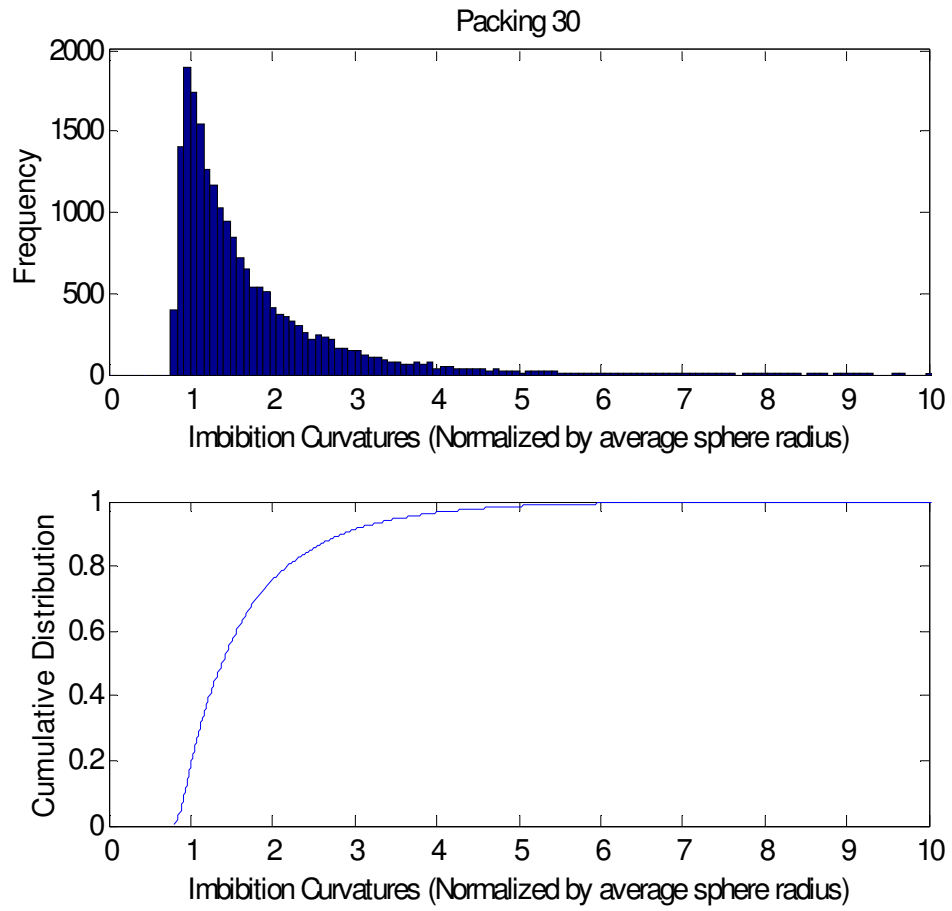


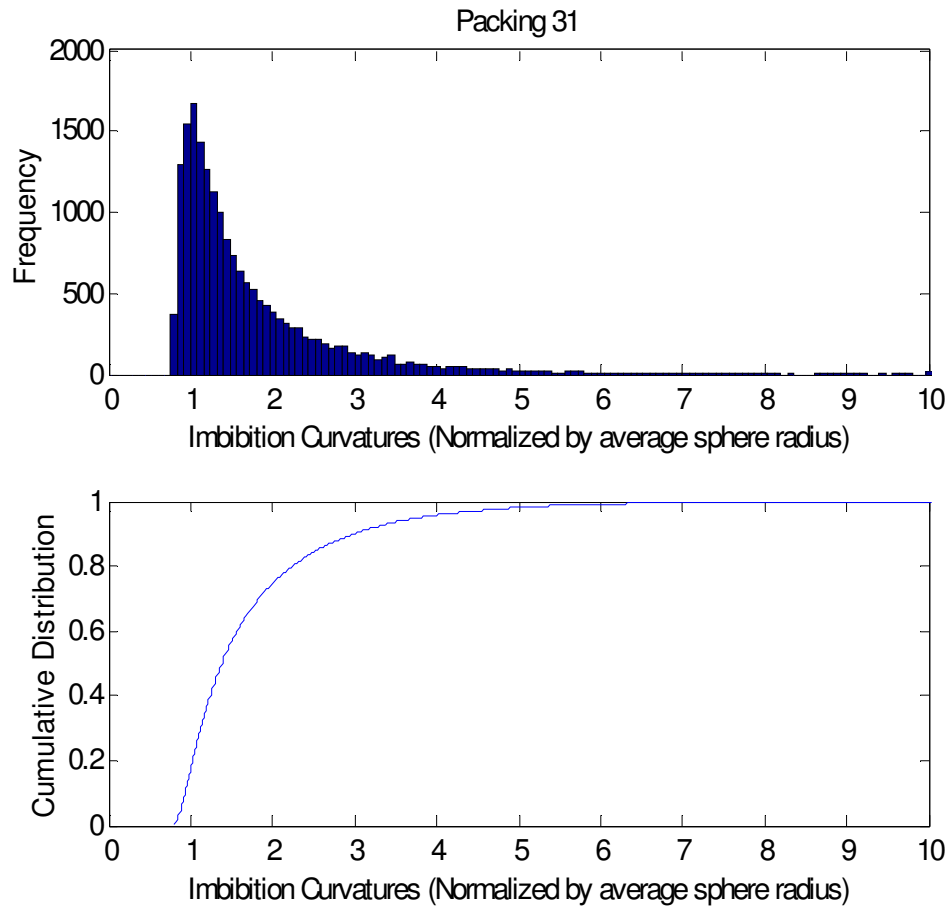


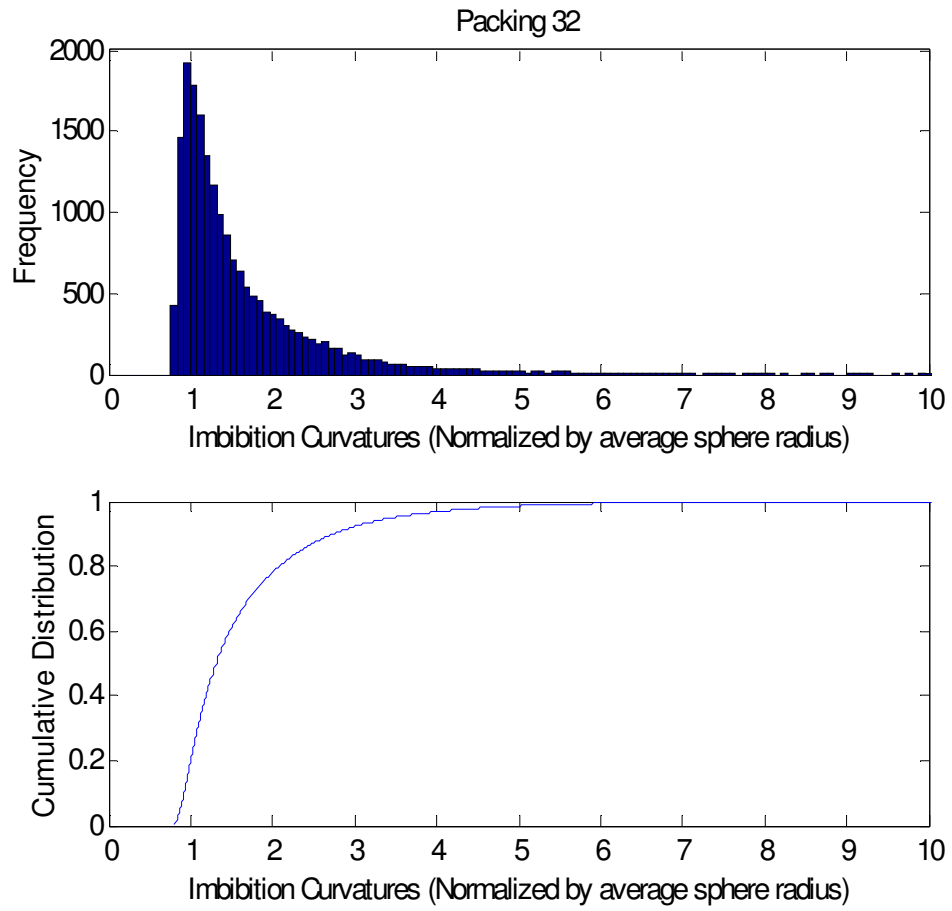


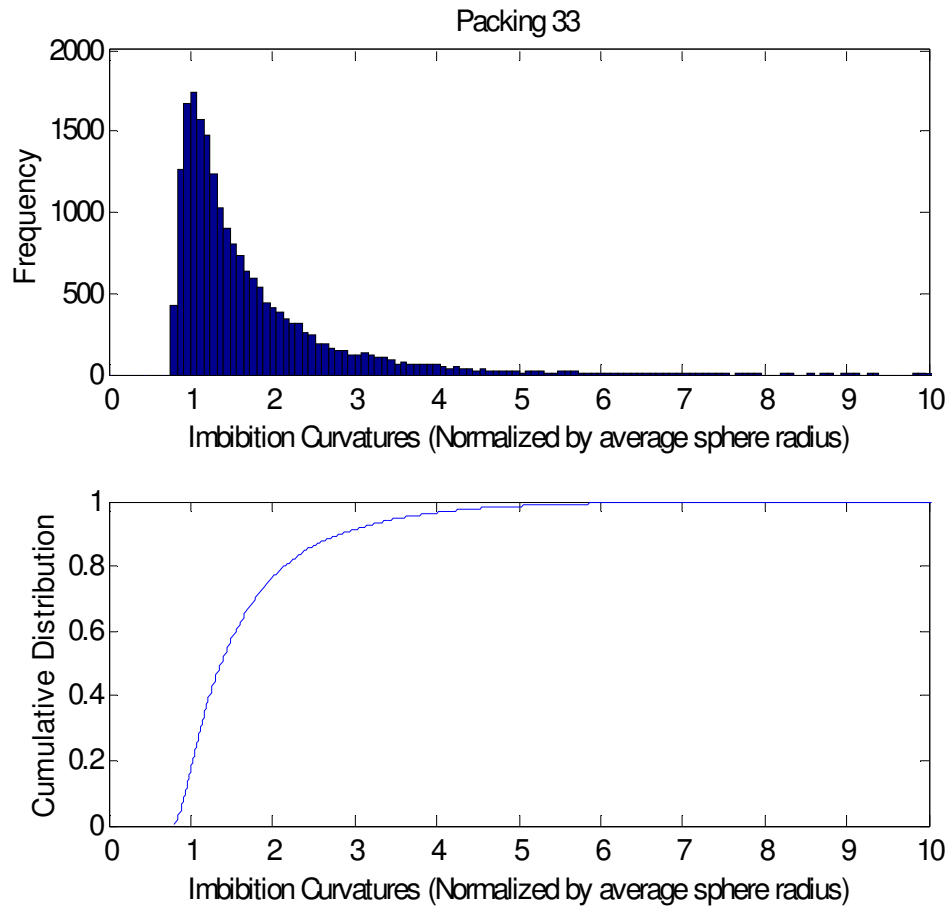


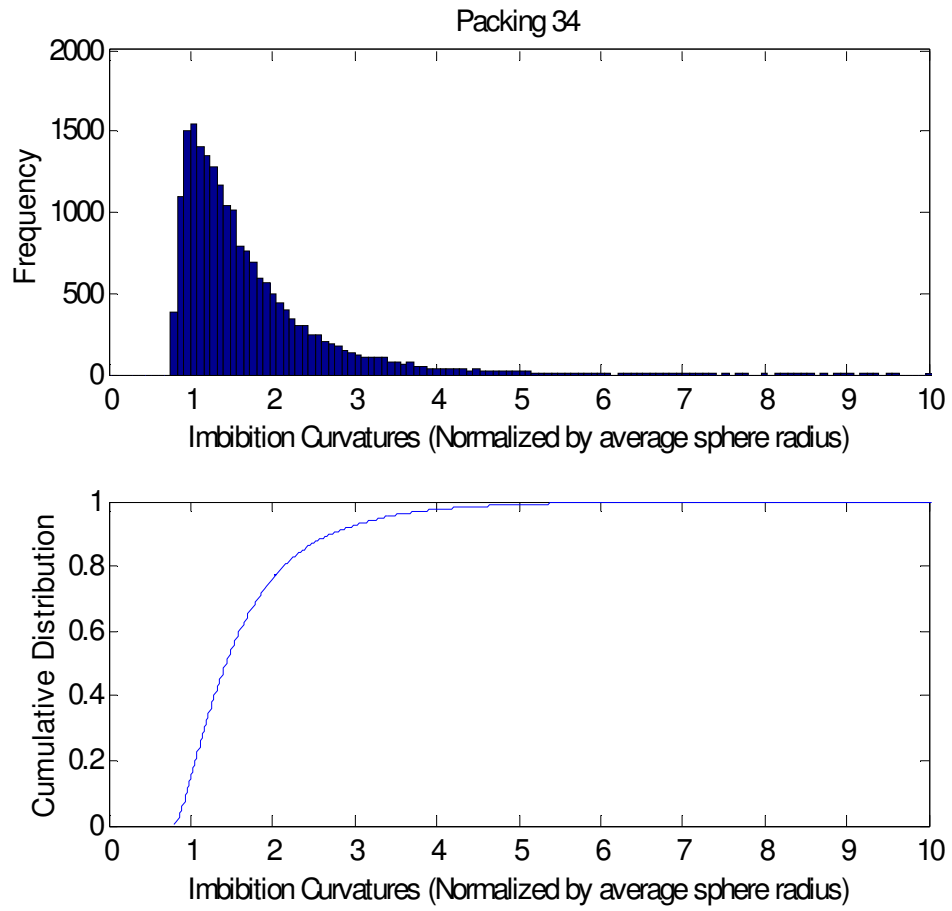


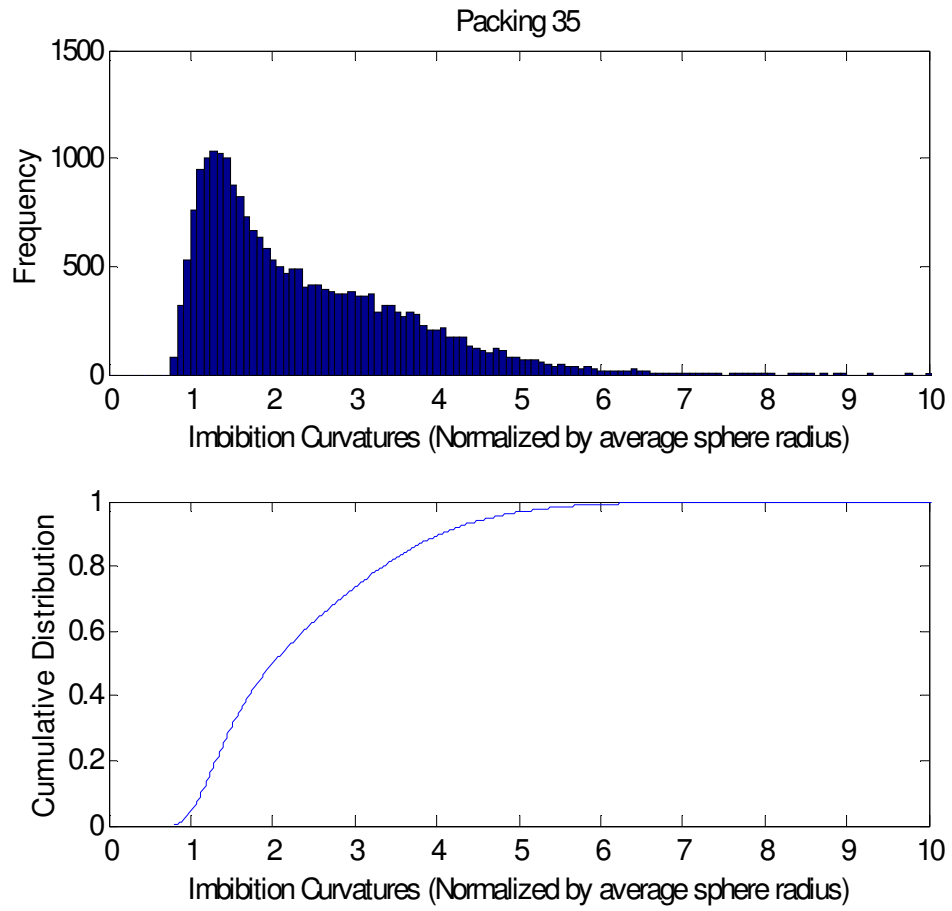


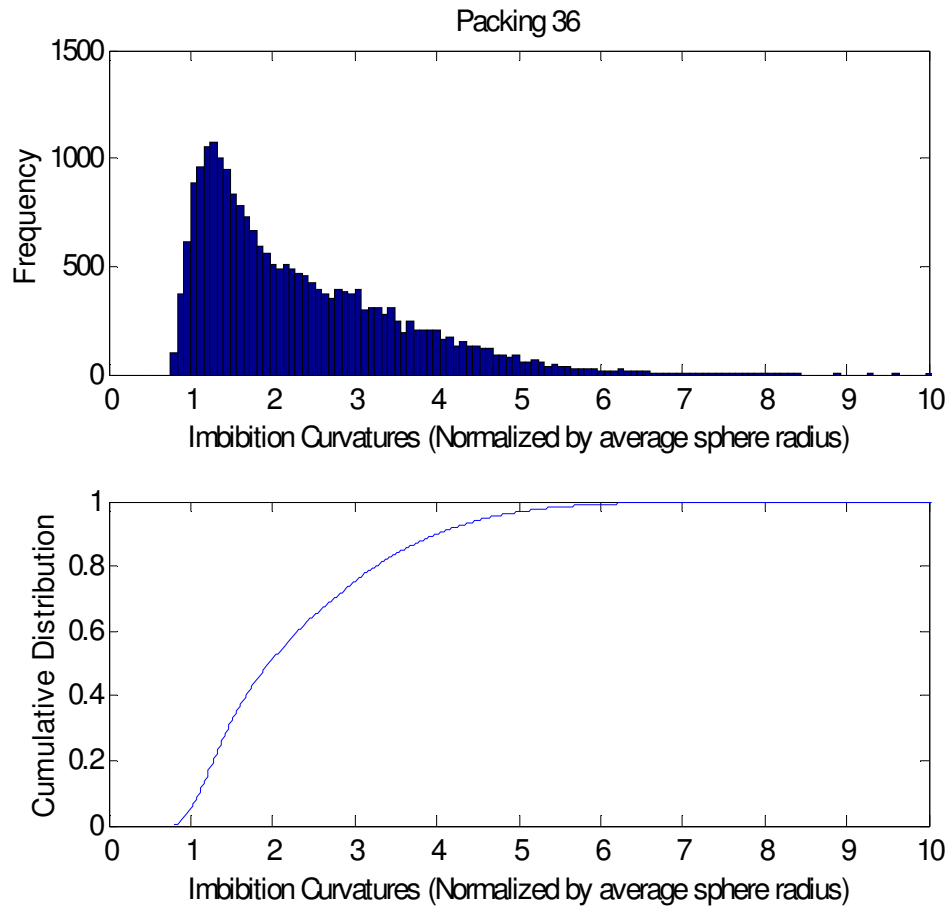


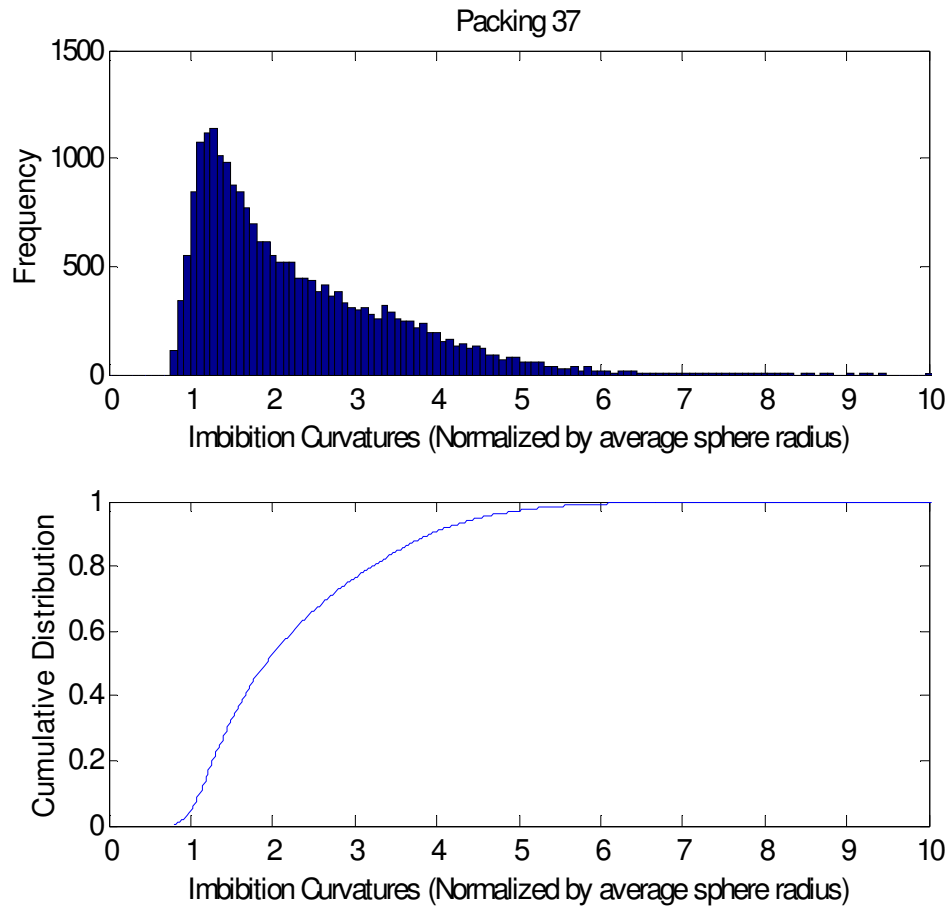


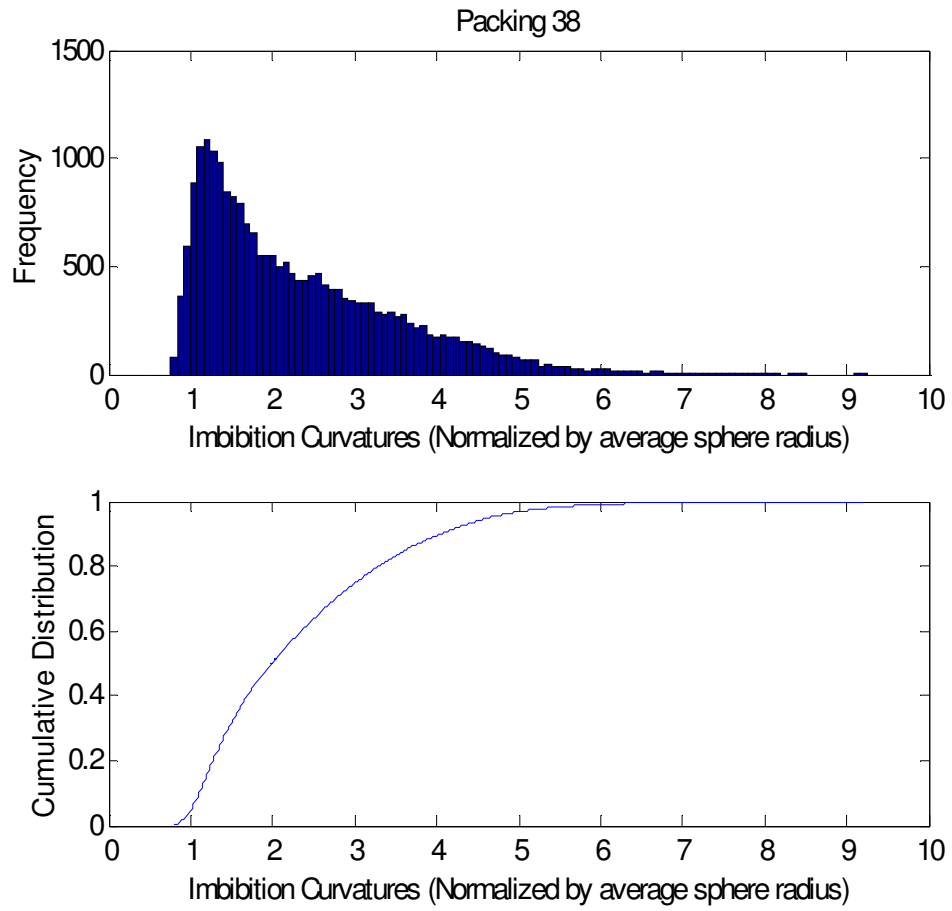


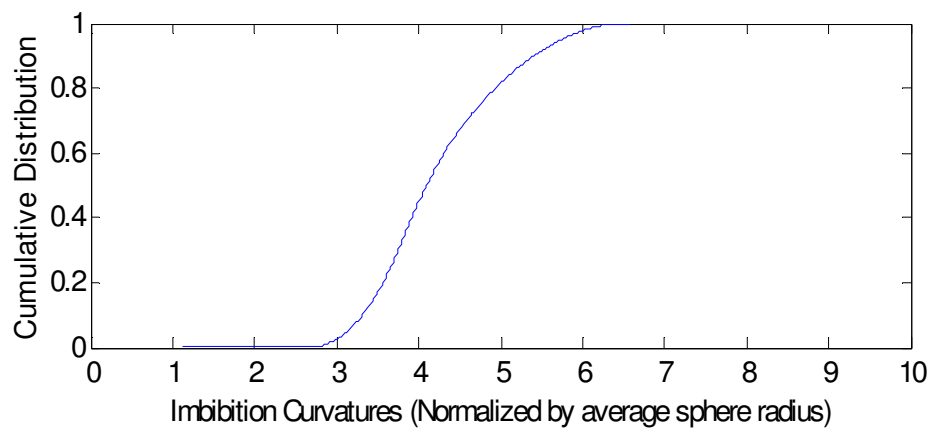
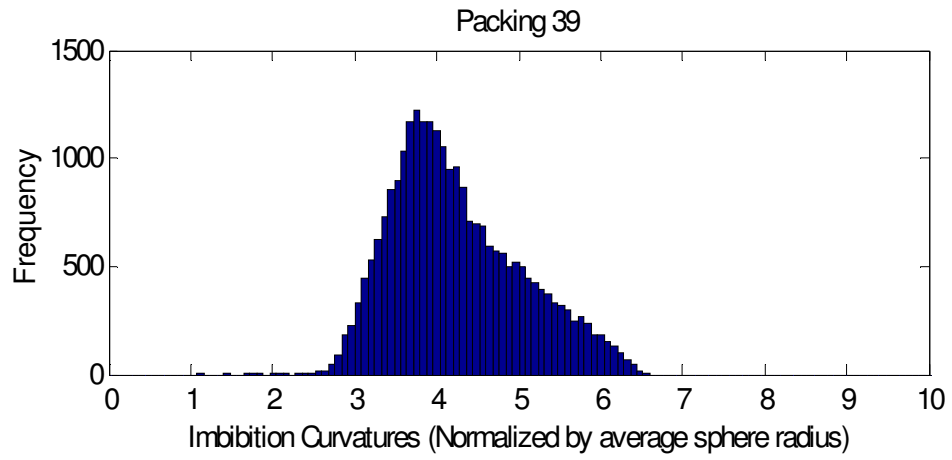


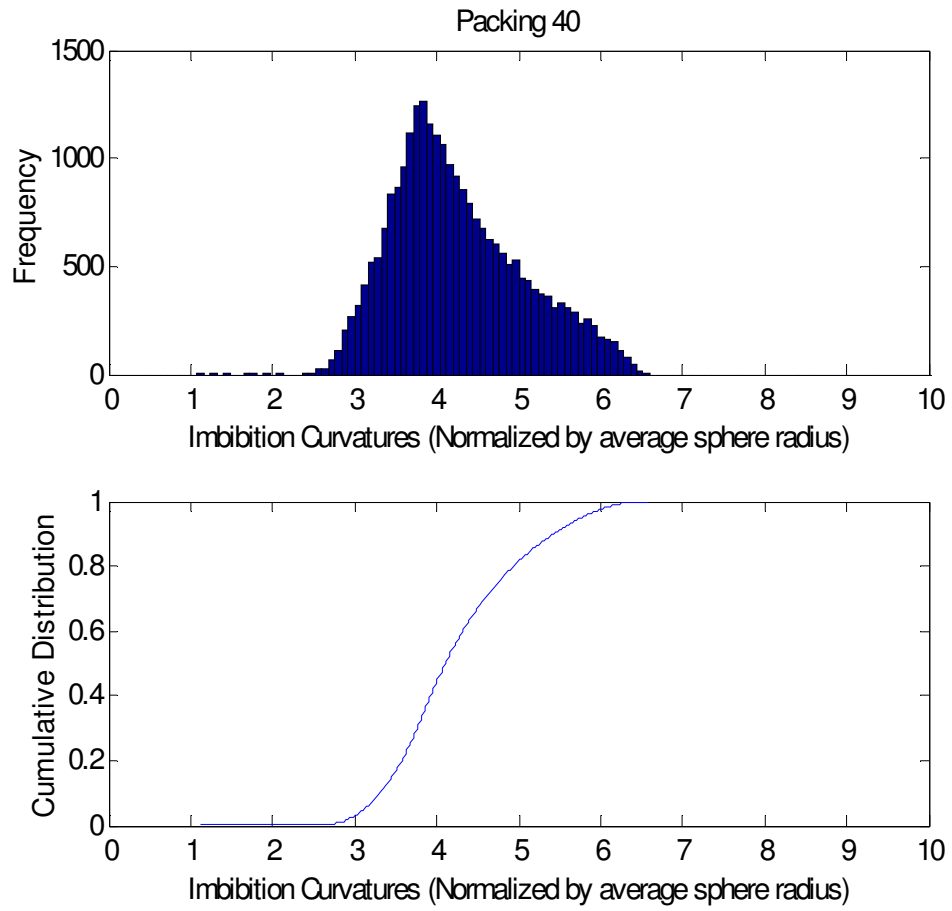


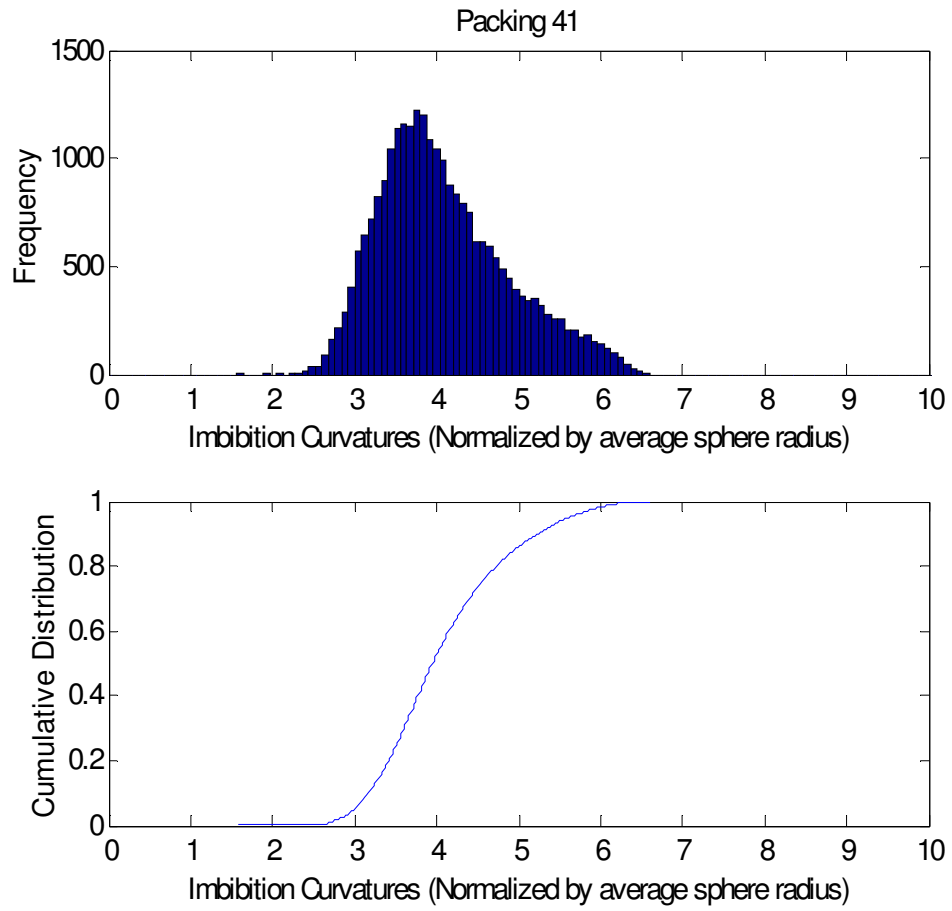


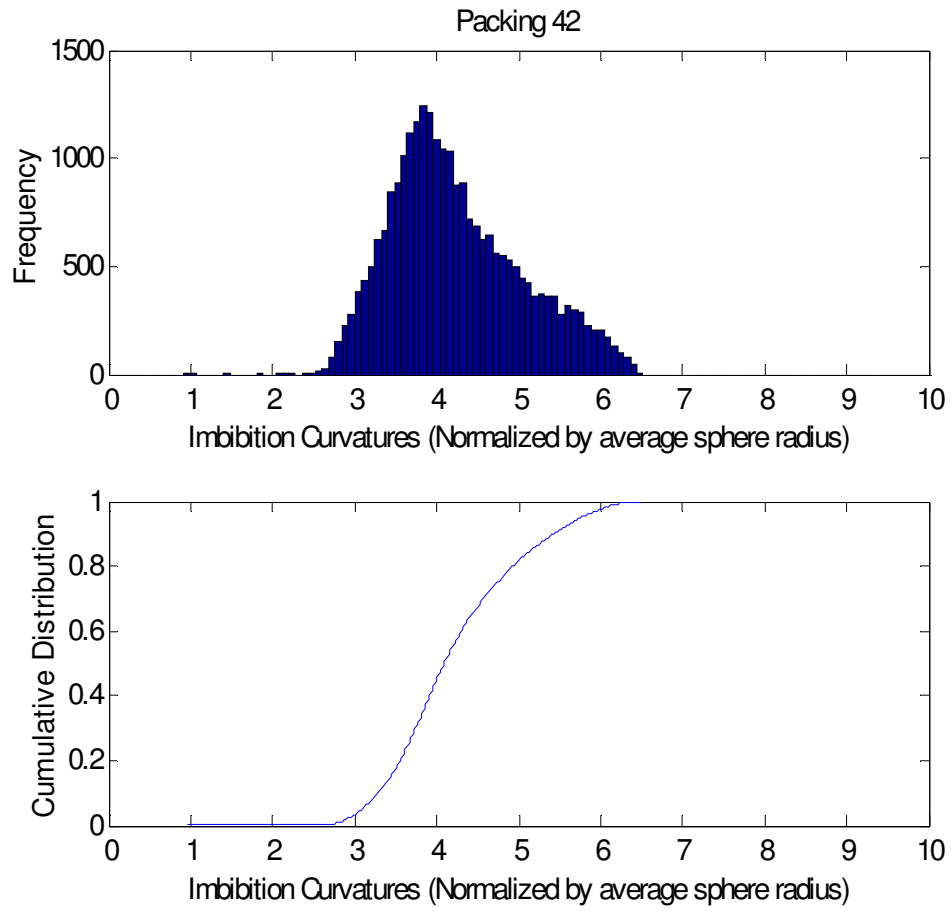


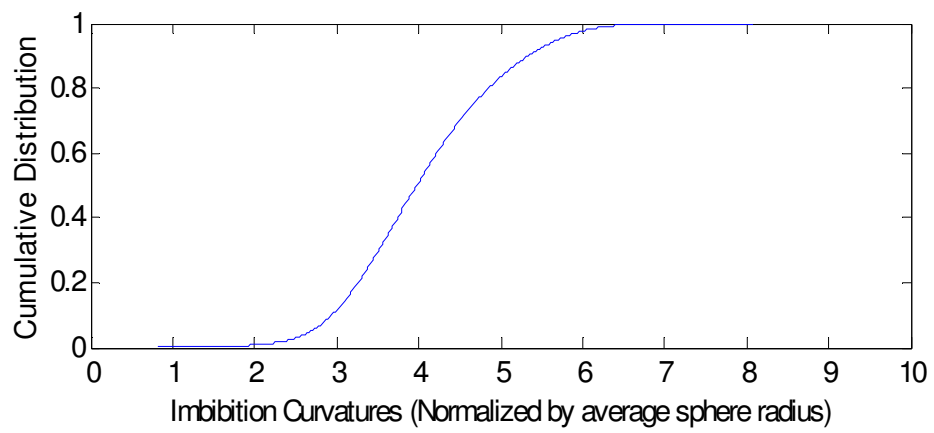
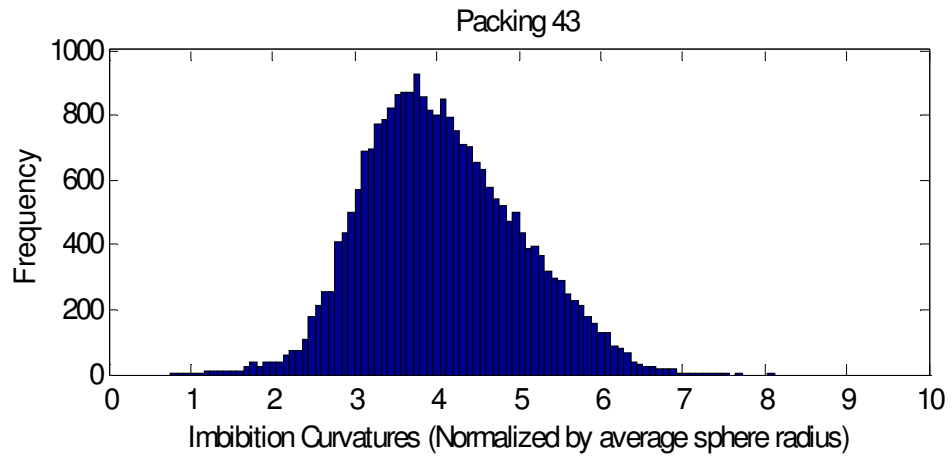


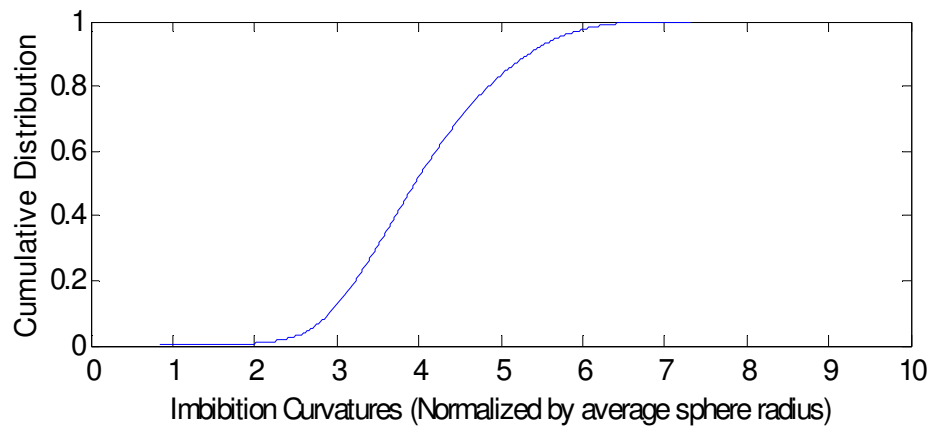
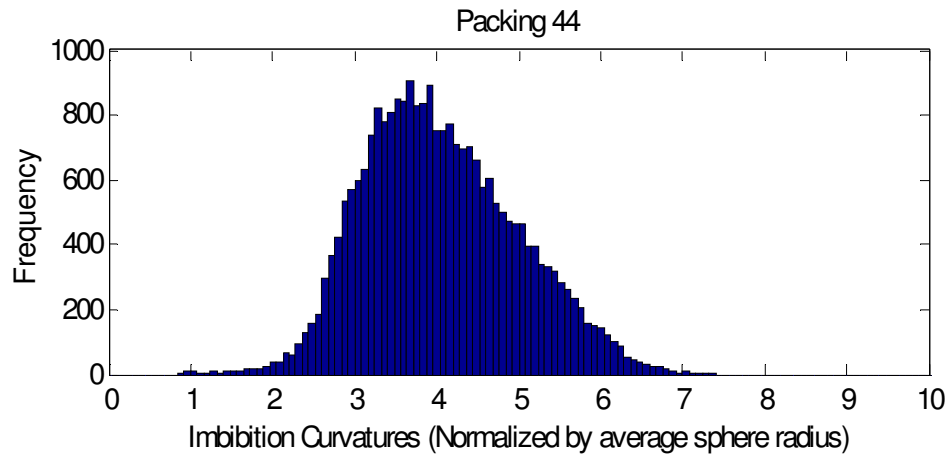


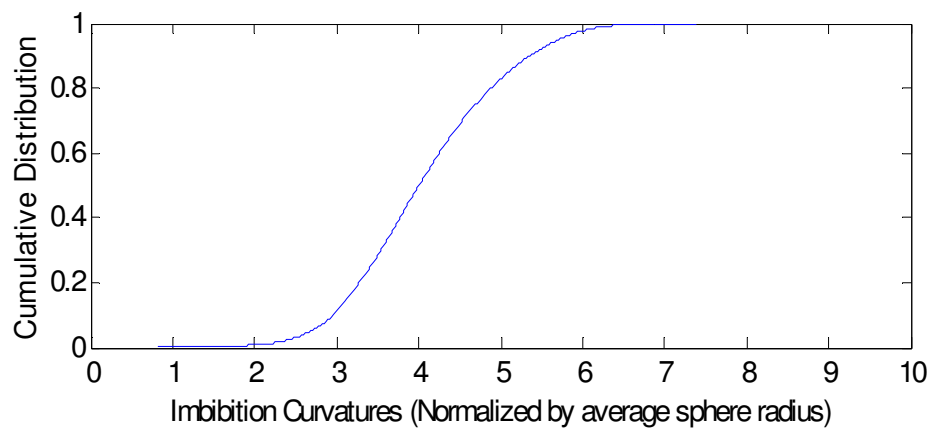
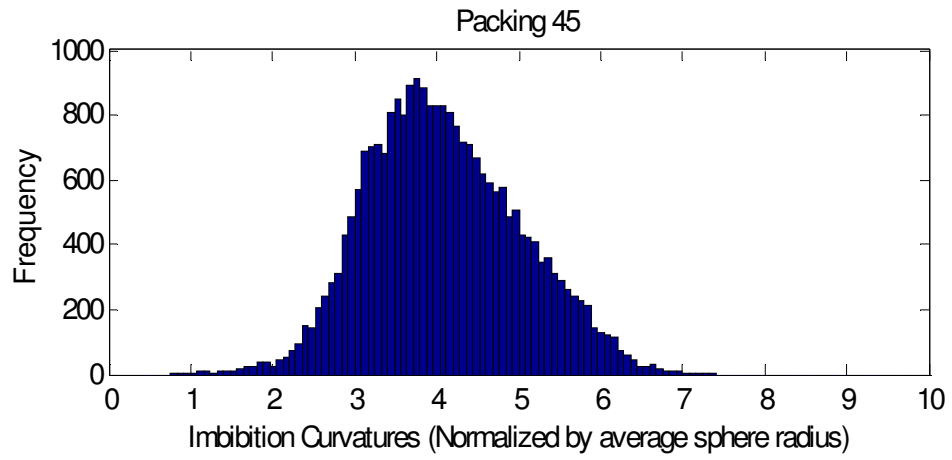


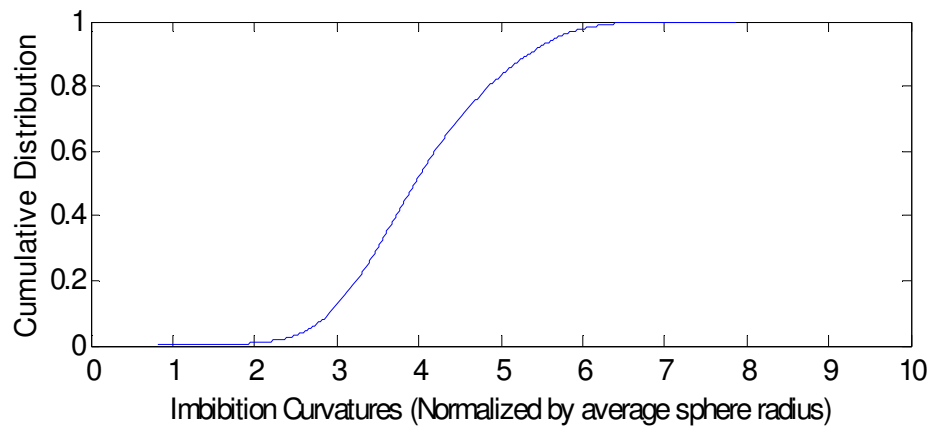
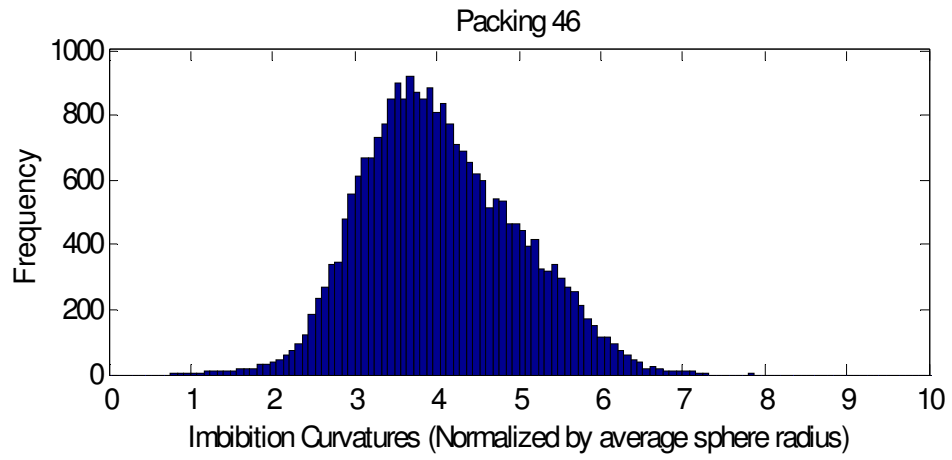


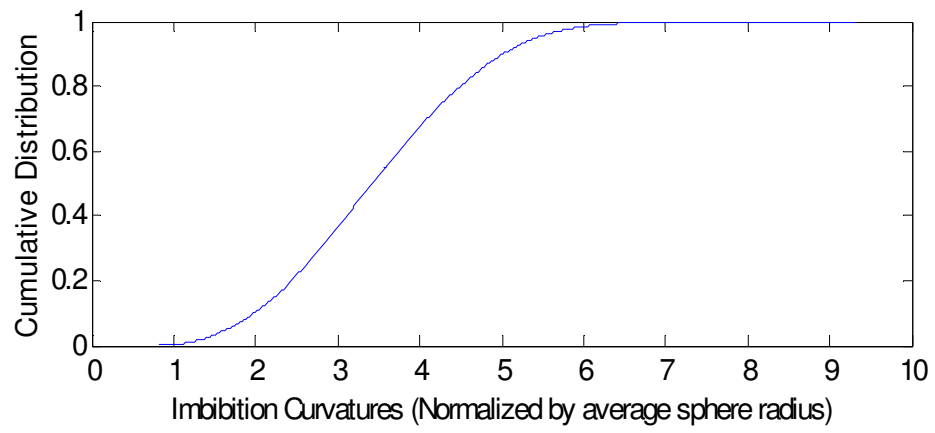
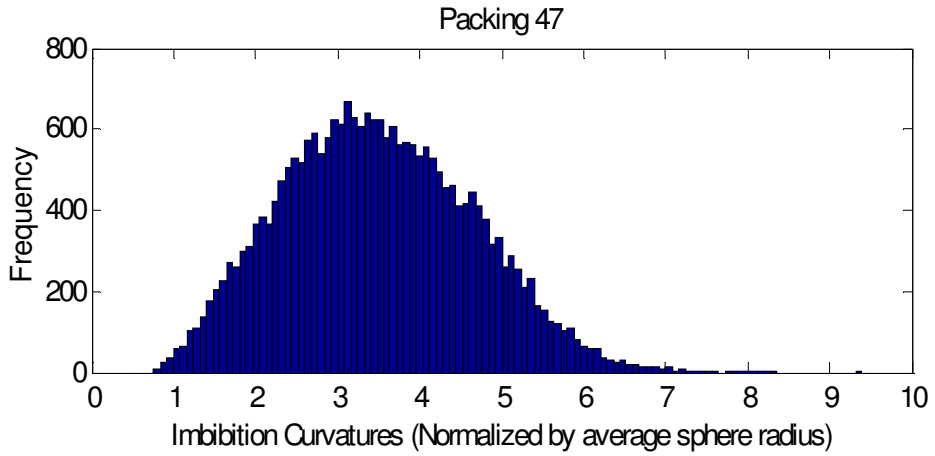


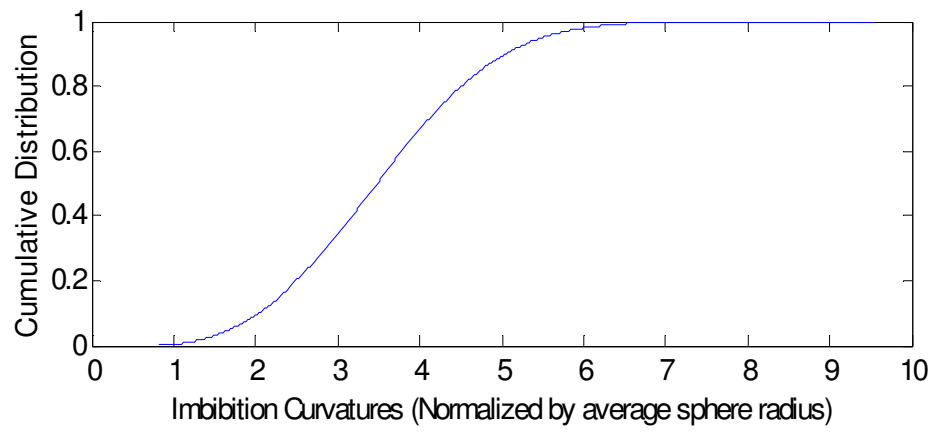
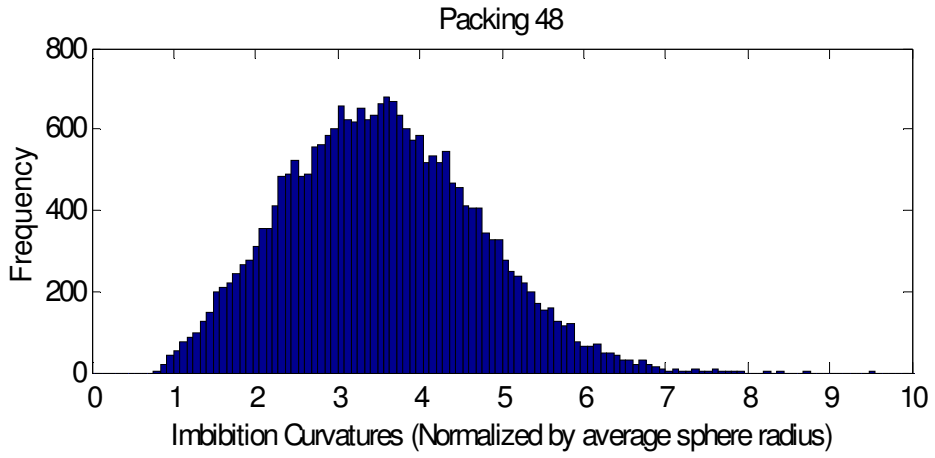


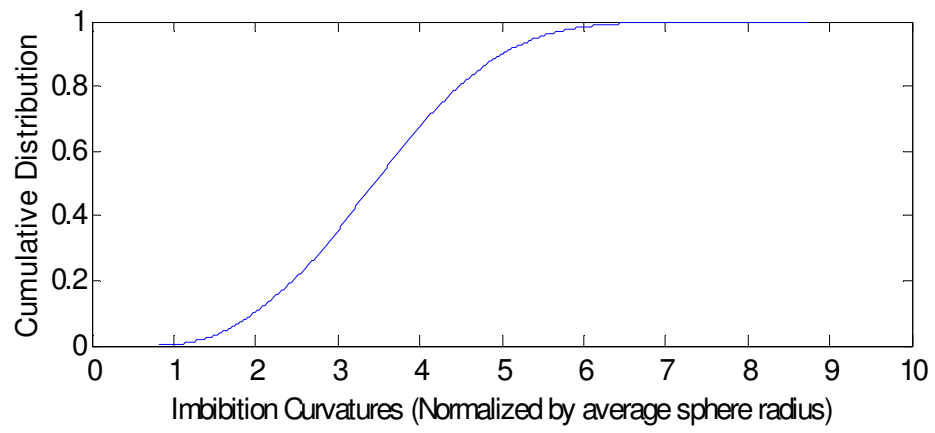
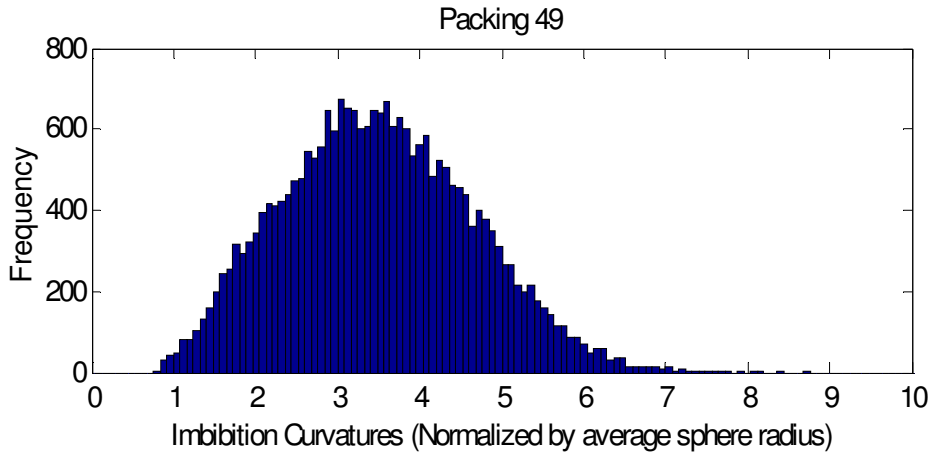


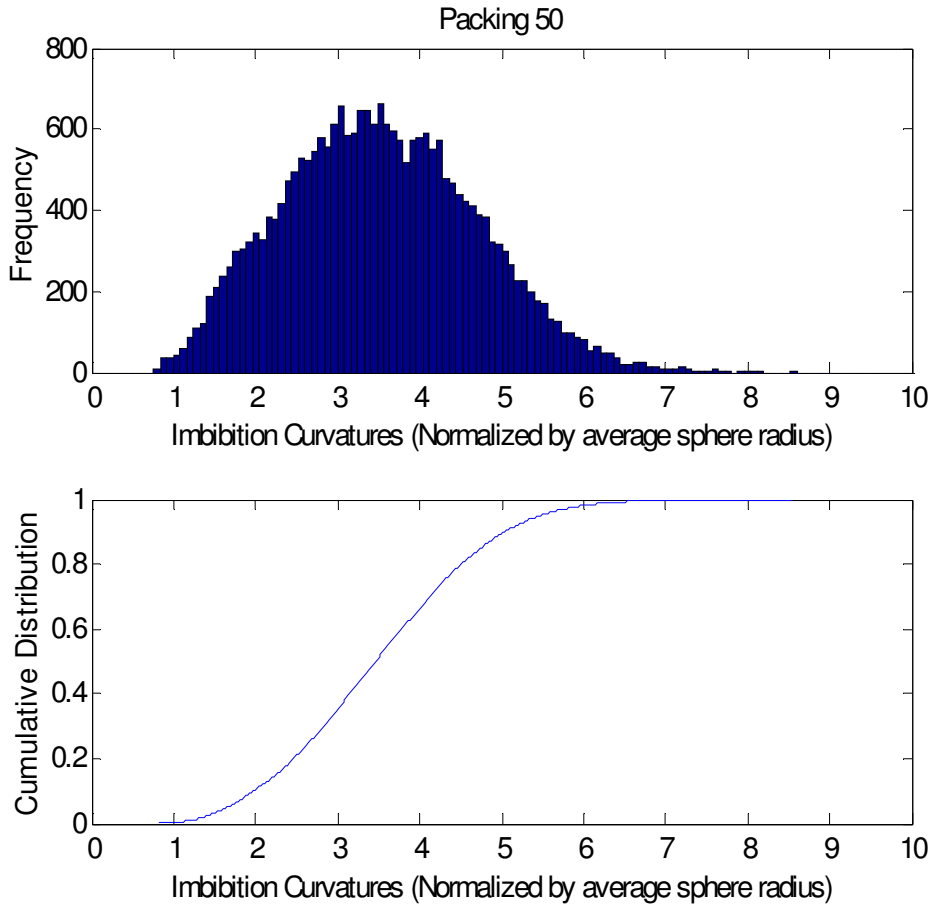


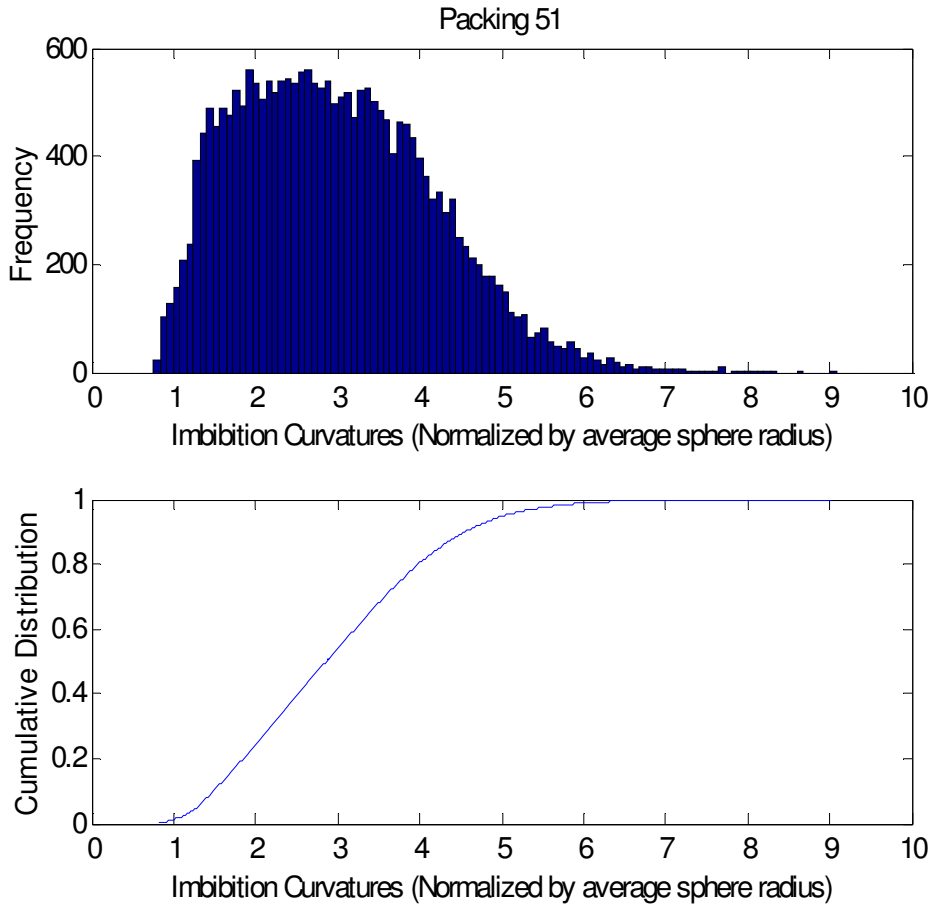


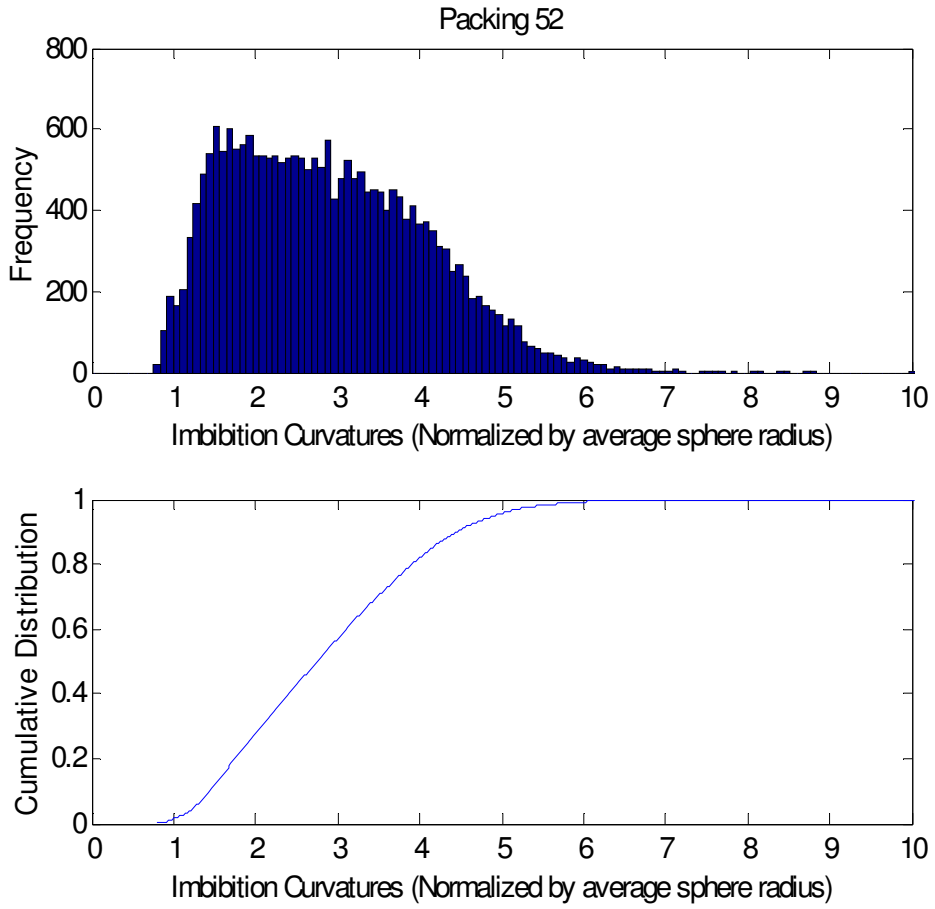


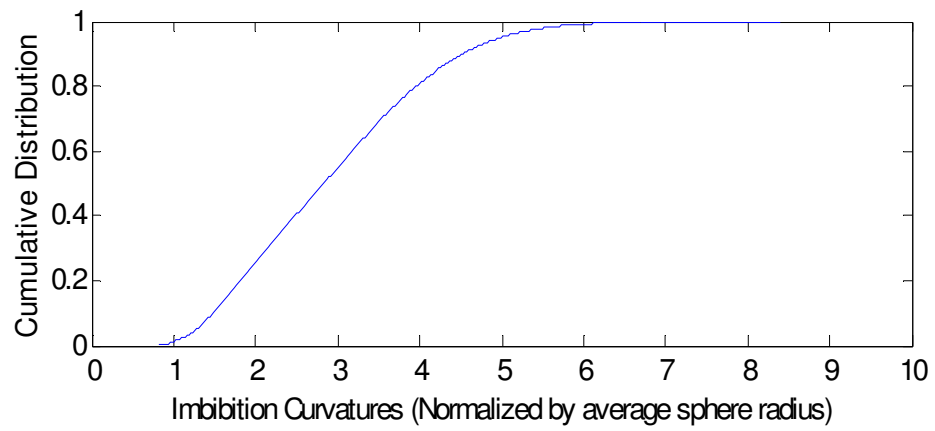
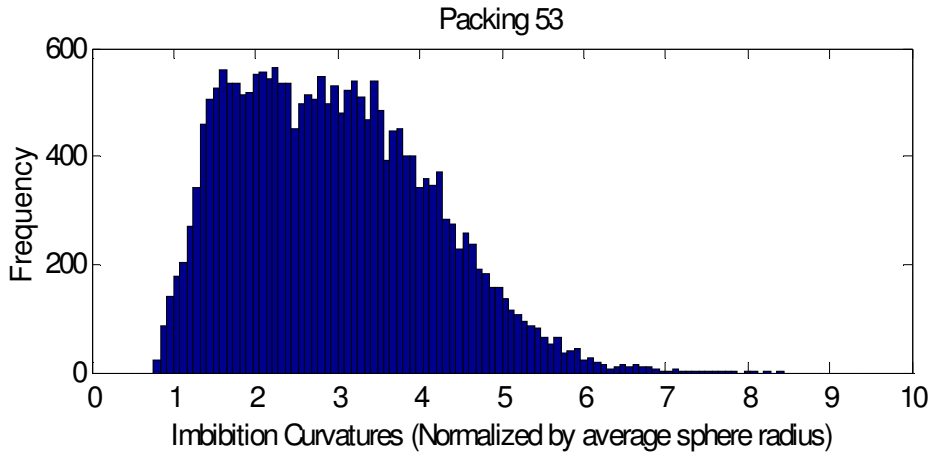


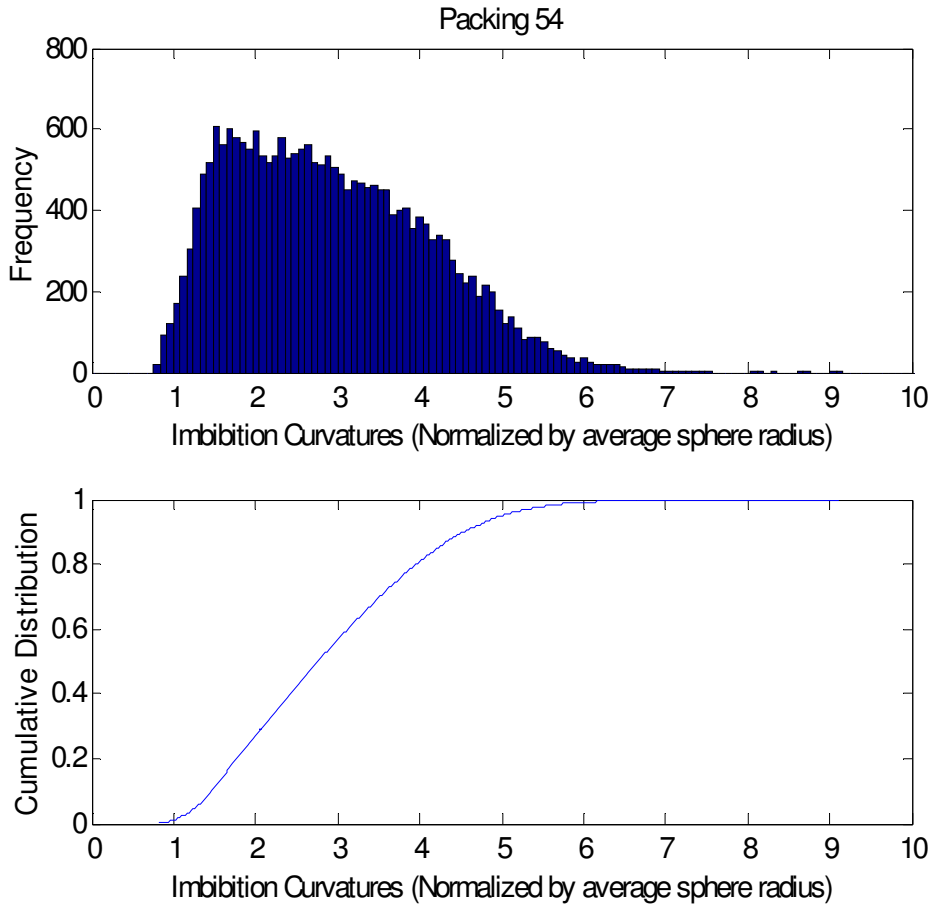


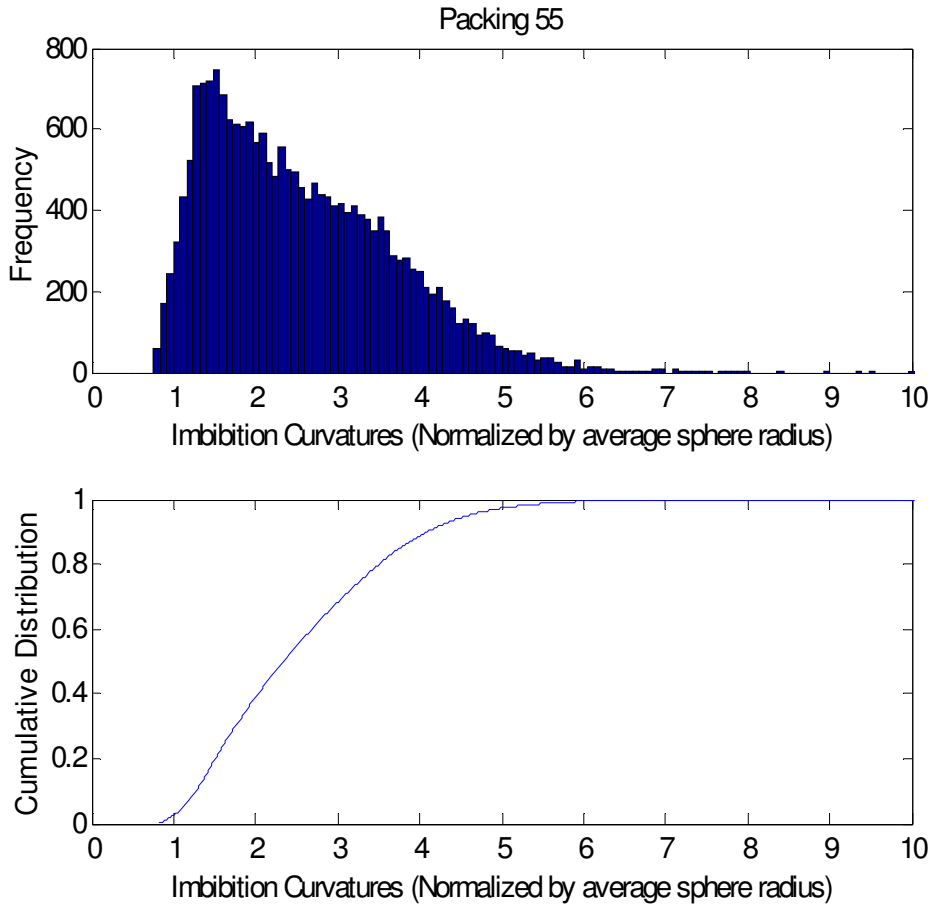


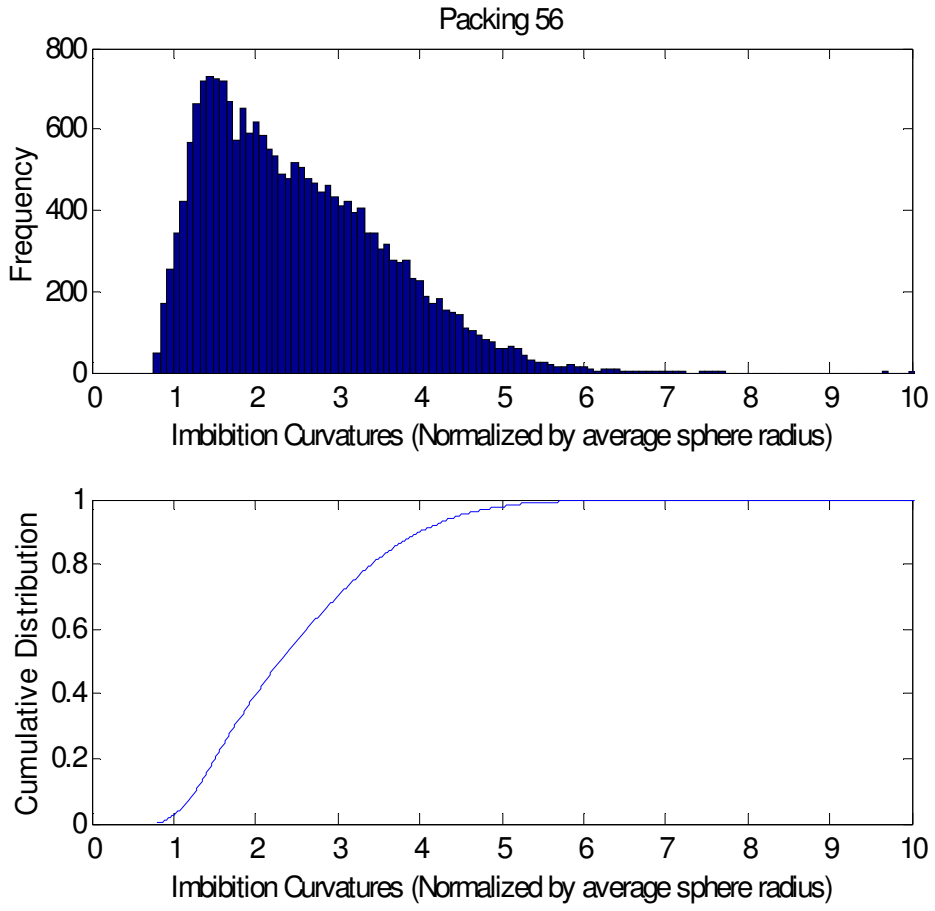




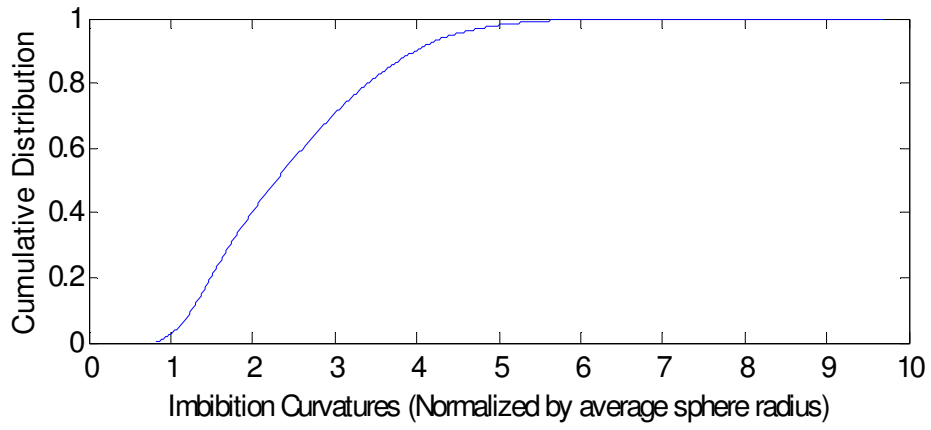
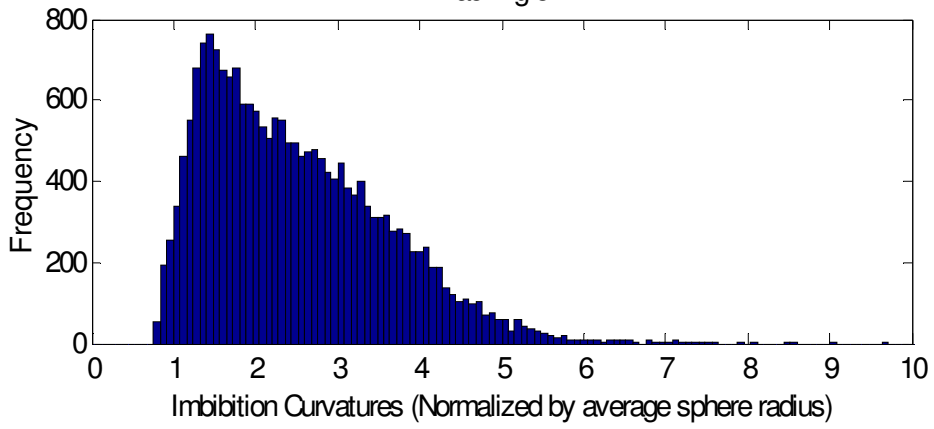


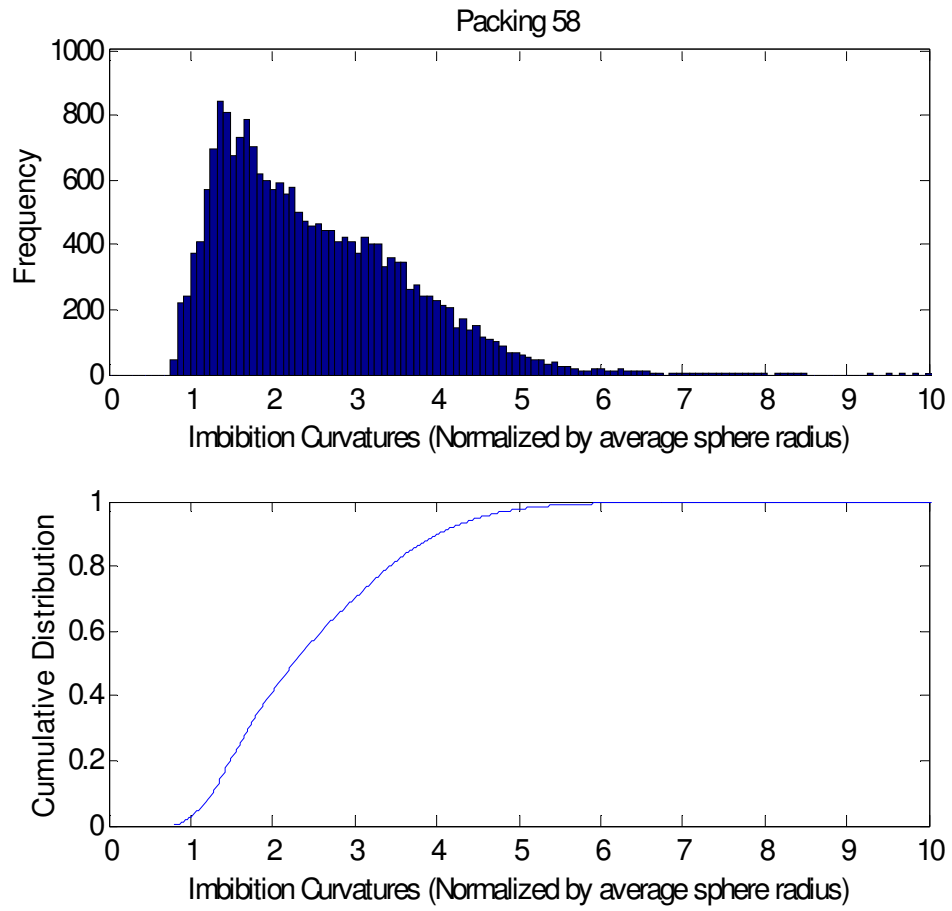


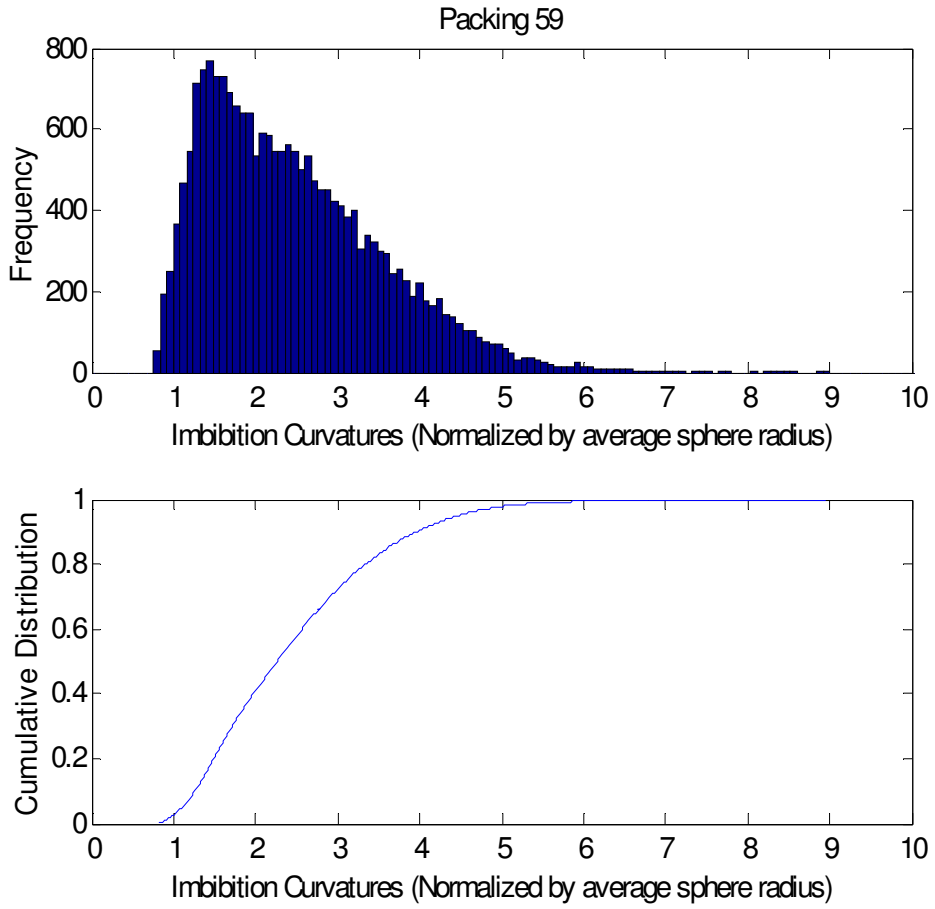


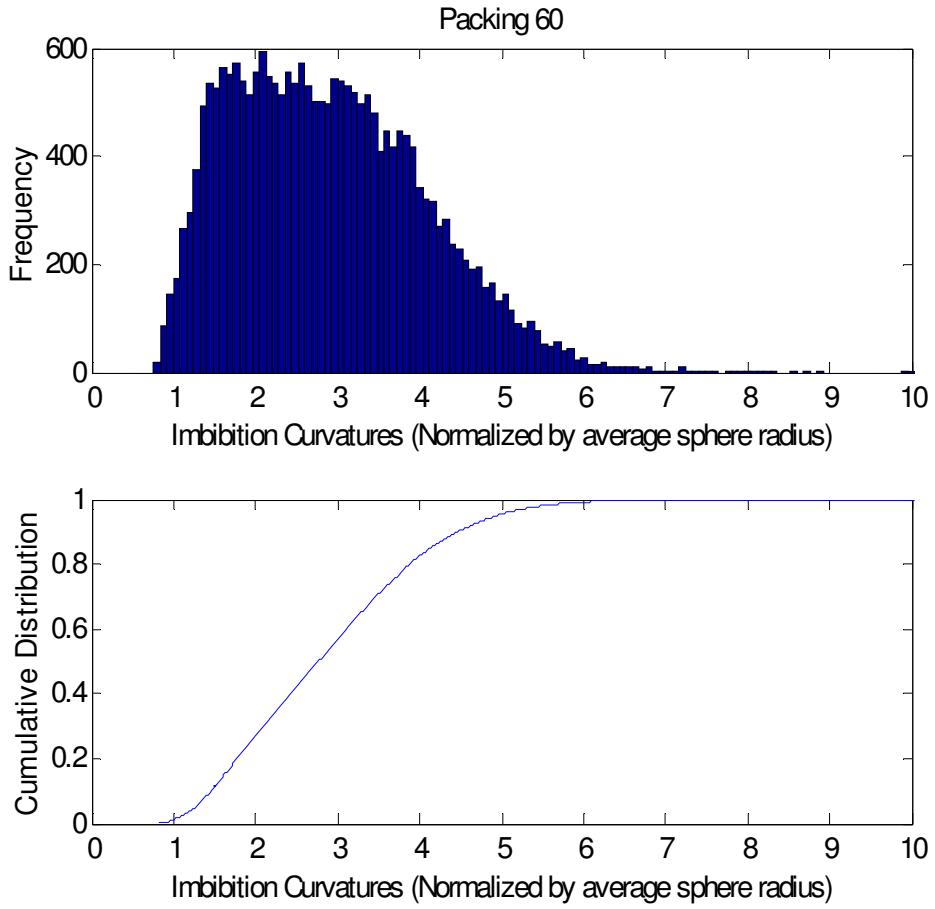


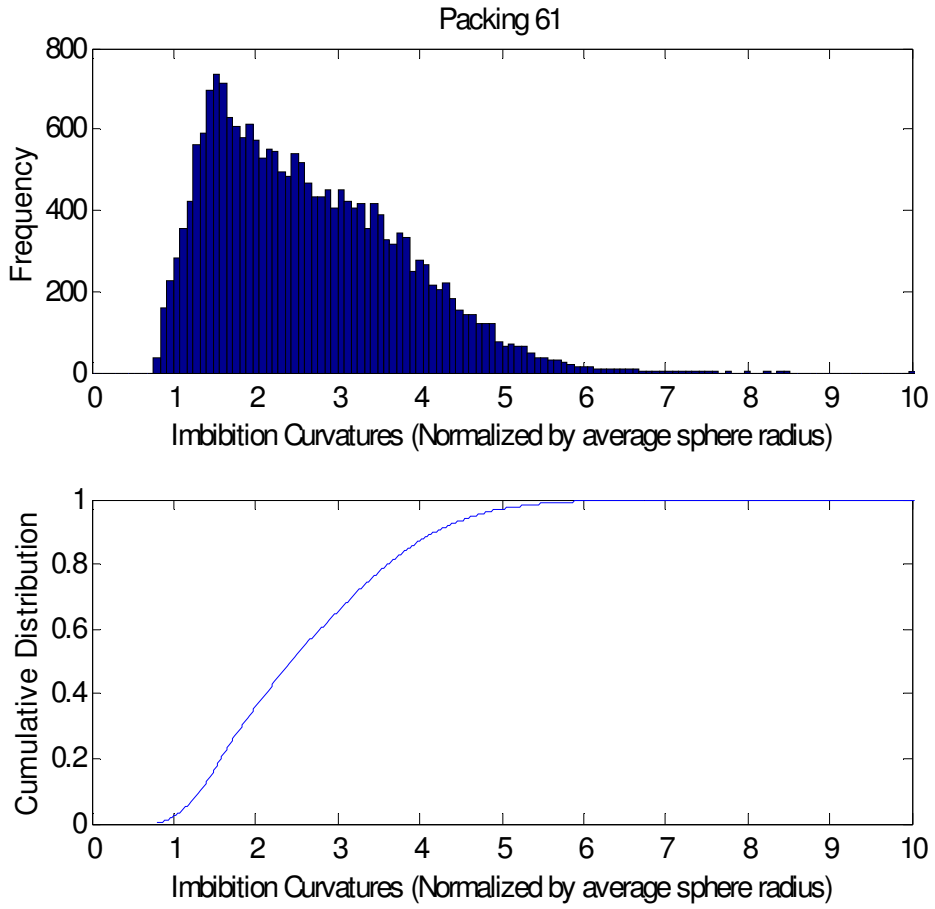
Packing 57

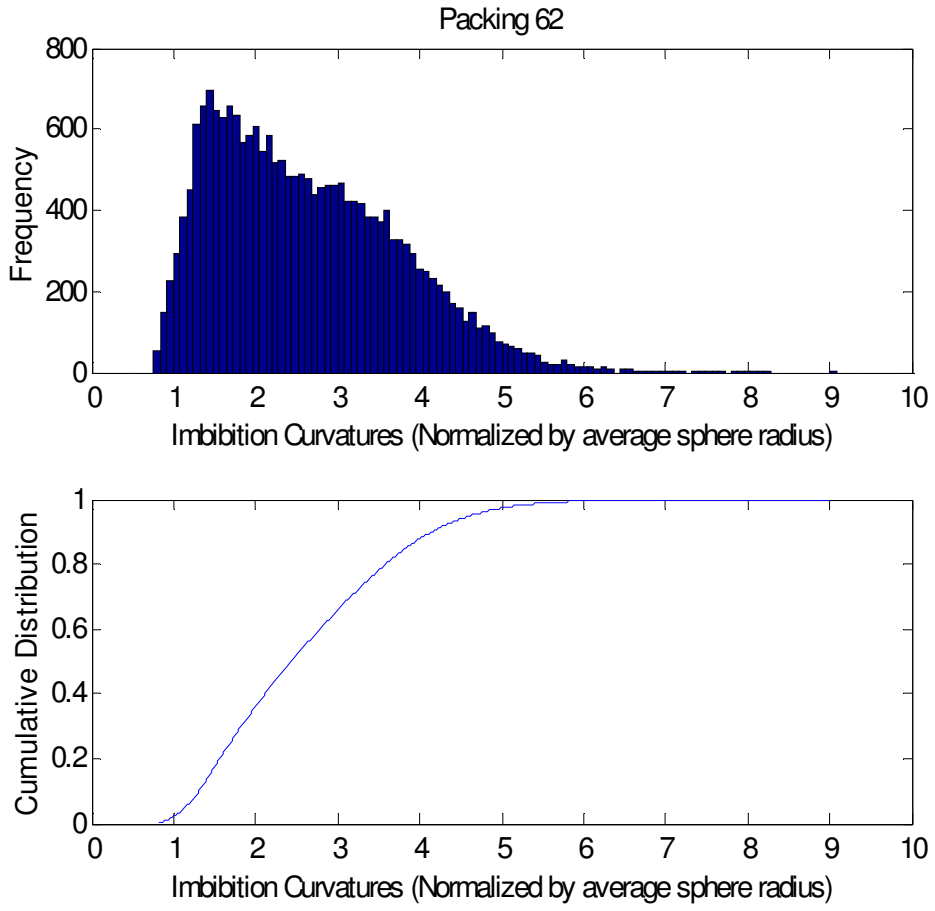


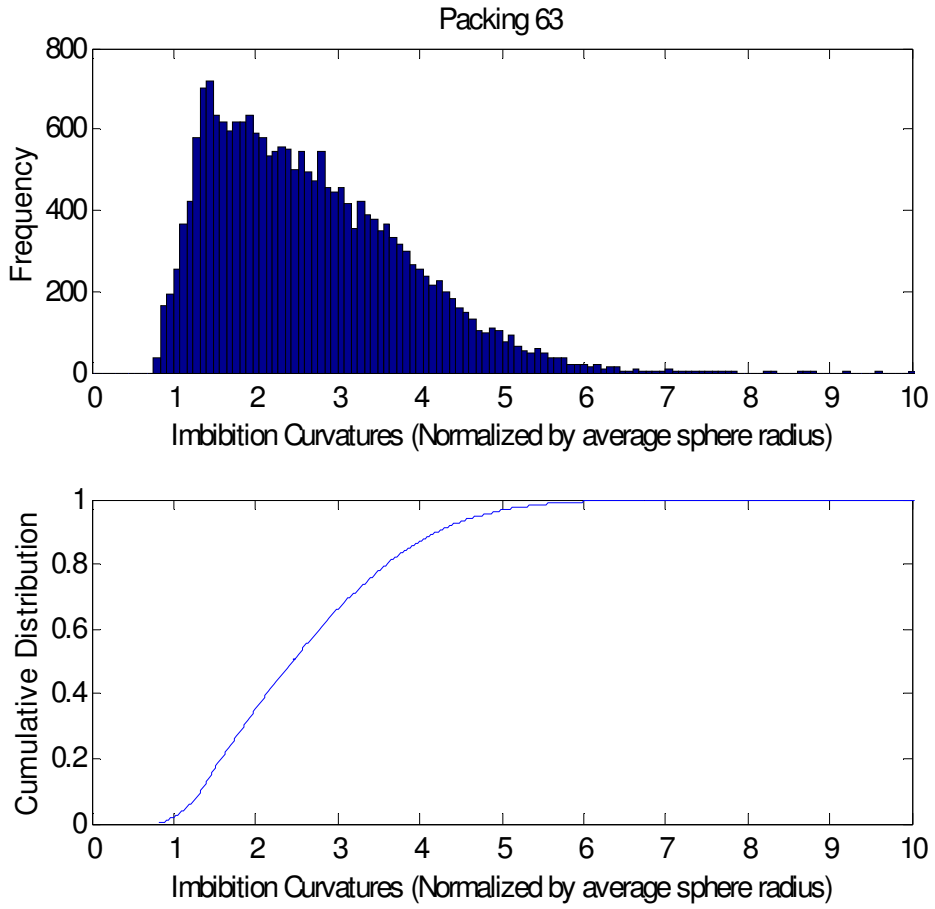


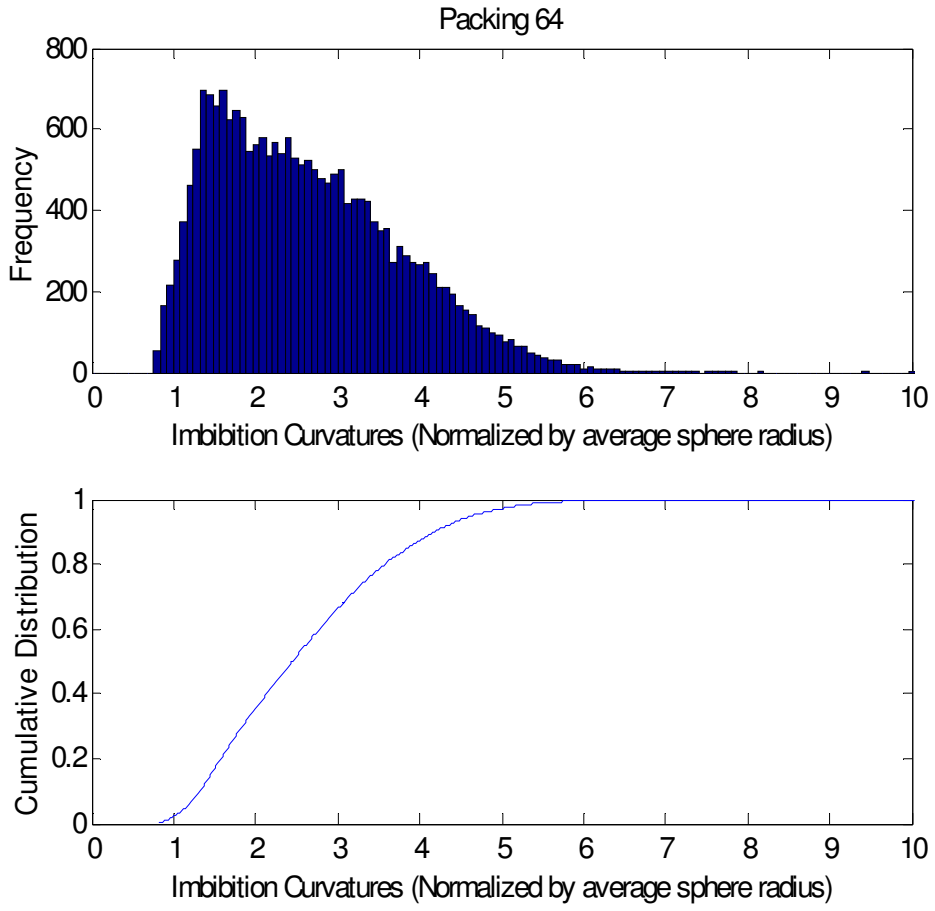


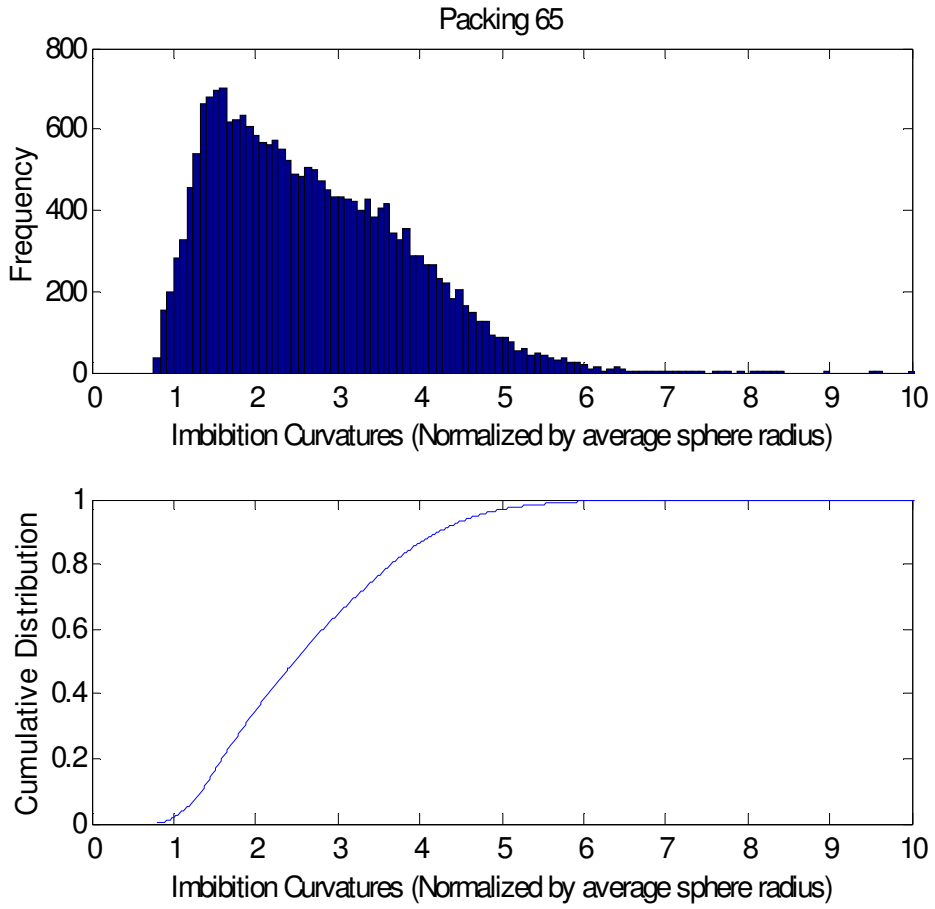


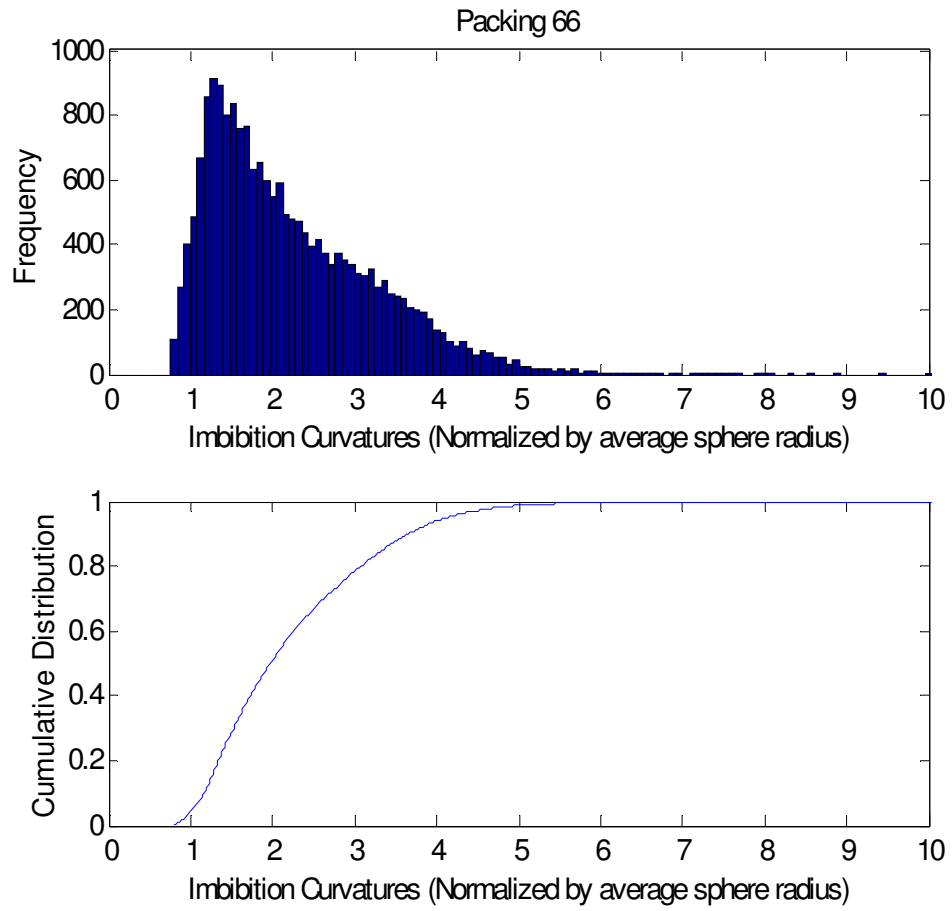


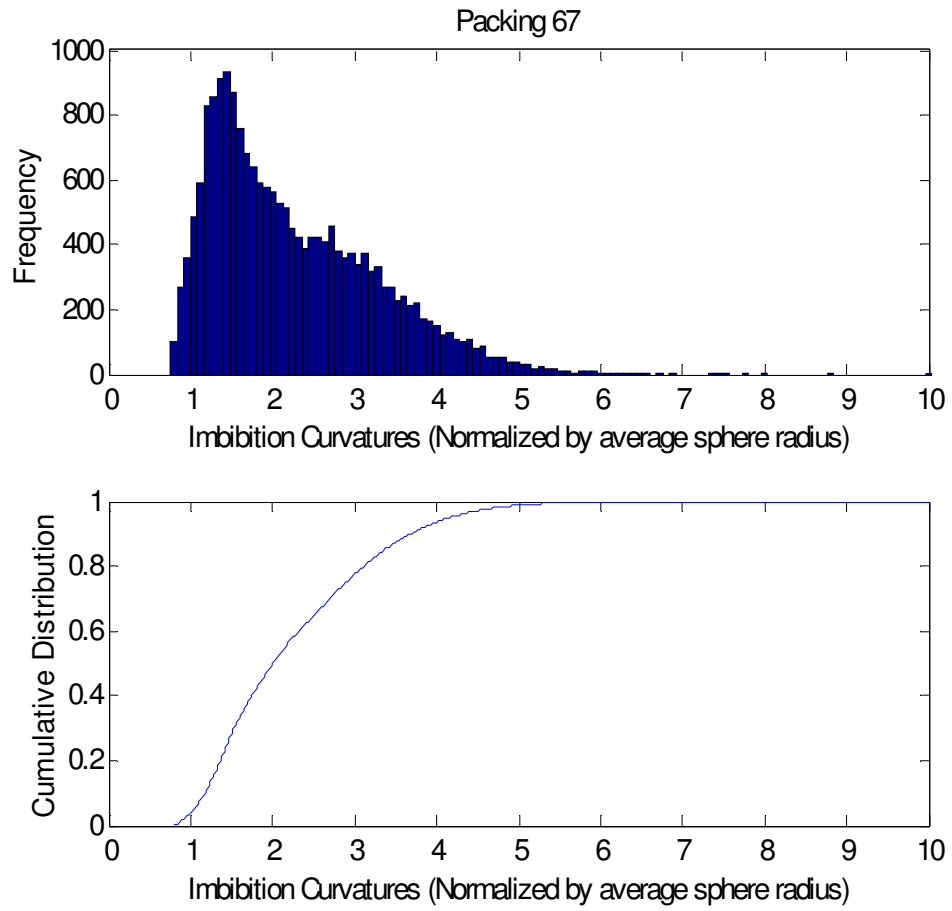


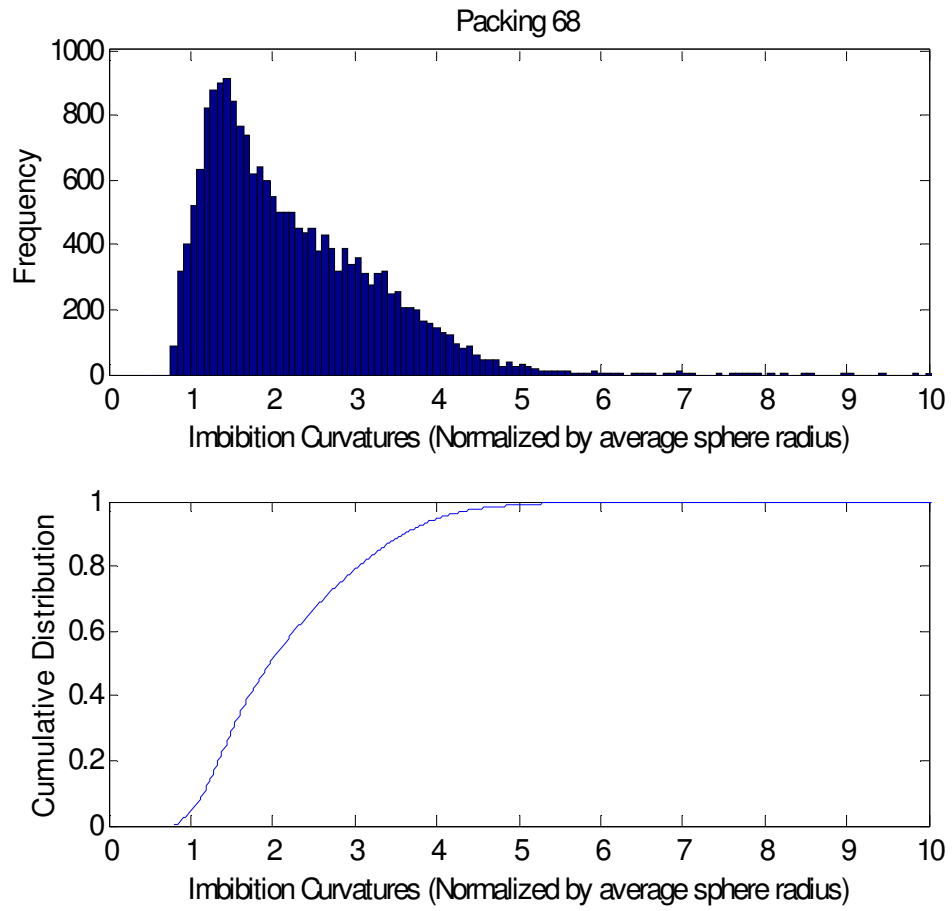


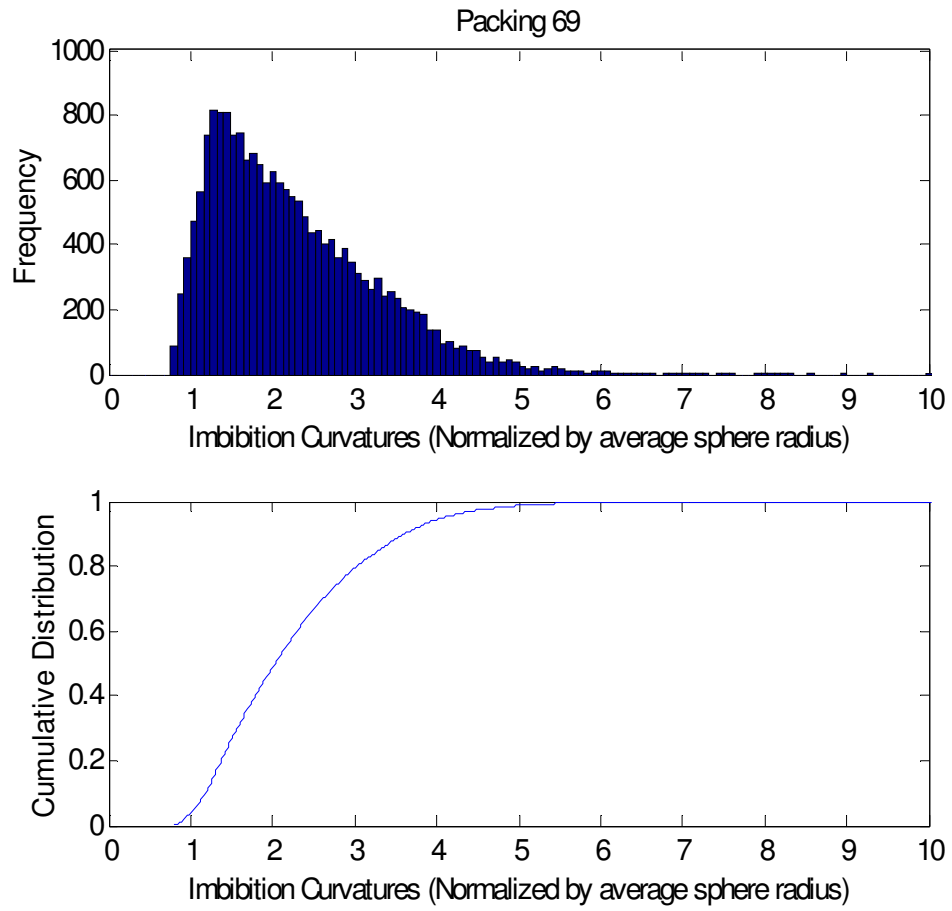


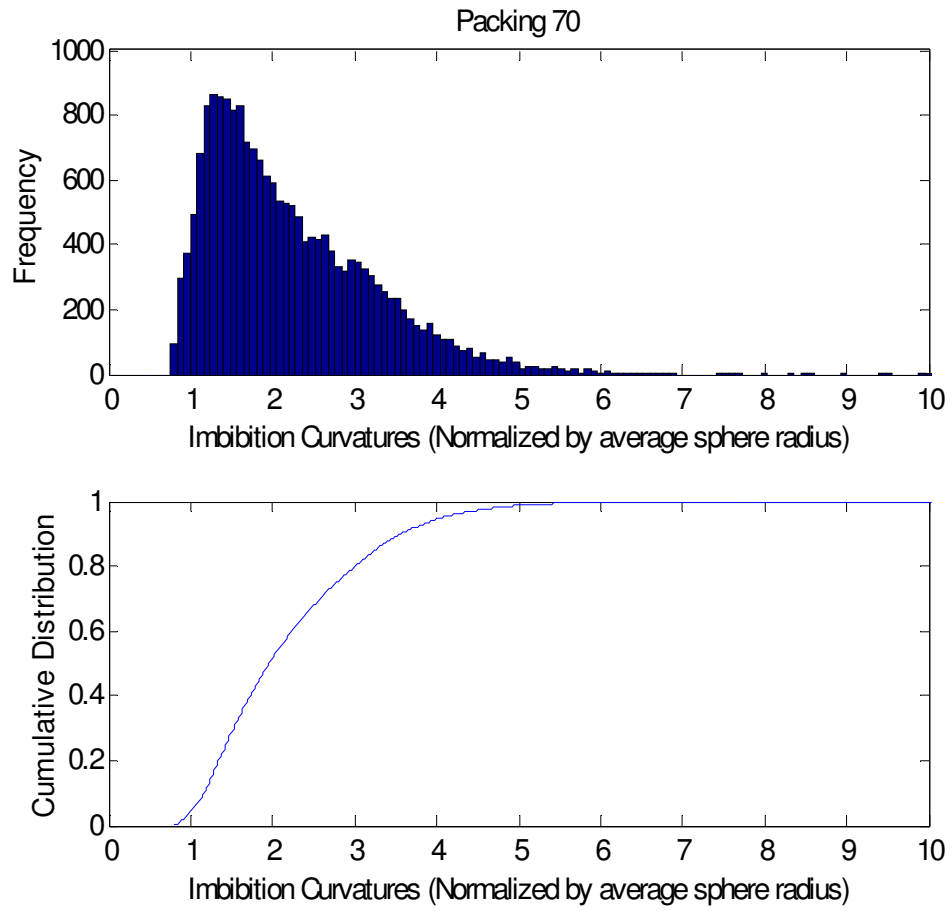


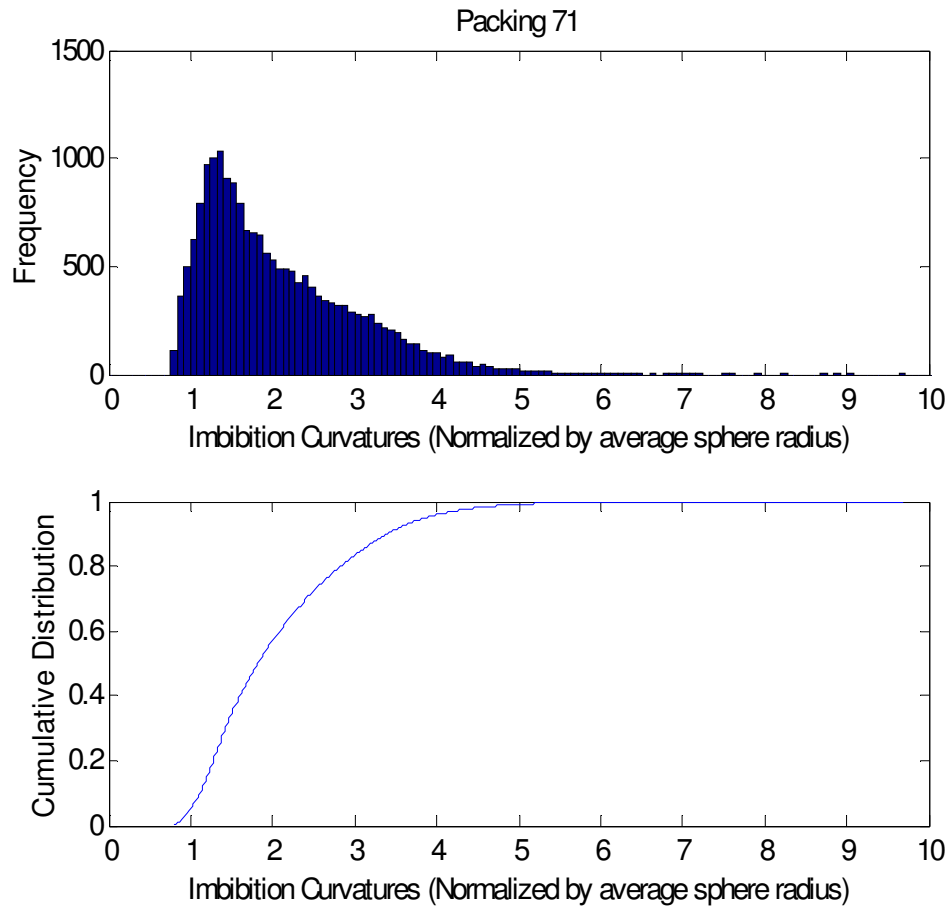


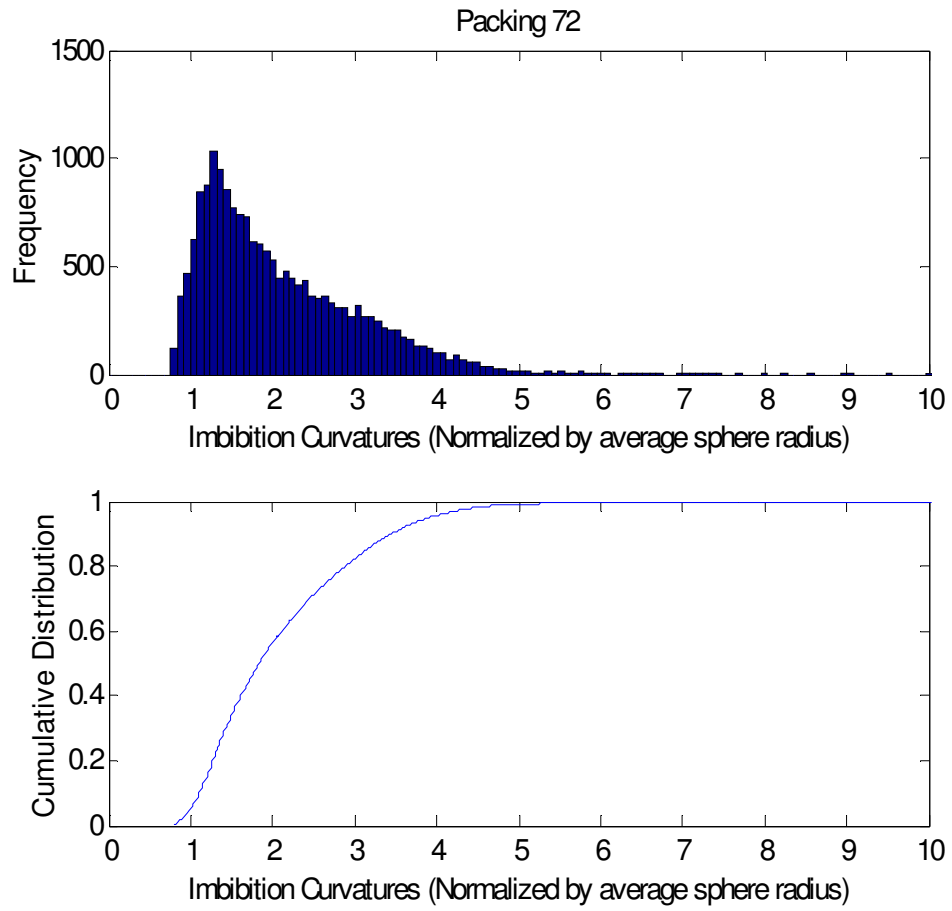


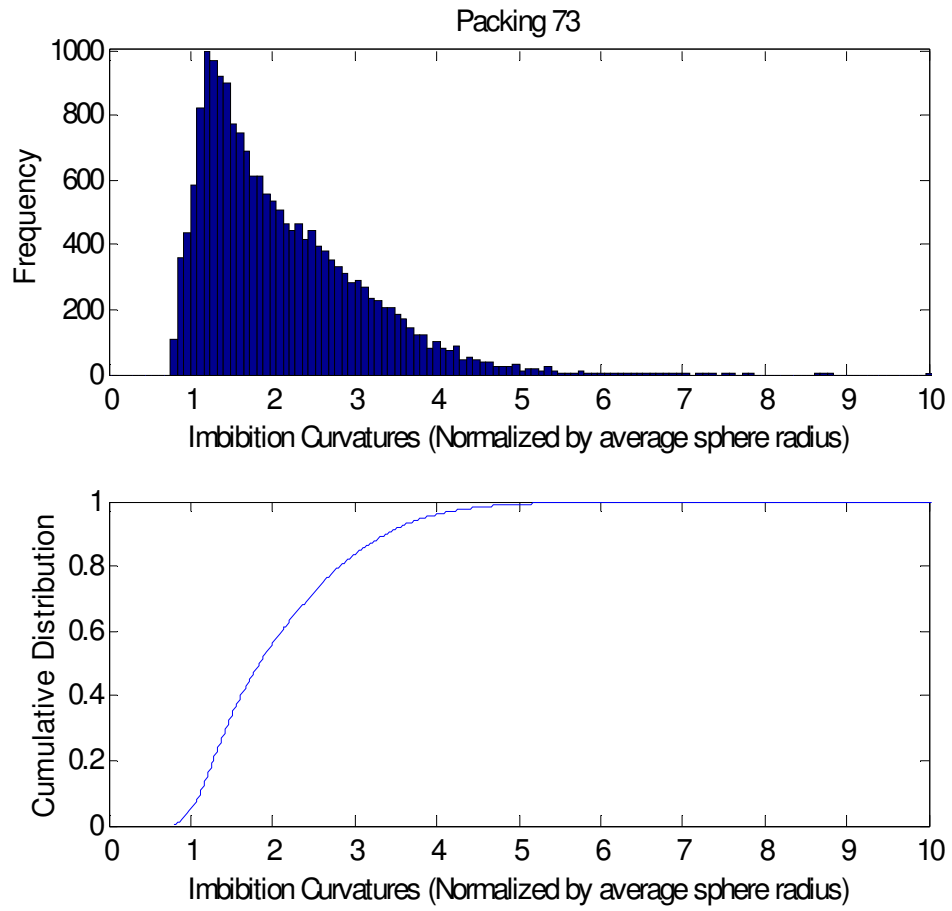


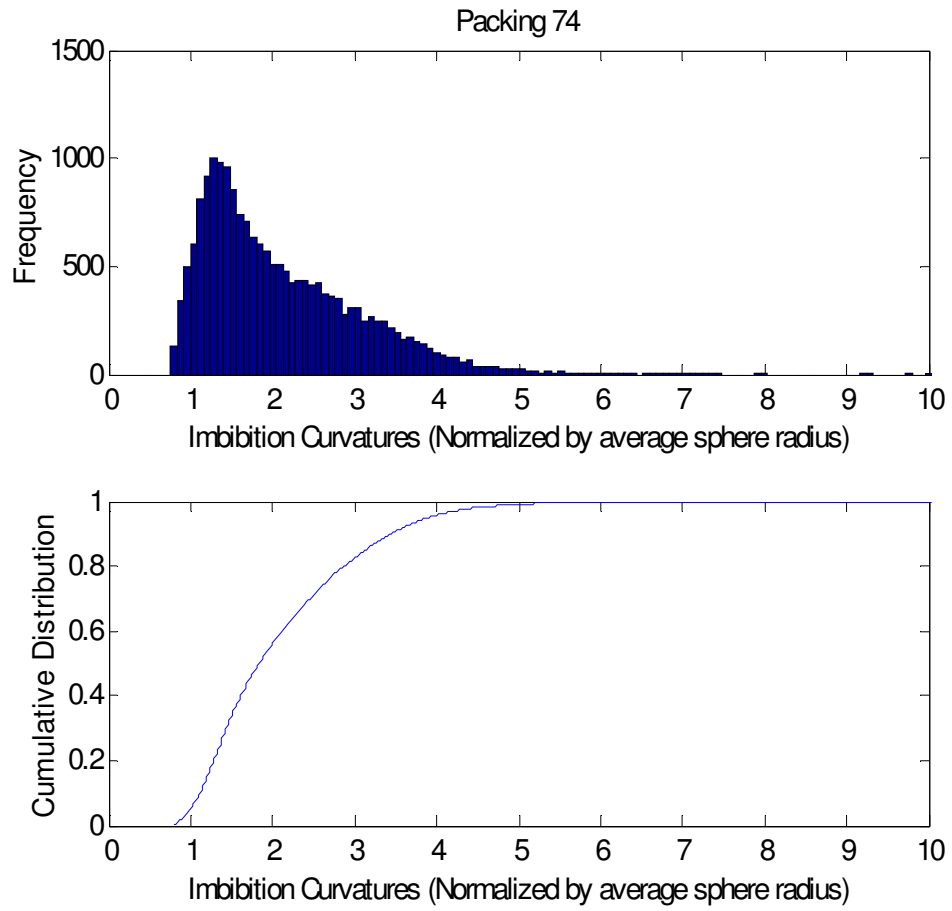


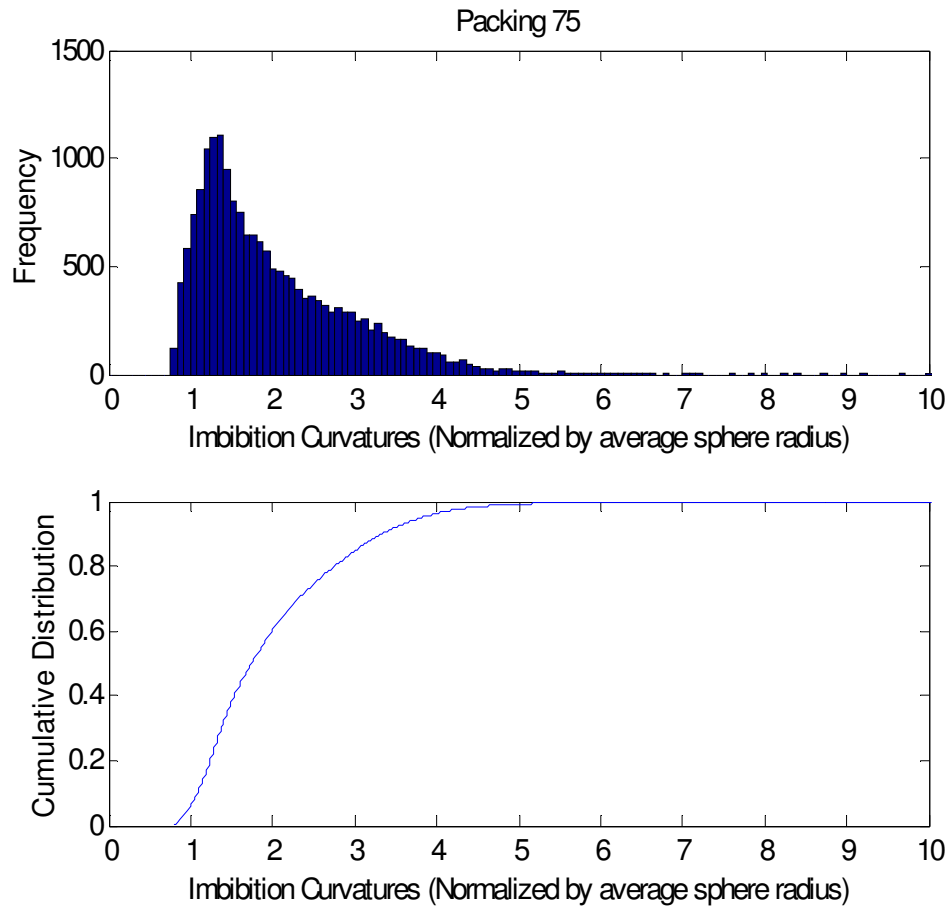


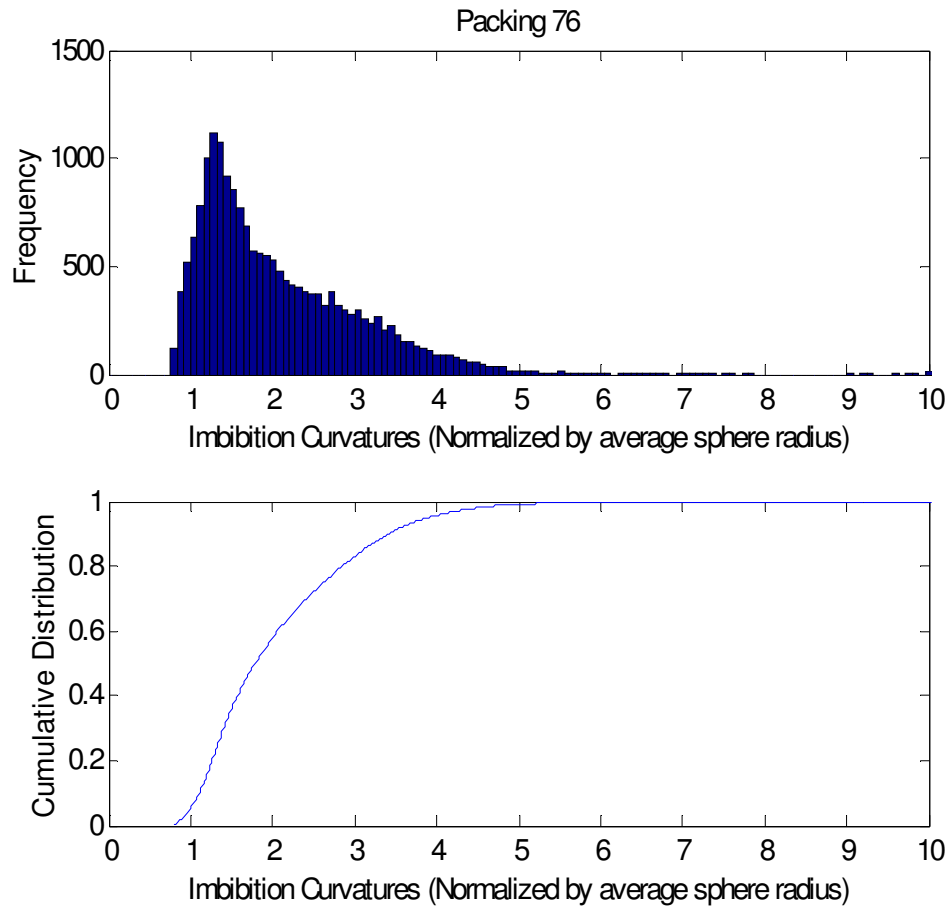












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