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Quantitative Geometric Model of Connected Carbonaceous Material in Mudrocks

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Quantitative Geometric Model of Connected Carbonaceous Material in Mudrocks

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Thesis
Presented to the Faculty of the Graduate School of
The University of Texas at Austin
in Partial Fulfillment
of the Requirements
for the Degree of

Master of Science in Engineering

The University of Texas at Austin
December 2010
Dedication

This thesis is dedicated to my mentors, parents and friends.
Acknowledgements

I would like to thank my supervisor Dr. Steven L. Bryant for his support, patience and encouragement throughout this research. Thanks to geoscientists of Bureau of Economic Geology for providing useful comments in my thesis. I am thankful to Dr. Jon T. Holder for reading this thesis and adding valuable comments.

I express my gratitude to the faculty and staff of the Petroleum and Geosystems Engineering Department. And last, but not the least, I would like to thank my friends and fellow graduate students at The University of at Texas who made my time at Austin even more enjoyable.

I acknowledge the financial support of ExxonMobil for this research.

December 3rd, 2010
Abstract

Quantitative Geometric Model of Connected Carbonaceous Material in Mudrocks

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Unconventional gas resources have become important as an environment-friendly source of fuel. It is important to understand the pore level geometries of grains and voids in mudrocks in order to understand the flow potential of gas from these rocks.

Recent observations of nanopores within carbonaceous material in mudrocks have led to the hypothesis that such material provides conduits for gas migration within the mudrock matrix. This hypothesis requires that the carbonaceous material exist not as isolated grains but as connected clusters of grains within the mudrock. To examine this hypothesis, we develop an algorithm for the grain-scale modeling of the spatial distribution of grains of carbonaceous matter in a matrix of non-carbonaceous material (silt, clay). The algorithm produces a grain-scale model of the sediment which is
precursor to a mudrock, then a sequence of models of the grain arrangement as burial compacts the sediment into mudrock.

The carbonaceous material is approximated by the simplest possible geometric model of spherical grains. These grains are distributed randomly within a population of other spheres that represent silt and clay grains. A cooperative rearrangement algorithm is used to generate a disordered packing of the grain mixture having a prescribed initial porosity. This model represents the sediment precursor of the shale in its original depositional setting. Periodic boundary conditions are imposed on the packing to eliminate wall-induced artifacts in the grain arrangement; in effect the packing extends infinitely in all three coordinate directions. We simulate compaction of the model sediment by incrementally rescaling the vertical coordinate axis, repeating the cooperative rearrangement calculation with periodic boundaries after each increment.

We determine the size distribution of clusters of touching carbonaceous grains, focusing particularly upon the approach toward percolation (when a cluster spans the entire packing). The model allows estimation of threshold fraction of carbonaceous material for significantly connected clusters to form. Beyond a threshold degree of compaction, connected clusters become much more prevalent. Other factors affecting the threshold fraction such as ductility of the carbonaceous material is also evaluated. Ductility is modeled by taking a grain consisting inner rigid core covered by the outer soft shell which can be penetrated and deformed during geometrical transformation.

The emergence of large numbers of clusters, or of a few large clusters, increases the probability that nanoporous conduits within the clusters would intersect a fracture in
the mudrock. This should correlate with greater producibility of gas from the mudrock. Thus the dependence of the statistics of the clusters upon other parameters, such as the fraction of carbonaceous material, porosity, degree of compaction, etc., could be useful for estimating resource quality. For example, it is observed that the threshold concentration of carbonaceous material in the initial sediments for “significant clustering” enough to approach percolation is about 20 percent of the volume fraction. The degree of compaction needed to get “significant clustering” is 50%.
# Table of Contents

List of Tables ......................................................................................................................... xi

List of Figures .......................................................................................................................... xix

Chapter 1: Overview ............................................................................................................. 1
  1.1 Problem statement........................................................................................................ 1
  1.2 Pore System and Transport Mechanism in Mudrocks ............................................ 1
  1.3 Previous Work on Modeling Gas Transport in Shale ............................................... 3
  1.4 Organization of thesis ............................................................................................... 6

Chapter 2: Methods for modeling the sediments ................................................................. 7
  2.1 Introduction.................................................................................................................... 7
  2.2 Cooperative rearrangement algorithm......................................................................... 7
  2.3 Algorithm for simulating compaction......................................................................... 10
  2.4 Rescaling in the direction of compaction................................................................... 13
  2.5 Rescaling in the direction of compaction without cooperative rearrangement ........ 14
  2.6 Rescaling in the direction of compaction with cooperative rearrangement .............. 14
  2.7 Cluster formation ....................................................................................................... 16

Chapter 3: Effect of volume fraction of carbonaceous material on number of clusters in model sediments ........................................................................................................... 21
  3.1 Algorithm for creating packings with prescribed volume fraction of grains .......... 21
  3.2 Carbonaceous material only (one component sphere packing) ................. 25
  3.3 Carbonaceous material with matrix (two component sphere packing) .......... 29
  3.4 Cluster length Analysis .............................................................................................. 35
  3.5 Geometrical Transformation ...................................................................................... 37
  3.6 Aspect Ratio ............................................................................................................... 39
3.7 Inherent clustering of spheres induced by cooperative rearrangement algorithm

Chapter 4: Effect of compaction on clustering of carbonaceous material

4.1 Rescaling in the direction of compaction without cooperative rearrangement: application to one component packings

4.2 Rescaling in the direction of compaction without cooperative rearrangement: application to two component packings

4.3 Rescaling in the direction of compaction with cooperative rearrangement: application to two component packings

4.3.1 Rigid carbonaceous material and silt/clay grains

4.3.2 Both carbonaceous and silt/clay grains are ductile

4.3.3 Carbonaceous material is ductile and silt/clay grains are rigid

4.4 Relationship of cluster statistics to porosity

4.5 Discussion of clustering trends

Chapter 5: Conclusions and Future directions

5.1 Conclusions

5.2 Future directions

Appendix

Example 1

All grains are rigid – one component sphere packing

Example 2

All grains are ductile- two component sphere packing

Example 3

Only carbonaceous grains are ductile- two component sphere packing

Bibliography

Vita
List of Tables

Table: 3.1 One component sphere packing representing carbonaceous material used for analysis with prescribed solid volume representing carbonaceous material .................................................................25

Table: 3.2 Normalized maximum cluster size for various volume fraction of carbonaceous material for 100 spheres for $D=0.001R$ ......................26

Table: 3.3 Normalized maximum cluster size for various volume fraction of carbonaceous material for 500 spheres for $D=0.001R$ ......................26

Table: 3.4 Normalized maximum cluster size for various volume fraction of carbonaceous material for 1000 spheres for $D=0.001R$ .....................26

Table: 3.5 Normalized maximum cluster size for various volume fraction of carbonaceous material for 2500 spheres for $D=0.001R$ .....................27

Table: 3.6 Normalized maximum cluster size for various volume fraction of carbonaceous material for 3000 spheres for $D=0.001R$ .....................27

Table: 3.7 Normalized maximum cluster size for various volume fraction of carbonaceous material for 3500 spheres for $D=0.001R$ .....................27

Table: 3.8 Normalized maximum cluster size for various volume fraction of carbonaceous material for 5000 spheres for $D=0.001R$ .....................28

Table: 3.9 Composition of two component packings: Carbonaceous material with other grains for target porosity of 70%; the desired number of carbonaceous material spheres is 1000. Volume fraction refers sediment bulk volume .................................................................30
Table: 3.10 Composition of two component packings: Carbonaceous material with other grains for target porosity of 60%; the desired number of carbonaceous material spheres is 1000. Volume fraction refers sediment bulk volume .................................................................31

Table: 3.11 Composition of two component packings: Carbonaceous material with other grains for target porosity of 50%; the desired number of carbonaceous material spheres is 1000. Volume fraction refers sediment bulk volume .................................................................31

Table 3.12: Cluster length and cluster aspect ratios for $D=0.001R$ and 5 percent carbonaceous material of bulk volume and 100 spheres with radius = 3.56 units for one component sphere packing after the geometrical transformation .................................................................40

Table 3.13: Cluster length and cluster aspect ratios for $D=0.001R$ and 10 percent carbonaceous material of bulk volume and 100 spheres with radius = 4.42 units for one component sphere packing after the geometrical transformation .................................................................41

Table 3.14: Cluster length and cluster aspect ratios for $D=0.001R$ and 15 percent carbonaceous material of bulk volume and 100 spheres with radius = 5.03 units for one component sphere packing after the geometrical transformation .................................................................42

Table 3.15: Cluster length and cluster aspect ratios for $D=0.001R$ and 20 percent carbonaceous material of bulk volume and 100 spheres with radius = 5.52 units for one component sphere packing after the geometrical transformation .................................................................43
Table 3.16: Cluster length and cluster aspect ratios for $D=0.001R$ and 25 percent carbonaceous material of bulk volume and 100 spheres with radius = 5.89 units for one component sphere packing after the geometrical transformation.................................................................43

Table 3.17: Cluster length and cluster aspect ratios for $D=0.001R$ and 30 percent carbonaceous material of bulk volume and 100 spheres with radius = 6.83 units for one component sphere packing after the geometrical transformation........................................................................44

Table 3.18: Maximum, minimum and average aspect ratios for one component sphere packing of 100 spheres for $D=0.001R$ ..............................................44

Table 4.1: Cluster frequency distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains. .................................................................................64

Table 4.2: Number of spheres distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains. .................................................................................64

Table 4.3: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains. ....................................................................................66
Table 4.4: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains. .................................................................67

Table 4.5: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.9R ........................................70

Table 4.6: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.9R ........................................71

Table 4.7: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.9R ........................................74

Table 4.8: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.9R ........................................74
Table 4.9: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.8R ........................................77

Table 4.10: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.8R ........................................77

Table 4.11: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.8R ........................................80

Table 4.12: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.8R ........................................80

Table 4.13: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.7R ........................................83
Table 4.14: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.7R$ .................................83

Table 4.15: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.7R$ .................................86

Table 4.16: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.7R$ .................................86

Table 4.17: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.9R$ and silt/clay being rigid ......................89

Table 4.18: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.9R$ and silt/clay being rigid ......................90
Table 4.19: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.9R$ and silt/clay being rigid ......................93

Table 4.20: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.9R$ and silt/clay being rigid .......................93

Table 4.21: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid ......................96

Table 4.22: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid .......................96

Table 4.23: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid ......................99
Table 4.24: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.8$R$ and silt/clay being rigid...............99

Table 4.25: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.7 $R$ and silt/clay being rigid .................102

Table 4.26: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.7$R$ and silt/clay being rigid....................102

Table 4.27: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.7 $R$ and silt/clay being rigid....................105

Table 4.28: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.7$R$ and silt/clay being rigid....................105
List of Figures

Figure 1.1: Scanning electron micro-image of Ar-ion-beam milled surface showing pores in organic matter (Wang and Reed, 2009) ................................2

Figure 1.2: Connected carbonaceous material in typical SEM image of shale gas sample (Barnett shale). The connections are interpreted to have formed as smaller, separate pieces of material come into contact during burial and compaction. (Courtesy Dr. K Milliken, University of Texas Bureau of Economic Geology) .................................................................3

Figure 1.3: Schematic diagram showing high-permeability elements in gas shale: organic matter, natural fractures, and hydraulic fractures. (Reed et al. 2009) ..................................................................................................5

Figure 2.1: Concept of periodicity as implemented in the sphere packing code. The spheres in the unit cell are shown in the projected y-z plane in the center of the diagram; four copies of the unit cell are placed around the center cell. Red spheres are real spheres and green spheres are their images. A sphere at or near one face of unit cell can thus be in virtual contact with a sphere at or near the opposite face. Such contacts are accounted for during the cooperative rearrangement steps. .............................................9

Figure 2.2: Schematic showing various stages of compaction. Original model sediment is uncompacted (c=1). The final state corresponds to mudrock. ...........................................................................................................11

Figure 2.3: Schematic showing the relative motion of spheres within a box in mechanical compaction ........................................................................................................13
Figure 2.4: Illustration of rigid and ductile grains. For rigid grain, the rigid radius equals grain radius \( R \). For ductile grains, the rigid radius is less than the grain radius \( R \).

Figure 2.5: The criterion for touching spheres is whether the gap \( D \) between the spheres is less than a user-specified tolerance.

Figure 2.6: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value \( D = 1.0 \ R \).

Figure 2.7: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value \( D = 0.1 \ R \).

Figure 2.8: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value \( D = 0.01 \ R \).

Figure 2.9: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value \( D = 0.001 \ R \).

Figure 2.10: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value \( D = 0.0001 \ R \).

Figure 2.11: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value \( D = 0.00001 \ R \).

Figure 3.1: Periodic packing of 100 spheres showing 5% (left) and 10% (right) of cell volume occupied by solid.

Figure 3.2: Periodic packing of 1000 spheres showing 5% (left) and 10% (right) of cell volume occupied by solid.

Figure 3.3: Initial point generation (Left) and particle growth (Right) in one component sphere packing representing only carbonaceous material in the original sediment.
Figure 3.4: Initial point generation (Left) and particle growth (Right) in two component sphere packing, red colored spheres representing carbonaceous material and green colored spheres representing silt/clay

Figure 3.5: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material for one component sphere packing

Figure 3.6: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material in sediment for packing of carbonaceous material with matrix. Sediment porosity is 70 percent. Curves refer to sets of packings in which number of carbonaceous material grains is constant

Figure 3.7: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material in sediment for packing of carbonaceous material with matrix. Sediment porosity is 60 percent. Curves refer to sets of packings in which number of carbonaceous material grains is constant

Figure 3.8: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material in sediment for packing of carbonaceous material with matrix. Sediment porosity is 50 percent. Curves refer to sets of packings in which number of carbonaceous material grains is constant

Figure 3.9: Cluster Length calculation in X direction

Figure 3.10: Selected cluster length analysis for 5 percent carbonaceous material for one component sphere packing of 100 spheres representing carbonaceous material with radius $= 3.56$ units
Figure 3.11: Geometrical transformation for the biggest cluster from one component sphere packing of 100 spheres representing carbonaceous material with radius = 3.56 units

Figure 3.12: Variation of LX and LY in new coordinate system showing a phase difference of 90 degrees between them for the biggest cluster from one component sphere packing of 100 spheres with radius = 3.56 units

Figure 3.13: Maximum aspect ratio of clusters vs. volume fraction of carbonaceous material for one component sphere packing of 100 spheres for $D=0.001R$

Figure 3.13: Aspect ratio of largest cluster vs. volume fraction of carbonaceous material for one component sphere packing of 100 spheres for $D=0.001R$

Figure 3.14: Comparison of cluster frequency vs. cluster size for $D=0.001R$ of the compaction stages of one component packing created by Thane’s code and dispersed spheres represented by suffix-2 (1000 rigid spheres of carbonaceous material)

Figure 3.15: Comparison of number of spheres vs. cluster size for $D=0.001R$ of the compaction stages of one component packing created by Thane’s code and dispersed spheres represented by suffix-2 (1000 rigid spheres of carbonaceous material)

Figure 3.16: Comparison of cluster frequency vs. cluster size for $D=0.001R$ of the compaction stages of two component packing created by Thane’s code and dispersed spheres represented by suffix-2 (1000 rigid spheres of carbonaceous material and 70 % target porosity)
Figure 3.17: Comparison of number of spheres vs. cluster size for $D=0.001R$ of the compaction stages of two component packing created by Thane’s code and dispersed spheres represented by suffix-2 (1000 rigid spheres of carbonaceous material and 70% target porosity)..........................51

Figure 4.1: Grain packing showing the effect of compaction.................................54

Figure 4.2: Cluster frequency vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for one component sphere packing (1000 spheres of carbonaceous material)..................55

Figure 4.3: Number of spheres in cluster size vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for one component sphere packing (1000 spheres of carbonaceous material).................56

Figure 4.4: Cluster frequency vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 10 percent of carbonaceous material in the initial bulk volume for one component sphere packing (1000 spheres of carbonaceous material)..............57

Figure 4.5: Number of spheres in cluster size vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 10 percent of carbonaceous material in the initial bulk volume for one component sphere packing (1000 spheres of carbonaceous material)....58
Figure 4.6: Cluster frequency vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for two component sphere packing (1000 spheres of carbonaceous material).................59

Figure 4.7: Number of spheres in cluster size vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for two component sphere packing (1000 spheres of carbonaceous material)...........................................................................................................60

Figure 4.8: Cluster frequency vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 10 percent of carbonaceous material in the initial bulk volume for two component sphere packing (1000 spheres of carbonaceous material).............61

Figure 4.9: Number of spheres in cluster size vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 10 percent of carbonaceous material in the initial bulk volume for two component sphere packing (1000 spheres of carbonaceous material)
...............................................................................................................................62

Figure 4.10: Cluster frequency distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains ..............................................................................................65
Figure 4.11: Number of spheres distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains. .................................................................66

Figure 4.12: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains. .................................................................68

Figure 4.13: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains. .................................................................69

Figure 4.14: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio =0.9$R$ .........................72

Figure 4.15: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio=0.9$R$ .................................................73
Figure 4.16: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.9R$.

Figure 4.17: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.9R$.

Figure 4.18: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.8R$.

Figure 4.19: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.8R$.

Figure 4.20: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.8R$. 

xxvi
Figure 4.21: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio = $0.8R$ .............................................82

Figure 4.22: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio = $0.7R$ ..............................84

Figure 4.23: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio = $0.7R$ .............................................85

Figure 4.24: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio = $0.7R$ ..............................87

Figure 4.25: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio = $0.7R$ .............................................88

xxvii
Figure 4.26: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.9$R$ and silt/clay being rigid.......................91

Figure 4.27: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.9$R$ and silt/clay being rigid......................92

Figure 4.28: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.9$R$ and silt/clay being rigid.......................94

Figure 4.29: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.9$R$ and silt/clay being rigid......................95

Figure 4.30: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.8$R$ and silt/clay being rigid.......................97
Figure 4.31: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid..........................98

Figure 4.32: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid .....................100

Figure 4.33: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid ....................101

Figure 4.34: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.7R$ and silt/clay being rigid ......................103

Figure 4.35: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.7R$ and silt/clay being rigid ......................104
Figure 4.36: Cluster frequency distribution for \( D=0.001R \) at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.7\( R \) and silt/clay being rigid .....................106

Figure 4.37: Number of spheres distribution for \( D=0.001R \) at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.7\( R \) and silt/clay being rigid ....................107

Figure 4.38: Relationship between number of clusters and sediment porosity with 5 percent of carbonaceous material in the initial bulk volume for initial sediment porosity of 70%. Values taken from Table 4.1, Table 4.5, Table 4.9, Table 4.13, Table 4.17, Table 4.21, Table 4.25 .............108

Figure 4.39: Relationship between number of spheres in cluster size and sediment porosity with 5 percent of carbonaceous material in the initial bulk volume for initial porosity 70%. Values taken from Table 4.2, Table 4.6, Table 4.10, Table 4.14, Table 4.18, Table 4.22, Table 4.26 ...........109

Figure 4.40: Relationship between number of clusters and sediment porosity with 10 percent of carbonaceous material in the initial bulk volume for initial porosity of 70%. Values taken from Table 4.3, Table 4.7, Table 4.11, Table 4.15, Table 4.19, Table 4.23, Table 4.27 ..............................110

xxx
Figure 4.41: Relationship between number of spheres in cluster size and sediment porosity with 10 percent of carbonaceous material in the initial bulk volume for initial porosity of 70%. Values taken from Table 4.4, Table 4.8, Table 4.12, Table 4.16, Table 4.20, Table 4.24, Table 4.28 ....111

Figure 5.1: Schematic diagram showing the roadmap of taking grain packing forward to commercial simulator for studying multiphase effect on gas phase permeability in mudrocks. ..............................................................115
Chapter 1: Overview

This Chapter gives an overview of the topics discussed in the thesis. The research is focused on grain-scale modeling of the unconventional reservoirs in mudrocks.

1.1 PROBLEM STATEMENT

Shale gas is one of the most important unconventional gas resources. It is increasingly becoming one of the most important energy sources for the world. Most of the shale gas reservoirs are explored in the United States and are exploited to meet the ever increasing demand of energy. It is important to understand the pore level geometries of grains and voids of the mudrocks which play an important role in the transport of hydrocarbons through them. The present work consists of making mechanistic models of certain aspects of the evolution of mudrocks. The models focus on the effect of mechanical compaction on the connectivity of carbonaceous material at the grain scale. The hypothesis is that the extent to which particles of organic matter touch each other determines the extent to which nanopores, which subsequently evolve within these particles, could be connected within the mudrock. Greater connectivity of nanopores should correlate with greater producibility once the mudrock has been stimulated.

1.2 PORE SYSTEM AND TRANSPORT MECHANISM IN MUDROCKS

The pore systems in mudrocks are generally composed of two types of pores:-

a) Intergranular Pores

b) Intragranular Pores
The former type of pores is not common in mudrocks, and the intragranular pore system is assumed to be the main network for storage and transport of the hydrocarbon throughout this study. Nanopores in carbonaceous material in gas-producing mudrocks, Figure 1.1, are attributed to thermal maturation and conversion of solid carbonaceous matter into a fluid hydrocarbon phase. Thermal cooking of this solid carbonaceous material results in increase of pressure within this material, resulting in the formation of nanopores. This leads to the hypothesis that carbonaceous material particles are the preferred conduits of hydrocarbon in mudrocks. The greater the extent to which carbonaceous particles are connected, Figure 1.2, the greater the conductivity of these conduits. The pore networks present in other lithofacies are generally small and isolated. As a limiting case, we assume that these other networks do not contribute to the flow of hydrocarbon in these types of unconventional reservoirs.

Figure 1.1: Scanning electron micro-image of Ar-ion-beam milled surface showing pores in organic matter (Wang and Reed, 2009)
1.3 Previous Work on Modeling Gas Transport in Shale

Javadpour (2009) observed that the gas production from mudrocks was greater than that anticipated from their Darcy permeability. Using images of nanopores obtained by Atomic Force Microscopy, he concluded that the gas flow in nanopores cannot be described simply by Darcy’s equation. Taking into account of Knudsen diffusion and slip flow he introduced an apparent permeability concept which is significant for the pore sizes smaller than 100 nm.

The mass balance equation can be written as follows:

\[ \frac{\partial c}{\partial t} + U \nabla c - D : \nabla^2 c - \kappa c = 0 \]  

(1)
The first term in Equation 1 is the accumulation term, the second one is advection, the third one is Knudsen diffusion and the last term is for desorption of fluid from the surface of carbonaceous material. The parameter $\kappa$ is the desorption constant, $D$ is the Knudsen diffusion and $U$ is the advective velocity. Knudsen diffusion is an important gas transport process in nanopores which are present in the carbonaceous material of the mudrock system and thus relevant to the hypothesis of this study.

Roy et al. (2003) proposed a model to predict the flow characteristics for reasonably high Knudsen number flow regimes through micro channels and nanopores. The Knudsen number ($Kn$) is defined as the ratio of the fluid mean-free path ($\lambda$) to the macroscopic length scale of the physical system ($\Lambda$):

$$Kn = \frac{\lambda}{\Lambda}$$  \hspace{1cm} (2)

where $\lambda = \frac{16\mu}{5\rho \sqrt{2\pi RT}}$; $\mu$ = viscosity; $T$ = temperature; $\Lambda = \rho / \frac{\partial \rho}{\partial x}$ and $\rho$ is fluid density; $R$ is the universal gas constant and $x$ is the direction of the pressure gradient. They developed a two dimensional microscale flow model to predict the overall flow characteristics for reasonably high Knudsen number flow in microchannels and nanopores. If connected paths of nanopores exist within the organic material in a mudrock, then this model could be applied to those paths to predict the macroscopic flow behavior in the mudrock.

Reed et al. (2009) identified four types of porous media in productive gas shale systems (shown in Figure 1.3):

a) Non organic matrix
b) Organic matrix
c) Natural fractures
d) Hydraulic fractures
They stated that organic matter pores, ranging from 5 to 1,000 nm have the ability to adsorb and store free gases. They noted that porosity in organic matter can be as high as five times that in material in a non organic matrix. As organic matter is oil wet, flow of gas in organic matter is predominantly single phase. All these factors tend to enhance gas permeability in gas shale. The pore network in organic matter could be the pathways to high gas production in gas shale when connected to natural and hydraulic fractures.

The hypothesis of this thesis is that the organic material provides the preferred conduits for gas flow in mudrocks. This organic material is a small volume fraction of the mudrock, so it can be expected that particles are distributed as isolated grains. However, to form conduits they must be present in clusters of touching particles within the mudrock. The results of simulations of compaction in the sediment model shows that the
grains of organic material come in contact and form clusters which are the representation of actual connected organic material in mudrocks.

1.4 Organization of Thesis

The thesis has been divided into five distinct chapters. The current chapter summarizes the background, hypothesis and research work done in the current study. Chapter 2 describes the cooperative rearrangement algorithm which is used for creating the grain packing. The chapter explains the two methodologies used for representing compaction in sediments: the unconserved volume approach and the conserved volume approach. Both rigid and ductile grains are defined. It analyzes the tolerance value used for defining a contact and the effect of the tolerance value on the cluster size distribution.

Chapter 3 describes the effect of the volume fraction of carbonaceous material on the number of clusters in the model sediment. It investigates the relationship of the maximum cluster size with the volume fraction of carbonaceous material and defines the threshold value of the volume fraction of carbonaceous material resulting in percolation. Cluster length and aspect ratios in model sediment are also studied in this chapter.

Chapter 4 explains the effect of compaction on clustering of carbonaceous material. It considers the significance of compaction in forming clusters in model sediment, and the threshold value of compaction resulting in “significant clustering” by studying the ductility of the carbonaceous material and silt/clay grains. Chapter 5 presents the conclusions and the future aspects of the current study.

A listing of codes for compaction with cooperative rearrangement and other analysis done in this study is given in the Appendix.
Chapter 2: Methods for modeling the sediments

2.1 INTRODUCTION

Sphere packings have been widely used to simulate sediments and soil and to examine any other process in which particles are packed in space (Rodriguez 2006, Thane 2005). Here we use a grain packing algorithm based on a cooperative rearrangement method. In this treatment touching of two or more grains leads to cluster formation. Cluster size distribution analysis is carried out to study the connectivity of the spheres which represent carbonaceous material. This chapter discusses the cluster formation, its size and frequency formed by the sphere packing algorithm.

A random loose packing with a user-defined solid fraction within a periodic cell is used to model sediments. The process of random packing models the arrangement of carbonaceous material in mudrock, and the main variable controlling cluster formation is the volume fraction of carbonaceous material. Burial compacts the model sediments into model mudrock.

2.2 COOPERATIVE REARRANGEMENT ALGORITHM

The cooperative rearrangement algorithm developed by Thane (2005) was used for this study. Her algorithm creates a dense disordered packing of grains in a defined space with periodic boundaries, referred to here as a “unit cell” or a “periodic cell”. Periodic boundaries eliminate artifacts in the packing due to rigid boundaries. The algorithm consists of three steps:-

1) Initial point generation – The points are randomly selected in a given 3D volume.

2) Growth of spheres – The points are allowed to grow into spheres incrementally in a concentric manner like an onion peel.
3) Removal of Overlaps- The growing of spheres may cause overlaps which are removed by moving the overlapped spheres away from each other in the direction of the line joining their centers.

Steps 2 and 3 are iterated until the packing reaches a user-specified density fraction, or alternatively, the densest possible arrangement. Thane’s original code produced the latter arrangement; for equal spheres such packings have porosity of 36%. The code was revised in this work to allow for stopping at an arbitrary solid volume fraction within the periodic cell.

Figure 2.1 shows an illustration of periodicity. The spheres in the unit cell are shown in the projected $y$-$z$ plane in the center of the diagram; four copies of the unit cell are placed around the center cell. The red spheres represent the real spheres in the unit cell and green spheres are their images. A sphere coming out of one face will have one image in the opposite face. A sphere coming out of a edge will have three images, and a sphere coming out from a corner will have seven images. The encircled regions in Figure 2.1 show the exact fitting of real spheres with their images (red spheres touching green spheres without overlap). The regions also show image spheres which fit with other image spheres (green spheres fitting with green ones).
Figure 2.1: Concept of periodicity as implemented in the sphere packing code. The spheres in the unit cell are shown in the projected $y$-$z$ plane in the center of the diagram; four copies of the unit cell are placed around the center cell. Red spheres are real spheres and green spheres are their images. A sphere at or near one face of unit cell can thus be in virtual contact with a sphere at or near the opposite face. Such contacts are accounted for during the cooperative rearrangement steps.
2.3 Algorithm for Simulating Compaction

Sphere packings created with the cooperative rearrangement algorithm above represent sediments in the original depositional environment. These model sediments are subjected to geometric transformation intended to model the process of compaction. The effect of compaction on connectivity of carbonaceous material is studied at multiple stages. The compaction is modeled by compacting the sediments uniaxially. This is achieved by decreasing a compaction factor \( c \) (\( c < 1.0 \)) in increments while maintaining periodic boundaries. The factor \( c \) scales the vertical dimension of the assembly of packed spheres relative to its initial value as shown in Figure 2.2. The \( z \) coordinate of the spheres is rescaled by the same factor. Thus the value \( c=1 \) does not change the sphere locations or unit cell volume. As \( c \) decreases, the amount of compaction increases.

The approach accounts for the relative motion of spheres within the unit cell and the shape of spheres is not distorted during compaction. This motion is representative of the motion of grains in nature and in uniaxial compaction experiments of sediments at the macroscopic level. A single compaction factor is applied to the unit cell. However, in layered natural sediments the compaction of each layer may be different and depends mainly on the mechanical property of each layer.
Figure 2.2: Schematic showing various stages of compaction. Original model sediment is uncompacted ($c=1$). The final state corresponds to mudrock.
It is useful to compare the relative motion of spheres in the compacted unit cell with grains in a sediment during burial or in a bench-scale resedimentation experiment. As depicted in Figure 2.3, let \( Z^0_{\text{top}} \) and \( Z^0_{\text{bottom}} \) be the distance from the datum of top and bottom of a layer of sediment undergoing compaction. Let \( Z'_{\text{top}} \) and \( Z'_{\text{bottom}} \) be the layer final position, and let \( d_{\text{top}} \) and \( d_{\text{bottom}} \) be the distance traversed by the top and bottom of the layer during compaction. During compaction the thickness \( H \) of the layer of grains decreases representing consolidation of sediments in that layer. The extent of translation of grains in the direction of compaction also decreases with depth. The deformation can be described by

\[
H^0 = Z^0_{\text{bottom}} - Z^0_{\text{top}} \quad \text{(Initial thickness of layer of grains)}
\]
\[
H' = Z'_{\text{bottom}} - Z'_{\text{top}} \quad \text{(Final thickness of layer of grains)}
\]
\[
\frac{H^0}{H'} = \frac{Z^0_{\text{bottom}} - Z^0_{\text{top}}}{Z'_{\text{bottom}} - Z'_{\text{top}}} = \frac{1}{c}
\]
\[
H^0 - H' = d_{\text{top}} - d_{\text{bottom}}
\]
\[
\frac{(H^0 - H')}{H^0} = \frac{(d_{\text{top}} - d_{\text{bottom}})}{H^0} = c
\]

Relative motion of grains as well as translation of the layer’s bottom (from \( Z^0_{\text{bottom}} \) to \( Z'_{\text{bottom}} \)) happens in nature. In the model, the top of the periodic cell moves downward, but the bottom of the cell remains stationary. The grains are forced to move relative to each other as the rescaling of grain center locations cause overlaps that are removed by cooperative rearrangement. However, the grains in the model have the same experience as in nature when the value of \( c \) of the compaction model corresponds to the overall compaction \( c \) in nature. Rescaling the grains in compaction model is representative of overall compaction of a sediment layer in nature.
Figure 2.3: Schematic showing the relative motion of spheres within a box in mechanical compaction

2.4 Rescaling in the direction of compaction

Using this procedure connectivity of carbonaceous material is simulated for 5 and 10 percent of carbonaceous material as a function of compaction stages (values of \( c \)). The percentage refers to the total bulk volume of the model sediment which undergoes compaction. Connectivity is studied in two scenarios:

a) Rescaling in the direction of compaction without cooperative rearrangement (Unconserved volume approach). Some solid volume is lost in rescaling due to non removal of overlaps and hence the grain volume is not conserved.
b) Rescaling in the direction of compaction with cooperative rearrangement (Conserved volume approach). The overlap created by rescaling is removed by moving the spheres apart in the line joining their centres to conserve the grain volume.

2.5 Rescaling in the direction of compaction without cooperative rearrangement

In this scenario, the effect of mechanical compaction is studied by rescaling the grain packing in the direction of compaction without cooperative rearrangement. The mechanical compaction is assumed to be uniaxial. It is imposed geometrically by incrementally rescaling the z-coordinate of the spheres and the box containing the packing.

\[ Z' = Z^0 \cdot c \]

where \( Z' \) is the final z-coordinate and \( Z^0 \) is the initial z-coordinate. This procedure is repeated for a series of values of \( c \). This process results in an overlap of spheres. The overlap of the spheres is not removed in any of the compaction stages. Thus this method does not conserve mass or volume. A more rigorous approach is defined next.

2.6 Rescaling in the direction of compaction with cooperative rearrangement

In this simulation the effect of mechanical compaction is also studied by rescaling the grain packing in the direction of compaction, and then allowing cooperative rearrangement after each increment. The overlaps created by rescaling are removed by moving the spheres apart in the line joining their centre. Overlap is removed in an iterative manner while keeping all the boundaries periodic. The algorithm stops when more compaction would cause unremovable overlaps for rigid grains or greater than
allowable overlap for the ductile grains. The compaction is done in stages with a constant decrement of 0.02 in the value of \( c \) starting from 1.00.

This approach is used to study connectivity of both rigid and ductile grains. Following Thane (2005), the rigid grain is represented by a hard sphere whereas a ductile grain is represented by a hard core with soft shell around it as shown in Figure 2.4. Ductility of a grain is defined in terms of the ratio of the rigid radius to the initial sphere radius. For example, a sphere of 0.9 rigid radius means that the hard core comprises 0.9 times the radius of the sphere with an outer shell of thickness 0.1\( R \). The ductility of the grains is simulated for rigid radius ratios of 0.9, 0.8 and 0.7.

![Rigid and Ductile Grains](image)

**Figure 2.4:** Illustration of rigid and ductile grains. For rigid grain, the rigid radius equals grain radius \( R \). For ductile grains, the rigid radius is less than the grain radius \( R \).
2.7 Cluster formation

In this work, a code was developed for studying the connectivity of the grains created by the cooperative rearrangement algorithm. Initially all the spheres of the packing are assigned a null cluster ID. All spheres are then tested for connectivity. Two spheres are said to be connected if the distance between their centers is equal to the sum of the radius of the spheres within some tolerance value. If the gap between the spheres ($D$) is more than the tolerance value the spheres are not considered to be connected as shown in Figure 2.5. A tolerance value ($D$) of 0.001 $R$ was chosen in all the simulations. Rodriguez (2006) studied the gap size distribution in packings of equal spheres created with Thane’s code and found that a tolerance of $|10^{-3}| R$ gives the experimentally observed average number of neighbors in a dense packing of porosity ~36%. Connected spheres form clusters and a distinct cluster ID assigned to these arrays of spheres. The cluster algorithm accounts for the periodic boundaries of the packing, That is, a sphere at or near one face of the cubic space (unit cell) can be in contact with a sphere at or near the opposite face.

Standard outputs of the simulation code consist of the size and frequency of the various cluster IDs. The size of a cluster is defined by the number of spheres in that cluster and its frequency gives the number of such clusters formed. The plot of cluster size versus cluster frequency gives the cluster size distribution of a sphere packing.
Figure 2.5: The criterion for touching spheres is whether the gap $D$ between the spheres is less than a user-specified tolerance.

The sensitivity of cluster numbers to the tolerance $D$ on a sphere packing of 100 spheres with a solid volume fraction of 0.05 is illustrated in Figures 2.6-2.11. The maximum cluster size is very large at a tolerance of $1.0R$ which is expected since tolerance and radius of sphere are of the same order. The maximum cluster size decreases as the tolerance value is decreased from $0.1R$ to $0.00001R$. The cluster distribution remains qualitatively similar from a tolerance value of $0.1R$ to $0.00001R$. In this work we use $D=0.001R$ to define touching spheres.
Figure 2.6: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value $D = 1.0 \, R$

Figure 2.7: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value $D = 0.1 \, R$
Figure 2.8: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value $D = 0.01 \ R$

Figure 2.9: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value $D = 0.001 \ R$
Figure 2.10: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value $D = 0.0001\ R$

Figure 2.11: Cluster size distribution for 100 spheres for one component sphere packing for tolerance value $D = 0.00001$
Chapter 3: Effect of volume fraction of carbonaceous material on number of clusters in model sediments

3.1 ALGORITHM FOR CREATING PACKINGS WITH PRESCRIBED VOLUME FRACTION OF GRAINS

As discussed in Chapter 2, the cooperative rearrangement algorithm developed by Thane (2005) was revised in this study to allow stopping at an arbitrary solid volume fraction within the periodic cell with a user-defined number of spheres. The variable of density fraction (equivalent to user-defined density fraction in the original code) was used to perform the above analysis. The number of spheres and the desired solid volume as a percentage of total cell volume are the inputs. Figure 3.1 and 3.2 show a periodic packing of 5% and 10% of the cell volume occupied by solid for 100 and 1000 spheres, respectively.

Figure 3.1: Periodic packing of 100 spheres showing 5% (left) and 10% (right) of cell volume occupied by solid
Figure 3.2: Periodic packing of 1000 spheres showing 5% (left) and 10% (right) of cell volume occupied by solid

The simplest model assumes that the other material in the sediment (silt, clay, etc.) does not influence the ability of carbonaceous grains to come into contact. In this case we need not model the other material explicitly. This case can be simulated by creating “one component sphere packings”, Figure 3.3, whose solid volume fraction corresponds to the volume fraction of organic material in sediments. All the grains in these model sediments represent carbonaceous material, hence the term “one component”. The number of spheres is varied from 100 to 5000 to check that the statistics are representative. This scenario involves a single independent parameter, the initial volume fraction of organic material.

The idea behind this approach is to study the connectivity of particles grown in an unrestricted growth environment assuming that the growth of carbonaceous material is not affected by other material around it, Figure 3.3. This decoupling may not accurately
reflect what happens in nature. Thus, a more realistic model explicitly includes grains that represent other constituents of the sediment. This case is simulated with two component sphere packings representing carbonaceous and silt grains mixed together with varying fraction of carbonaceous material.

![Figure 3.3: Initial point generation (Left) and particle growth (Right) in one component sphere packing representing only carbonaceous material in the original sediment](image)

In Figure 3.4, only a prescribed fraction of grains in the packing represent carbonaceous material. The idea of this approach is to model the interference of other grains on the clustering material as the sediment precursor is compacted into mudrock. This scenario involves two parameters, the initial volume fraction of organic material and the prescribed porosity of the initial model sediment.

To create a two component model, the same grain packing code described in Chapter 2 is used to generate a packing of spheres of two slightly different sizes. The size difference is a simple way to identify a subset of the grains and assign them the attribute of being carbonaceous. The ratio of the sphere sizes is kept close to one (1.01) so that the
effect of the relative size of the grains on grain rearrangement and connectivity is negligible. In these models both sizes of sphere are grown simultaneously. The number fraction of larger spheres is chosen to give the desired volume fraction of organic material. Target sediment porosities of 50%, 60% and 70% are considered in this scenario which is assumed to be representative of the sediment precursor to mudrock.

Figure 3.4: Initial point generation (Left) and particle growth (Right) in two component sphere packing, red colored spheres representing carbonaceous material and green colored spheres representing silt/clay
3.2 Carbonaceous Material Only (One Component Sphere Packing)

The grain packing code described above was used to make numerous one component sphere packings. Packings of 500, 1000, 2500, 3000, 3500 and 5000 spheres were created with prescribed solid volume fraction ranging from 0.05 to 0.30 in step size of 0.05 (Table 3.1). As it is one component sphere packing all the solid volume corresponds to carbonaceous material.

Plots of cluster size and cluster frequency were made to characterize the span of clusters in 3D. The volume fraction of the solids representing carbonaceous matter was varied and maximum cluster size with varying density fraction was simulated. Normalized maximum cluster size (maximum cluster size / total number of spheres in the packing) was tabulated (Tables 3.2-3.8) and plotted against volume fraction of carbonaceous material (Figure 3.5).

Table: 3.1 One component sphere packing representing carbonaceous material used for analysis with prescribed solid volume representing carbonaceous material

<table>
<thead>
<tr>
<th>Packing Number</th>
<th>Prescribed volume fraction of carbonaceous material</th>
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<tbody>
<tr>
<td>1</td>
<td>0.05</td>
</tr>
<tr>
<td>2</td>
<td>0.10</td>
</tr>
<tr>
<td>3</td>
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</tr>
<tr>
<td>4</td>
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<td>6</td>
<td>0.30</td>
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</table>
Table: 3.2 Normalized maximum cluster size for various volume fraction of carbonaceous material for 100 spheres for $D=0.001R$

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Maximum Cluster size</th>
<th>Normalized cluster size</th>
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</thead>
<tbody>
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Table: 3.3 Normalized maximum cluster size for various volume fraction of carbonaceous material for 500 spheres for $D=0.001R$

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<th>Volume fraction of carbonaceous material</th>
<th>Maximum Cluster size</th>
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Table: 3.4 Normalized maximum cluster size for various volume fraction of carbonaceous material for 1000 spheres for $D=0.001R$

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Maximum Cluster size</th>
<th>Normalized cluster size</th>
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Table: 3.5 Normalized maximum cluster size for various volume fraction of carbonaceous material for 2500 spheres for $D=0.001R$

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Maximum Cluster size</th>
<th>Normalized cluster size</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>7</td>
<td>0.002</td>
</tr>
<tr>
<td>0.10</td>
<td>12</td>
<td>0.004</td>
</tr>
<tr>
<td>0.15</td>
<td>42</td>
<td>0.016</td>
</tr>
<tr>
<td>0.20</td>
<td>203</td>
<td>0.081</td>
</tr>
<tr>
<td>0.25</td>
<td>1328</td>
<td>0.531</td>
</tr>
<tr>
<td>0.30</td>
<td>2146</td>
<td>0.858</td>
</tr>
</tbody>
</table>

Table: 3.6 Normalized maximum cluster size for various volume fraction of carbonaceous material for 3000 spheres for $D=0.001R$

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Maximum Cluster size</th>
<th>Normalized cluster size</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>10</td>
<td>0.003</td>
</tr>
<tr>
<td>0.10</td>
<td>21</td>
<td>0.007</td>
</tr>
<tr>
<td>0.15</td>
<td>38</td>
<td>0.012</td>
</tr>
<tr>
<td>0.20</td>
<td>137</td>
<td>0.045</td>
</tr>
<tr>
<td>0.25</td>
<td>1894</td>
<td>0.631</td>
</tr>
<tr>
<td>0.30</td>
<td>2643</td>
<td>0.881</td>
</tr>
</tbody>
</table>

Table: 3.7 Normalized maximum cluster size for various volume fraction of carbonaceous material for 3500 spheres for $D=0.001R$

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Maximum Cluster size</th>
<th>Normalized cluster size</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>13</td>
<td>0.003</td>
</tr>
<tr>
<td>0.10</td>
<td>22</td>
<td>0.005</td>
</tr>
<tr>
<td>0.15</td>
<td>59</td>
<td>0.012</td>
</tr>
<tr>
<td>0.20</td>
<td>491</td>
<td>0.067</td>
</tr>
<tr>
<td>0.25</td>
<td>2896</td>
<td>0.545</td>
</tr>
<tr>
<td>0.30</td>
<td>3321</td>
<td>0.867</td>
</tr>
</tbody>
</table>
Table: 3.8 Normalized maximum cluster size for various volume fraction of carbonaceous material for 5000 spheres for $D=0.001R$

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Maximum Cluster size</th>
<th>Normalized cluster size</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>8</td>
<td>0.001</td>
</tr>
<tr>
<td>0.10</td>
<td>15</td>
<td>0.003</td>
</tr>
<tr>
<td>0.15</td>
<td>62</td>
<td>0.012</td>
</tr>
<tr>
<td>0.20</td>
<td>229</td>
<td>0.045</td>
</tr>
<tr>
<td>0.25</td>
<td>2999</td>
<td>0.599</td>
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<tr>
<td>0.30</td>
<td>4324</td>
<td>0.864</td>
</tr>
</tbody>
</table>

Figure 3.5: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material for one component sphere packing
As shown in Figure 3.5, model sediments that assume carbonaceous material arrangement unaffected by other grains have a characteristic trend of maximum cluster size. The normalized maximum cluster size starts increasing with the volume fraction of carbonaceous material and makes a ‘S’ shaped profile. A rapid increase in normalized maximum cluster size is observed at 0.2 volume fraction of carbonaceous material for tolerance value \( D = 0.001R \). This is the point at which smaller different sized clusters mingle to form a big cluster which may result in percolation.

These results suggest that, if mudrocks have a volume fraction of carbonaceous material from 0.20 to 0.25, we can expect a pore network of connected carbonaceous material leading to percolation. Such rocks should have significantly larger permeability to gas than rocks with carbonaceous material volume fraction less than 0.20. However, it is observed that cooperative rearrangement leads to clustering (section 3.7), as there is enough void space to accommodate all the spheres without any formation of clusters. Thus these results predict more clustering that may occur in nature.

### 3.3 Carbonaceous Material with Matrix (Two Component Sphere Packing)

The same grain packing code was used to make numerous two component sphere packing by using slightly different size of spheres to distinguish their chemical identity (carbonaceous material or silt/clay).

Packings of 100, 500, 1000 and 2000 spheres of carbonaceous material were created. The volume fraction of carbonaceous material ranged from 0.05 to 0.30 in step size of 0.05. Target porosities of 50%, 60% and 70% were used to represent a range of
sediments. In this scenario, porosities represent the void volume in the mixtures of carbonaceous material and silt/clay which are sediment precursor to mudrock.

Each set of packings with a given amount of carbonaceous grains had a range of numbers of silt grains. The values were chosen to yield different porosities and volume fractions of carbonaceous material. This results in a “probability factor”, the fraction of the total number of spheres that are carbonaceous material. The cooperative rearrangement code allows specifying this fraction to be carbonaceous, so the resulting packing does not have exactly the desired number of carbonaceous spheres. The fraction and the total number of spheres for packings containing 1000 spheres (desired number) representing carbonaceous material are tabulated in the tables 3.9 to 3.11. Similar tables can be constructed for packings in which 100, 500 or 2000 spheres are carbonaceous and others non carbonaceous. The plots are shown in Figure 3.6-3.8.

Table: 3.9 Composition of two component packings: Carbonaceous material with other grains for target porosity of 70%; the desired number of carbonaceous material spheres is 1000. Volume fraction refers sediment bulk volume

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Probability factor for carbonaceous material</th>
<th>Total number of spheres in packing</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.1666</td>
<td>6000</td>
</tr>
<tr>
<td>0.10</td>
<td>0.3333</td>
<td>3000</td>
</tr>
<tr>
<td>0.15</td>
<td>0.5000</td>
<td>2000</td>
</tr>
<tr>
<td>0.20</td>
<td>0.6666</td>
<td>1500</td>
</tr>
<tr>
<td>0.25</td>
<td>0.8333</td>
<td>1200</td>
</tr>
<tr>
<td>0.30</td>
<td>1.0000</td>
<td>1000</td>
</tr>
</tbody>
</table>
Table: 3.10 Composition of two component packings: Carbonaceous material with other grains for target porosity of 60%; the desired number of carbonaceous material spheres is 1000. Volume fraction refers sediment bulk volume

<table>
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<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Probability factor for carbonaceous material</th>
<th>Total number of spheres in packing</th>
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</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.1250</td>
<td>8000</td>
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<tr>
<td>0.10</td>
<td>0.2500</td>
<td>4000</td>
</tr>
<tr>
<td>0.15</td>
<td>0.3750</td>
<td>2667</td>
</tr>
<tr>
<td>0.20</td>
<td>0.5000</td>
<td>2000</td>
</tr>
<tr>
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<td>0.6250</td>
<td>1600</td>
</tr>
<tr>
<td>0.30</td>
<td>0.7500</td>
<td>1334</td>
</tr>
</tbody>
</table>

Table: 3.11 Composition of two component packings: Carbonaceous material with other grains for target porosity of 50%; the desired number of carbonaceous material spheres is 1000. Volume fraction refers sediment bulk volume

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<th>Volume fraction of carbonaceous material</th>
<th>Probability factor for carbonaceous material</th>
<th>Total number of spheres in packing</th>
</tr>
</thead>
<tbody>
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<td>0.1</td>
<td>10000</td>
</tr>
<tr>
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<td>0.2</td>
<td>5000</td>
</tr>
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<td>0.15</td>
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<td>3334</td>
</tr>
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</tr>
<tr>
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<td>0.5</td>
<td>2000</td>
</tr>
<tr>
<td>0.30</td>
<td>0.6</td>
<td>1667</td>
</tr>
</tbody>
</table>
Figure 3.6: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material in sediment for packing of carbonaceous material with matrix. Sediment porosity is 70 percent. Curves refer to sets of packings in which number of carbonaceous material grains is constant.
Figure 3.7: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material in sediment for packing of carbonaceous material with matrix. Sediment porosity is 60 percent. Curves refer to sets of packings in which number of carbonaceous material grains is constant.
Figure 3.8: Normalized maximum cluster size for $D = 0.001R$ vs. volume fraction of carbonaceous material in sediment for packing of carbonaceous material with matrix. Sediment porosity is 50 percent. Curves refer to sets of packings in which number of carbonaceous material grains is constant.

Similar to the one component packing Figure 3.5, packing of carbonaceous material with other grains also yields a ‘S’ shaped curve in the plot of normalized maximum cluster size vs. volume fraction of carbonaceous material. The maximum cluster size starts increasing when the volume fraction of carbonaceous material reaches about 0.15. Rapid changes in normalized maximum cluster sizes are again observed at 0.2 volume fraction of carbonaceous material for a tolerance value ($D$) of 0.001$R$. 
Similar to the results of one component packing discussed in the section 3.2, even in the presence of other component like silt/clay we can expect a pore network of connected carbonaceous material leading to percolation for a mudrock having 0.2-0.25 volume fraction of carbonaceous material.

3.4 Cluster Length Analysis

The clusters formed from the sphere packing in the previous section were subjected to cluster length analysis to study their span in 3D, based on the presumption that connected carbonaceous materials are the preferred conduits of gas migration in mudrocks. The length distribution of each cluster in x, y, and z directions was calculated and with the help of suitable geometric transformation its extent was studied in 3D. The 3D envelope made by the geometrical transformation gives an idea of the ranges of lateral extent of the clusters observed in slices cut through any plane for SEM (Scanning Electron Microscope) analysis. For example in Figure 3.9, length in the X direction is calculated as:

\[ \text{Length in } X \text{ direction } (L_X) = X_{\text{max}} - X_{\text{min}} + R_1 + R_2 \]

where \( X_{\text{max}} \) and \( X_{\text{min}} \) are the maximum and minimum x coordinates of spheres in a particular cluster ID and \( R_1 \) and \( R_2 \) are the radii of them. Similarly length in Y and Z directions \( L_Y \) and \( L_Z \) were also calculated and the length distribution was studied. The results, Figure 3.10, showed that the distribution of the length in x y and z directions were quite uniform; i.e. no preferred direction which should be the case as the spheres in the packing were randomly generated.
Figure 3.9: Cluster Length calculation in X direction

Figure 3.10: Selected cluster length analysis for 5 percent carbonaceous material for one component sphere packing of 100 spheres representing carbonaceous material with radius = 3.56 units
As an example shown in Figure 3.10, it is observed that the cluster ID 223 corresponds to biggest cluster (size =5) for one component sphere packing of 100 spheres with radius 3.56 units.

3.5 Geometrical Transformation

A geometrical transformation was carried out in order to study the 3D envelope of clusters formed. It gives a better idea about the span of cluster with the coordinate axes. The geometrical transformation includes the translation as well as the rotation of the coordinate axes. The spheres nearest and farthest from the origin are identified. The origin of the coordinate system is shifted to the centre of the sphere which is nearest to the old origin with the help of translation. Then the coordinate axes are rotated in such a manner that the z axis of the new coordinate system coincides with the line joining the centre of the spheres identified above (as shown in Figure 3.11). The whole cluster is rotated about this new z axis at steps of 10 degrees from 0 to 180 degrees and its length in the x and y direction is reported. It is observed that the variation in length of the cluster with angle of rotation is sinusoidal shown in Figure 3.12. The maximum value of cluster length in the x direction is at the minimum value of cluster length in the y direction indicating a constant phase shift of 90 degrees between the two length values.
Figure 3.11: Geometrical transformation for the biggest cluster from one component sphere packing of 100 spheres representing carbonaceous material with radius = 3.56 units
Figure 3.12: Variation of LX and LY in new coordinate system showing a phase difference of 90 degrees between them for the biggest cluster from one component sphere packing of 100 spheres with radius = 3.56 units

3.6 ASPECT RATIO

The aspect ratio of a cluster is defined as the ratio of the maximum cluster length to the minimum cluster length in coordinate directions. The aspect ratios of the clusters were also calculated and reported for different volume fractions of the carbonaceous material. The aspect ratio gives an idea about the appearance of a cluster in 3D for a particular volume fraction of the carbonaceous material. The geometrical transformation with aspect ratios tabulated below in Tables 3.12-3.18.
Table 3.12: Cluster length and cluster aspect ratios for $D=0.001R$ and 5 percent carbonaceous material of bulk volume and 100 spheres with radius = 3.56 units for one component sphere packing after the geometrical transformation

<table>
<thead>
<tr>
<th>Cluster number</th>
<th>length$_{xmax}$</th>
<th>length$_{xmin}$</th>
<th>length$_{ymax}$</th>
<th>length$_{ymin}$</th>
<th>length$_{zmax}$</th>
<th>length$_{zmin}$</th>
<th>Aspect ratio</th>
<th>Number of spheres in cluster</th>
</tr>
</thead>
<tbody>
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<td>1</td>
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<td>7.12</td>
<td>7.12</td>
<td>7.12</td>
<td>14.24</td>
<td>14.24</td>
<td>2.00</td>
<td>2</td>
</tr>
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<td>9.54</td>
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</tr>
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</table>
Table 3.13: Cluster length and cluster aspect ratios for $D=0.001R$ and 10 percent carbonaceous material of bulk volume and 100 spheres with radius = 4.42 units for one component sphere packing after the geometrical transformation

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<th>length$_y$max</th>
<th>length$_y$min</th>
<th>length$_z$max</th>
<th>length$_z$min</th>
<th>Aspect ratio</th>
<th>Number of spheres in cluster</th>
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<td>17.68</td>
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Table 3.14: Cluster length and cluster aspect ratios for $D=0.001R$ and 15 percent carbonaceous material of bulk volume and 100 spheres with radius = 5.03 units for one component sphere packing after the geometrical transformation

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<th>length_y min</th>
<th>length_z max</th>
<th>length_z min</th>
<th>Aspect ratio</th>
<th>Number of spheres in cluster</th>
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<td>30.53</td>
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<td>3.43</td>
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<td>16.86</td>
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<td>10.06</td>
<td>20.13</td>
<td>20.13</td>
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</table>
Table 3.15: Cluster length and cluster aspect ratios for $D=0.001R$ and 20 percent carbonaceous material of bulk volume and 100 spheres with radius $= 5.52$ units for one component sphere packing after the geometrical transformation

<table>
<thead>
<tr>
<th>Cluster number</th>
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<th>length$_x$ min</th>
<th>length$_y$ max</th>
<th>length$_y$ min</th>
<th>length$_z$ max</th>
<th>length$_z$ min</th>
<th>Aspect ratio</th>
<th>Number of spheres in cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
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<td>85.02</td>
<td>69.05</td>
<td>88.61</td>
<td>88.61</td>
<td>1.28</td>
<td>48</td>
</tr>
<tr>
<td>3</td>
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<td>17.98</td>
<td>11.56</td>
<td>28.22</td>
<td>28.22</td>
<td>2.44</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>11.04</td>
<td>11.04</td>
<td>11.04</td>
<td>11.04</td>
<td>22.09</td>
<td>22.09</td>
<td>2.00</td>
<td>2</td>
</tr>
<tr>
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<td>11.04</td>
<td>11.04</td>
<td>11.04</td>
<td>22.09</td>
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<td>2</td>
</tr>
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<td>11.04</td>
<td>11.04</td>
<td>11.04</td>
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<td>22.09</td>
<td>2.00</td>
<td>2</td>
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<td>11.04</td>
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</tr>
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<td>2.13</td>
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<tr>
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<td>11.04</td>
<td>22.09</td>
<td>22.09</td>
<td>2.00</td>
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Table 3.16: Cluster length and cluster aspect ratios for $D=0.001R$ and 25 percent carbonaceous material of bulk volume and 100 spheres with radius $= 5.89$ units for one component sphere packing after the geometrical transformation

<table>
<thead>
<tr>
<th>Cluster number</th>
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<th>length$_x$ min</th>
<th>length$_y$ max</th>
<th>length$_y$ min</th>
<th>length$_z$ max</th>
<th>length$_z$ min</th>
<th>Aspect ratio</th>
<th>Number of spheres in cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>17.37</td>
<td>12.27</td>
<td>32.51</td>
<td>32.51</td>
<td>2.65</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>11.78</td>
<td>11.78</td>
<td>11.78</td>
<td>11.78</td>
<td>23.57</td>
<td>23.57</td>
<td>2.00</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>11.78</td>
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<td>11.78</td>
<td>11.78</td>
<td>23.57</td>
<td>23.57</td>
<td>2.00</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
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<td>11.78</td>
<td>11.78</td>
<td>11.78</td>
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<td>23.57</td>
<td>2.00</td>
<td>2</td>
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<td>5</td>
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<td>94.19</td>
<td>77.59</td>
<td>125.06</td>
<td>125.06</td>
<td>1.61</td>
<td>73</td>
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Table 3.17: Cluster length and cluster aspect ratios for $D=0.001R$ and 30 percent carbonaceous material of bulk volume and 100 spheres with radius = 6.83 units for one component sphere packing after the geometrical transformation

<table>
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<th>Cluster number</th>
<th>length_x max</th>
<th>length_x min</th>
<th>length_y max</th>
<th>length_y min</th>
<th>length_z max</th>
<th>length_z min</th>
<th>Aspect ratio</th>
<th>Number of spheres in cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>22.32</td>
<td>12.77</td>
<td>22.32</td>
<td>12.77</td>
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<td>2.33</td>
<td>3</td>
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<tr>
<td>2</td>
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<td>101.54</td>
<td>85.02</td>
<td>114.08</td>
<td>114.08</td>
<td>1.34</td>
<td>87</td>
</tr>
</tbody>
</table>

The maximum aspect ratio increases with the volume fraction of the carbonaceous material. It reaches a maximum value near percolation and then starts decreasing gradually as shown in Figure 3.13.

The aspect ratio of the large clusters increases with volume fraction of carbonaceous material reaches a maximum value (2.06 for cluster size of 16 for 15 percent of carbonaceous material packing) and then starts decreasing with increase in volume fraction of carbonaceous material (1.34 for cluster size of 87 for 30 percent of carbonaceous material packing).

Table 3.18: Maximum, minimum and average aspect ratios for one component sphere packing of 100 spheres for $D=0.001R$

<table>
<thead>
<tr>
<th>Volume fraction of carbonaceous material</th>
<th>Max Aspect ratio</th>
<th>Min Aspect ratio</th>
<th>Avg Aspect ratio</th>
</tr>
</thead>
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<td>0.05</td>
<td>2.90</td>
<td>2.00</td>
<td>2.14</td>
</tr>
<tr>
<td>0.10</td>
<td>3.49</td>
<td>2.00</td>
<td>2.57</td>
</tr>
<tr>
<td>0.15</td>
<td>3.43</td>
<td>1.56</td>
<td>2.31</td>
</tr>
<tr>
<td>0.20</td>
<td>2.74</td>
<td>1.28</td>
<td>2.07</td>
</tr>
<tr>
<td>0.25</td>
<td>2.65</td>
<td>1.61</td>
<td>2.05</td>
</tr>
<tr>
<td>0.30</td>
<td>2.33</td>
<td>1.34</td>
<td>1.83</td>
</tr>
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</table>
Figure 3.13: Maximum aspect ratio of clusters vs. volume fraction of carbonaceous material for one component sphere packing of 100 spheres for $D=0.001R$
Figure 3.13: Aspect ratio of largest cluster vs. volume fraction of carbonaceous material for one component sphere packing of 100 spheres for $D=0.001R$.

### 3.7 Inherent Clustering of Spheres Induced by Cooperative Rearrangement Algorithm

The algorithm for rescaling the grains with and without cooperative rearrangement was also assessed for inducing clustering of spheres. The cooperative rearrangement algorithm by its nature is conducive to creating clusters, because overlapping spheres are moved until they just touch. Packings in which the grains occupy small volume fractions, e.g. 15%, can easily be arranged to have no grains touching at all.
Thus it is of interest to quantify how much clustering is inherent in the method used to create model sediments.

A one component packing of 0.25 solid volume fraction was considered for analysis. The radius of all the spheres in the packing was reduced so that the packing had a 0.05 solid volume fraction. This method ensured that no sphere was touching with another in the initial sediment precursor. In fact it ensures that the distance between spheres was at least 1.42 sphere radii. The packing was then rescaled in the direction of compaction without cooperative rearrangement. The statistics of cluster frequency and number of spheres associated with particular cluster size class were generated and shown in Figure 3.14-3.15 (bar labeled with suffix-2). They are compared with the statistics of the packing having a 0.05 solid fraction created by Thane’s code (Figure 3.14-3.15). That is, two packing have same initial solid fraction (0.05), one containing contacts inherent to the cooperative rearrangement algorithm, the other having all spheres separated, are subjected to the same compaction simulation.
Figure 3.14: Comparison of cluster frequency vs. cluster size for $D=0.001R$ of the compaction stages of one component packing created by Thane’s code and dispersed spheres represented by suffix-2 (1000 rigid spheres of carbonaceous material)
The cluster frequency and the number of spheres associated with a particular cluster size class were significantly different in the two model sediments. The one with no initially touching spheres yielded fewer large clusters during compaction. The clustering of spheres in this scenario, however, depended on the initial position of spheres as there was no rearrangement of spheres at any compaction stage.

To test the same effect for the algorithm of rescaling in the direction of compaction with cooperative rearrangement, two component packing of target porosity
50% having 5 percent carbonaceous material by bulk volume having rigid spheres was taken into consideration. The above packing was changed to 70% porosity by reducing the radius of all the spheres by the same ratio ensuring that no spheres touch each other at the initial stage. The distance between spheres was at least 0.09 sphere radii. The packing was subjected to compaction with cooperative rearrangement. Meanwhile another two-component sphere packing of 70% initial porosity was created with the modified Thane’s code that uses cooperative rearrangement. It was subjected to the same process of compaction with cooperative rearrangement. The results are shown in Figure 3.16-3.17.

Figure 3.16: Comparison of cluster frequency vs. cluster size for $D=0.001R$ of the compaction stages of two component packing created by Thane’s code and dispersed spheres represented by suffix-2 (1000 rigid spheres of carbonaceous material and 70% target porosity)
The cluster frequency and the number of spheres associated with a particular cluster size class were quite different for the above compared scenarios. The isolated spheres were more in case of dispersed sediments in which spheres were not touching each other at every stage of compaction. Even compaction with cooperative rearrangement for the dispersed sediments did not give enough big clusters of cluster size 5 to 10 and no cluster of size 10 to 50 at 48 percent compaction when compared to...
compaction of the sphere packing created by Thane’s code. The results showed some biasing of cluster formation in the sphere packing created from Thane’s code. This suggests that the cluster statistics reported in this chapter and the next are biased toward cluster formation. This could represent behavior in nature if carbonaceous particles have some affinity for each other. If this were the case, small clusters of particles could form during deposition, and then the models described above, in which the initial grains are forced to be separated, would be more representative. Further research is needed to evaluate which model is applicable.
Chapter 4: Effect of compaction on clustering of carbonaceous material

In this section the sphere packing of Chapter 3, created from the cooperative rearrangement algorithm in Chapter 2, was subjected to mechanical compaction using algorithms of Chapter 2. The resulting change in connectivity of the carbonaceous material was investigated at the grain scale (Figure 4.1). Compaction of carbonaceous material only (one component sphere packing) and carbonaceous material with matrix (two component sphere packing) were considered. For each class of model sediments, plots of cluster frequency and number of spheres in cluster size ranges were analyzed as a function of cluster size for rescaling in the direction of compaction with and without cooperative rearrangement. The former plot gives the number of clusters present in each cluster size class while the latter gives the number of spheres associated with that cluster size class.
4.1 Rescaling in the Direction of Compaction without Cooperative Rearrangement: Application to One Component Packings

One component sphere packing representing only carbonaceous material is carried out by rescaling the grain packing in the direction of compaction without cooperative rearrangement. Packings of 0.05 and 0.10 volume fraction of carbonaceous material were compacted to various reductions of the initial bulk volume 10%, 30%, 50% and 70%. Plots of cluster frequency vs. cluster size are shown in Figure 4.2-4.5.

The stages of volume reduction are related to the compaction factor of Chapter 2 $(c)$ by:

\[
\text{Compaction factor } (c) = \frac{\text{Volume of cell at compacted stage}}{\text{Initial volume of the cell}}
\]
As shown in Figures 4.2-4.3, the compaction resulted in increase in cluster size and in numbers of spheres associated with larger cluster sizes. The effect of compaction on connectivity is greater for the case of 0.10 volume fraction than in 0.05 volume fraction of carbonaceous material for these model sediments. Because this model of compaction does not conserve the volume of solid grains, the results are not applicable to mudrocks. However, they are useful for establishing the range of behavior that might be observed in more realistic compaction models, discussed in Section 4.3.

Figure 4.2: Cluster frequency vs. cluster size for $D = 0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for one component sphere packing (1000 spheres of carbonaceous material)
Figure 4.3: Number of spheres in cluster size vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for one component sphere packing (1000 spheres of carbonaceous material)
Figure 4.4: Cluster frequency vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 10 percent of carbonaceous material in the initial bulk volume for one component sphere packing (1000 spheres of carbonaceous material)
4.2 RESCALING IN THE DIRECTION OF COMPACTION WITHOUT COOPERATIVE REARRANGEMENT: APPLICATION TO TWO COMPONENT PACKINGS

Two component sphere packing in which the carbonaceous material and clay/silt were combined, was compacted by rescaling the grain packing in the direction of compaction without cooperative rearrangement and studied in the similar way as one component sphere packing in the preceding section. The compaction stages of 10%, 30%, 50% and 70% were carried out for the 0.05 and 0.10 volume fraction of the carbonaceous material.
The result of compaction on the cluster size distribution was found to be (Figure 4.6 to Figure 4.9) similar to that of one component sphere packing (Figure 4.2 to Figure 4.5) representing only carbonaceous material. There is no significant effect of the presence of clay/silt grains on connectivity of carbonaceous material grains at various compaction stages. This may be due to the simplicity of the compaction simulation, which does allow arbitrary degrees of sphere overlap and does not conserve solid volume.

Figure 4.6: Cluster frequency vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for two component sphere packing (1000 spheres of carbonaceous material)
Figure 4.7: Number of spheres in cluster size vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 5 percent of carbonaceous material in the initial bulk volume for two component sphere packing (1000 spheres of carbonaceous material)
Figure 4.8: Cluster frequency vs. cluster size for $D=0.001R$ as a function of compaction without cooperative rearrangement with 10 percent of carbonaceous material in the initial bulk volume for two component sphere packing (1000 spheres of carbonaceous material)
Three scenarios for sediments were investigated by using this approach.

1) Rigid carbonaceous material and silt/clay grains
2) Both carbonaceous and silt/clay grains are ductile
3) Carbonaceous grains are ductile and silt/clay grains are rigid

Grain packings of prescribed porosity 70 %, having 0.05 and 0.10 volume fraction of carbonaceous material were used as a base case for this study. Compaction with
cooperative rearrangement was used to remove overlaps, thereby conserving solid volume, and periodic boundaries to allow unconfined grain motion. Thus these packings have a more realistic representation of the compaction process in nature.

4.3.1 Rigid Carbonaceous Material and Silt/Clay Grains

Under this scenario, both carbonaceous material and silt/clay grains are assumed to be rigid. Results for grain packing subjected to compaction and both cluster frequency vs. cluster size and numbers of spheres vs. cluster size are shown in Figure 4.10-4.13 and summarized in Table 4.1-4.4. We observe that the grain packing of prescribed porosity 70% is compacted to 48% (c= 0.52) giving a final porosity of approximately 42%. The final volume fraction of carbonaceous material for initial 5% and 10% volume fraction of carbonaceous material is 9.6% and 19.2% respectively. As the compaction increases, the number of larger clusters increases. At 52 percent compaction, for 5 percent carbonaceous material by bulk volume 1 cluster with associated 12 spheres is formed in cluster size class of 10 to 50 and for 10 percent carbonaceous material by bulk volume 2 clusters with associated 242 spheres in the class of 50-500 are formed.
Table 4.1: Cluster frequency distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.

<table>
<thead>
<tr>
<th>Compaction stage</th>
<th>Porosity</th>
<th>Max cluster size</th>
<th>Normalized max cluster size</th>
<th>Frequency of clusters by size</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
<td></td>
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</tr>
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<td>Initial</td>
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<td>7</td>
<td>0.007035</td>
<td>744</td>
</tr>
<tr>
<td>0.9</td>
<td>0.6700</td>
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</tr>
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<td>0.009045</td>
<td>580</td>
</tr>
<tr>
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<td>0.4288</td>
<td>12</td>
<td>0.012060</td>
<td>405</td>
</tr>
</tbody>
</table>

Table 4.2: Number of spheres distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.

<table>
<thead>
<tr>
<th>Compaction stage</th>
<th>Porosity</th>
<th>Max cluster size</th>
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<th>Total number of spheres in clusters of different size ranges</th>
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Figure 4.10: Cluster frequency distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.
Figure 4.11: Number of spheres distribution for $D=0.001R$ at different levels of compaction for two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.

Table 4.3: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.
Table 4.4: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.

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<th>Total number of spheres in clusters of different size ranges</th>
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<td>Initial</td>
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Figure 4.12: Cluster frequency distribution for \( D=0.001R \) at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.
Figure 4.13: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both rigid grains.

**4.3.2 Both Carbonaceous and Silt/Clay Grains Are Ductile**

Under this scenario, both carbonaceous material and silt/clay grains are assumed ductile. Grain packing is subjected to compaction, and both cluster frequency and number of spheres vs. cluster size are plotted in Figure 4.14-4.17 and summarized in Table 4.5-4.8. The grain packing of prescribed porosity 70% is compacted to 56% ($c=0.44$) for 0.9 rigid radius, 62% ($c=0.38$) for 0.8 rigid radius and 68% ($c=0.32$) for 0.7 rigid radius giving final residual porosity ~42%, ~23% and ~13% respectively.
The final volume fraction of carbonaceous material for initial volume fractions of 5% and 10% of carbonaceous material is 11.3% and 22.7% for 0.9 rigid radius, 13.1% and 26.3% for 0.8 rigid radius and 15.6% and 31.2% for 0.7 rigid radius respectively (Table 4.5-4.16 and Figure 4.14-4.25).

It is observed that as the compaction increases, the number of large clusters increases but the effect of compaction on connectivity of carbonaceous material is more pronounced as the grains are ductile in this scenario.

Table 4.5: Cluster frequency distribution for \( D=0.001R \) at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.9R

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<th>Porosity</th>
<th>Max cluster size</th>
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<td>0.3178</td>
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Table 4.6: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.9R$

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<th>Compaction stage</th>
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<td>0.3178</td>
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Figure 4.14: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.9R$. 

Cluster frequency

Cluster size

Initial stage
10 percent compaction
30 percent compaction
50 percent compaction
56 percent compaction
Figure 4.15: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio=$0.9R$
Table 4.7: Cluster frequency distribution for $D=0.001 R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.9R$

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<td>0.3116</td>
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<td>0.7925</td>
<td>68</td>
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Table 4.8: Number of spheres distribution for $D=0.001 R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.9R$

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<td>0.7925</td>
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</table>
Figure 4.16: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.9R$. 
Figure 4.17: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio=$0.9R$
Table 4.9: Cluster frequency distribution for $D = 0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $= 0.8R$

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<th>Frequency of clusters by size</th>
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Table 4.10: Number of spheres distribution for $D = 0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $= 0.8R$

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Figure 4.18: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.8R$
Figure 4.19: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio=$0.8R$
Table 4.11: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.8R$

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<td>0.2329</td>
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Table 4.12: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio $=0.8R$

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Figure 4.20: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.8R$
Figure 4.21: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio=0.8R
Table 4.13: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.7$R$

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Table 4.14: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.7$R$

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Figure 4.22: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio $=0.7R$. 
Figure 4.23: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio=$0.7R$
Table 4.15: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.7R

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Table 4.16: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid ratio =0.7R

<table>
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<tr>
<th>Compaction stage</th>
<th>Porosity</th>
<th>Max cluster size</th>
<th>Normalized max cluster size</th>
<th>Total number of spheres in clusters of different size ranges</th>
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<td>0.9178</td>
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86
Figure 4.24: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material and silt/clay both ductile grains with rigid radius ratio =0.7R
4.3.3 Carbonaceous material is ductile and silt/clay grains are rigid

Under this scenario, only carbonaceous material is assumed to be ductile. The grain packing used for the scenario of all the spheres to be rigid was considered for this analysis which ensured that there was no overlap of spheres in the initial sediment setting. The grain packing is subjected to compaction and both cluster frequency vs. cluster size and number of spheres vs. cluster size are plotted in Figure 4.26-4.37 and summarized in Table 4.17-4.28. It is observed that the grain packing of prescribed
porosity 70% is compacted to 50% ($c = 0.50$) for all the cases (0.9 rigid radius, 0.8 rigid radius and 0.7 rigid radius) giving a final porosity of approximately 40%. The final volume fractions of carbonaceous material for initial 5% and 10% volume fraction of carbonaceous material is 10% and 20% respectively.

The results (Figure 4.26-4.37) shows that as the compaction increases, number of large cluster increases. However, the effect of compaction on connectivity of carbonaceous material is less pronounced than the case of both carbonaceous material and silt/clay grains as ductile grains (Figure 4.13-4.25). There is a minor effect of ductility of carbonaceous material on connectivity observed in 0.05 and 0.10 volume fraction of carbonaceous material grain packing (Figure 4.26-4.37).

Table 4.17: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.9$R$ and silt/clay being rigid.
Table 4.18: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.9$R$ and silt/clay being rigid.

<table>
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<th>Compaction stage</th>
<th>Porosity</th>
<th>Max cluster size</th>
<th>Normalized max cluster size</th>
<th>Total number of spheres in clusters of different size ranges</th>
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</thead>
<tbody>
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<td>Initial</td>
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<td>744</td>
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<td>0.4007</td>
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<td>0.0111</td>
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Figure 4.26: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.9$R$ and silt/clay being rigid
Figure 4.27: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.9R$ and silt/clay being rigid.
Table 4.19: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.9R and silt/clay being rigid

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<th>Frequency of clusters by size</th>
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<td>0.5</td>
<td>0.4021</td>
<td>550</td>
<td>0.5753</td>
<td>83</td>
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</table>

Table 4.20: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.9R and silt/clay being rigid

<table>
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<tr>
<th>Compaction stage</th>
<th>Porosity</th>
<th>Max cluster size</th>
<th>Normalized max cluster size</th>
<th>Total number of spheres in clusters of different size ranges</th>
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<td>0.0178</td>
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<td>0.4021</td>
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<td>0.5753</td>
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Figure 4.28: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=$0.9R$ and silt/clay being rigid.
Figure 4.29: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.9R$ and silt/clay being rigid.
Table 4.21: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.8 $R$ and silt/clay being rigid.

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<th>Frequency of clusters by size</th>
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Table 4.22: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.8$R$ and silt/clay being rigid.

<table>
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<th>Compaction stage</th>
<th>Porosity</th>
<th>Max cluster size</th>
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<th>Total number of spheres in clusters of different size ranges</th>
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<td>0.3955</td>
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<td>0.0151</td>
<td>261 377 298 59 0</td>
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</table>
Figure 4.30: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.8$R$ and silt/clay being rigid.
Figure 4.31: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid
Table 4.23: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid

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<th>Frequency of clusters by size</th>
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<td>0.3400</td>
<td>60</td>
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Table 4.24: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid

<table>
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<th>Compaction stage</th>
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<th>Total number of spheres in clusters of different size ranges</th>
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<td>0.3974</td>
<td>325</td>
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</table>
Figure 4.32: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.8R and silt/clay being rigid.
Figure 4.33: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.8R$ and silt/clay being rigid
Table 4.25: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio =0.7 $R$ and silt/clay being rigid

<table>
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<th>Compaction stage</th>
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<th>Normalized max cluster size</th>
<th>Frequency of clusters by size</th>
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<td>0.3982</td>
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<td>0.0171</td>
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Table 4.26: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio=0.7$R$ and silt/clay being rigid

<table>
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<tr>
<th>Compaction stage</th>
<th>Porosity</th>
<th>Max cluster size</th>
<th>Normalized max cluster size</th>
<th>Total number of spheres in clusters of different size ranges</th>
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</table>
Figure 4.34: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.7R$ and silt/clay being rigid
Figure 4.35: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 5 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.7R$ and silt/clay being rigid.
Table 4.27: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio = 0.7 R and silt/clay being rigid

<table>
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<th>Max cluster size</th>
<th>Normalized max cluster size</th>
<th>Frequency of clusters by size</th>
</tr>
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<tr>
<td>Initial</td>
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<td>0.0220</td>
<td>250 142 38 7 0</td>
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<td>0.3974</td>
<td>161</td>
<td>0.1684</td>
<td>78 48 12 14 5</td>
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Table 4.28: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio = 0.7R and silt/clay being rigid

<table>
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<th>Compaction stage</th>
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<td>0.3974</td>
<td>161</td>
<td>0.1684</td>
<td>78 130 79 232 437</td>
</tr>
</tbody>
</table>
Figure 4.36: Cluster frequency distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.7R$ and silt/clay being rigid.
Figure 4.37: Number of spheres distribution for $D=0.001R$ at different levels of compaction of two component packing with 10 percent of carbonaceous material in the initial bulk volume. Cooperative rearrangement, 1000 spheres of carbonaceous material, carbonaceous material being ductile with rigid radius ratio $=0.7R$ and silt/clay being rigid.

4.4 Relationship of Cluster Statistics to Porosity

Cluster statistics generated in the previous section for all the three scenarios were analyzed and related to the porosity values of the grain packing for 5 and 10 percent of carbonaceous material, considering all grains rigid, all grains ductile with rigid radius ratios of 0.9, 0.8 and 0.7 and only carbonaceous material ductile with rigid ratios of 0.9, 0.8 and 0.7 with target porosity of 70% as shown in plots in Figure 4.38-4.41. A relationship between porosity and number of clusters and porosity and number of spheres in different cluster sizes is observed. Isolated grains and small cluster sizes 2 to 5
decreased with decrease in porosity while large cluster size 5 to 10 and 10 to 50 increased with decrease in porosity for 5 percent and 10 percent of carbonaceous material by bulk volume grain packing of the scenarios discussed in the previous section. A porosity of 0.40 was observed as a critical point for clustering for the packing having 10 percent of carbonaceous for the above scenarios which corresponded to 50% of compaction.

Figure 4.38: Relationship between number of clusters and sediment porosity with 5 percent of carbonaceous material in the initial bulk volume for initial sediment porosity of 70%. Values taken from Table 4.1, Table 4.5, Table 4.9, Table 4.13, Table 4.17, Table 4.21, Table 4.25
Figure 4.39: Relationship between number of spheres in cluster size and sediment porosity with 5 percent of carbonaceous material in the initial bulk volume for initial porosity 70%. Values taken from Table 4.2, Table 4.6, Table 4.10, Table 4.14, Table 4.18, Table 4.22, Table 4.26
Figure 4.40: Relationship between number of clusters and sediment porosity with 10 percent of carbonaceous material in the initial bulk volume for initial porosity of 70%. Values taken from Table 4.3, Table 4.7, Table 4.11, Table 4.15, Table 4.19, Table 4.23, Table 4.27
Figure 4.41: Relationship between number of spheres in cluster size and sediment porosity with 10 percent of carbonaceous material in the initial bulk volume for initial porosity of 70%. Values taken from Table 4.4, Table 4.8, Table 4.12, Table 4.16, Table 4.20, Table 4.24, Table 4.28

4.5 Discussion of Clustering Trends

The results discussed in the previous section 4.3 have significant implications for the mudrock system. In the scenario of all the spheres to be rigid (section 4.3.1), for 5 percent of carbonaceous material by bulk volume and for 48 percent compaction, the cluster frequency distribution plot show only 31 big clusters in cluster size 5-10 and 10 to 50 as shown in Figure 4.10. However the number of spheres associated with these classes is 190 which is 20 percent of all the spheres of carbonaceous material as shown
in Figure 4.11. Similarly, for 10 percent of carbonaceous material as shown in Figure 4.13, the number of spheres associated with cluster size 5-10, 10-50 and 50-500 collectively are around 601 which is 60 percent of all the spheres of carbonaceous material.

Ductility of grains plays an important role in the connectivity of organic material in mudrocks which was studied in section 4.3.2 and 4.3.3. For 5 percent of carbonaceous material by bulk volume at last compaction stage, the total number of spheres associated with cluster sizes 5-10 and 10-50 is 361 with ductility of rigid radius ratio 0.9 R, 314 with ductility of rigid radius ratio 0.8R and 478 with ductility of rigid radius ratio 0.7R which is in a range of 30-50 % of the total carbonaceous material. For 10 percent of carbonaceous material by bulk volume at last compaction stage, the number of spheres associated with cluster size 5-10, 10-50 and 50-500 is 889 with ductility of rigid radius ratio 0.9 R, 885 with ductility of rigid radius ratio 0.8R and 936 with ductility of rigid radius ratio 0.7R which is in a range of 80-95 % of the total carbonaceous material.

Thus these results show the significant effect of burial and compaction on clustering of organic material in mudrocks which is important for evaluating the resource quality.
Chapter 5: Conclusions and Future directions

5.1 Conclusions

This study suggests a mechanism whereby small amounts of carbonaceous material can occur not as just isolated grains but as connected clusters of grains within a mudrock. This supports the hypothesis that gas production from mudrock is along the connected paths within the carbonaceous material. The study focuses on the dependence of the statistics of the clusters upon volume fraction of carbonaceous material and degree of compaction. The dependence can be useful for estimating the resource quality.

Volume fraction of carbonaceous material has a significant effect on the clustering statistics. In the model sediment, the number and size of carbonaceous clusters are small, but they increase with increase in volume fraction of carbonaceous material (Figure 3.5-3.8). The grain packing reaches to a maximum number of clusters after which two or more distinct small clusters merge to form a big cluster. This phenomenon happens at 0.20 volume fraction of carbonaceous material which only happens with cooperative rearrangement algorithm which induces clustering. The big cluster continues to grow and eventually all the spheres of the packing touch each other to form one cluster.

Degree of compaction is identified as one more important factor controlling the cluster statistics. The numbers of clusters start increasing in number and size with increase in degree of compaction (c) and at a 50% compaction stage a significantly large cluster is formed which may lead to percolation (Figure 4.1-4.12). However, there is less clustering of spheres if in initial sediment carbonaceous material is forced apart.
Ductility of grains is another important aspect of this study. With the same volume fraction of carbonaceous material, ductility enhances the connectivity of carbonaceous material in mudrocks. The connectivity of carbonaceous material with compaction increases more in scenario of both carbonaceous material and silt/clay ductile than of only carbonaceous material being ductile (Figure 4.13-4.36).

5.2 Future directions

In general a reevaluation of the assumptions is needed in order to gain insight into the clustering mechanism. If after the revision the model succeeds, then it motivates further testing and validation through experiments.

Even if the grain packing of almost same size spheres captures the random spatial arrangements of grains in sediments, they are an oversimplification of grains naturally occurring in sediments. Therefore, these packings are not always representative of a physical system. A next step would be to study the cluster distribution of carbonaceous material with aspect ratios between the sizes of carbonaceous material and silt/clay.

In this study, grains are assumed to be spherical. It would be instructive to study the connectivity of carbonaceous material if these were angular or some random shape. This study may bring out any effect of shape on the connectivity of sediments.

A further extension of the current work can be taking the grain packing forward to commercial simulator for studying the multiphase effect on the gas permeability in mudrocks.
Figure 5.1: Schematic diagram showing the roadmap of taking grain packing forward to commercial simulator for studying multiphase effect on gas phase permeability in mudrocks.
Appendix

CODES

Some of the codes used in this thesis are showed in this appendix. Many of these codes refer to specific data files. Contact the author at email abhishek.kumar@mail.utexas.edu for more information.

Code for compaction with cooperative rearrangement

parameter (MAX =30000)
real array1(MAX,5)
real array(MAX,5),cm(MAX),cv(MAX),newarray(MAX,5)
real compaction, step, grainvolume, porosity, ff, gg
integer counter, iteration, ak, bk, sd, pin(MAX), ii, pinflag(MAX)
logical qq, ww, ee
real xx, yy, zz, mincomp, maxrad
integer p
real rb, rs
write('**') 'Number of Spheres'
read('**') p
write('**') 'Radius of big spheres'
read('**') rb
write('**') 'Radius of small spheres'
read('**') rs
write('**') 'Compaction Step'
step = 0.02
maxrad = 0
ductility = 0.35
open(5, file='new.txt', status='UNKNOWN')
!$$$$$$ reading the input file
do i = 1, p
read(5,*) array1(i,1:5)
if(maxrad.lt.array1(i,5)) maxrad = array1(i,5)
end do
close(5)
open(2, file='results.txt', status='UNKNOWN')
compaction = 1
array = 0
do i = 1,p
array(i,1)=array1(i,1)
array(i,2)= array1(i,2)
array(i,3)=array1(i,3)
array(i,4)=array1(i,4)
array(i,5)=array1(i,5)
enddo

!Compaction loop
    mincomp = (2*maxrad/70)+0.01
    compaction = compaction -step
    if (compaction.lt.mincomp) compaction = mincomp

! Initialization of the array containing spheres
do ii = 1,p
array(ii,2)= array(ii,2)*compaction/(compaction+step)
enddo

!-------------Making of Conjugates------------------------------------------------
array(p+1:MAX,:) =0
call conjugate(p,array,mp,pin,compaction,pinflag)
write(1,*) mp

counter = 1
iteration=0
do while(counter.gt.0 .and. iteration.lt.250)
    iteration = iteration +1
    write(1,*) 'Overlaps', counter
    write(2,*) 'Iteration', iteration
    counter =0
    do  ak= 1,mp
       do bk = 1,mp
          if(ak.ne.bk)then
             d =  ((array(ak,2)- array(bk,2))**2 + (array(ak,3)- array(bk,3))**2+(array(ak,4)-array(bk,4))**2)**0.5
             if( array(ak,5).eq.rb .and. array(bk,5) .eq. rb)then
                overlap = array(ak,5)+array(bk,5)- d
             else
                overlap = array(ak,5)+array(bk,5)- d
             endif
             if (overlap.gt. 0.01) then
                !---------------------------Removal of  overlap----------------------------------------------
            endif
          endif
       enddo
    enddo
    write(1,*) 'Overlaps', counter
    write(2,*) 'Iteration', iteration

117
counter = counter
dx= abs(array(ak,2)- array(bk,2))
dy=abs(array(ak,3)- array(bk,3))
dz= abs(array(ak,4)- array(bk,4))
!-----   X direction -----------------------------
      xx =  overlap*dx/(2*d)
      yy =  overlap*dy/(2*d)
      zz =  overlap*dz/(2*d)
      if (array(ak,2).gt.array(bk,2) )then
            array(ak,2)= array(ak,2) + xx
            array(bk,2)= array(bk,2) - xx
      else
            array(ak,2)= array(ak,2) - xx
            array(bk,2)= array(bk,2) + xx
            xx = -xx
      endif
!------  Y direction-----------------------------
      if (array(ak,3).gt.array(bk,3))then
            array(ak,3)= array(ak,3) + yy
            array(bk,3)= array(bk,3) - yy
      else
            array(ak,3)= array(ak,3) - yy
            array(bk,3)= array(bk,3) + yy
            yy = -yy
      endif
!--------- Z direction-----------------------------------------------------------------------
      if (array(ak,4).gt.array(bk,4))then
            array(ak,4)= array(ak,4) + zz
            array(bk,4)= array(bk,4) - zz
      else
            array(ak,4)=  array(ak,4) - zz
            array(bk,4)= array(bk,4) +  zz
            zz = -zz
      endif
!-------------MOVE CONJUGATES--------------------------------------------------------
      if ( pinflag(ak).eq.1 )   then
            array(pin(ak),2) = array(pin(ak),2)+xx ; array(pin(ak),3)=array(pin(ak),3)+yy
            array(pin(ak),4) = array(pin(ak),4) +zz
      endif
      if ( pinflag(bk).eq.1 )   then
            array(pin(bk),2) = array(pin(bk),2)-xx ; array(pin(bk),3)=array(pin(bk),3)-yy
            array(pin(bk),4) = array(pin(bk),4) -zz
endif

if ( pinflag(ak).eq.2 ) then
  if(ak.le.p) then
    do i = 0,2
       array(pin(ak)+i,2)=array(pin(ak)+i,2)+xx
       array(pin(ak)+i,3)=array(pin(ak)+i,3)+yy
       array(pin(ak)+i,4) = array(pin(ak)+i,4) +zz
    end do
  else
    array(pin(ak),2) = array(pin(ak),2)+xx ; array(pin(ak),3)=array(pin(ak),3)+yy
    array(pin(ak),4) = array(pin(ak),4) +zz
    do i = -2,2
      if( (i.ne.0).and.(pin(ak+i).eq.pin(ak)) ) then
        array(ak+i,2) = array(ak+i,2)+xx ; array(ak+i,3)=array(ak+i,3)+yy
        array(ak+i,4) = array(ak+i,4) +zz
      end if
    end do
  end if
endif

if ( pinflag(bk).eq.2 ) then
  if(bk.le.p) then
    do i = 0,2
       array(pin(bk)+i,2)=array(pin(bk)+i,2)-xx
       array(pin(bk)+i,3)=array(pin(bk)+i,3)-yy
       array(pin(bk)+i,4) = array(pin(bk)+i,4) -zz
    end do
  else
    array(pin(bk),2) = array(pin(bk),2)-xx ; array(pin(bk),3)=array(pin(bk),3)-yy
    array(pin(bk),4) = array(pin(bk),4) -zz
    do i = -2,2
      if( (i.ne.0).and.(pin(bk+i).eq.pin(bk)) ) then
        array(bk+i,2) = array(bk+i,2)-xx ; array(bk+i,3)=array(bk+i,3)-yy
        array(bk+i,4) = array(bk+i,4) -zz
      end if
    end do
  end if
endif

if ( pinflag(ak).eq.3 ) then
  if(ak.le.p) then
    do i = 0,6
       array(pin(ak)+i,2)=array(pin(ak)+i,2)+xx
       array(pin(ak)+i,3)=array(pin(ak)+i,3)+yy
       array(pin(ak)+i,4) = array(pin(ak)+i,4) +zz
    end do
  else
    array(pin(ak),2) = array(pin(ak),2)+xx ; array(pin(ak),3)=array(pin(ak),3)+yy
    array(pin(ak),4) = array(pin(ak),4) +zz
          
  end if
endif

if ( pinflag(bk).eq.3 ) then
  if(bk.le.p) then
    do i = 0,6
       array(pin(bk)+i,2)=array(pin(bk)+i,2)-xx
       array(pin(bk)+i,3)=array(pin(bk)+i,3)-yy
       array(pin(bk)+i,4) = array(pin(bk)+i,4) -zz
    end do
  else
    array(pin(bk),2) = array(pin(bk),2)-xx ; array(pin(bk),3)=array(pin(bk),3)-yy
    array(pin(bk),4) = array(pin(bk),4) -zz
          
  end if
endif
array(pin(ak)+i,4) = array(pin(ak)+i,4) +zz 
end do 
else 
array(pin(ak),2) = array(pin(ak),2)+xx ; array(pin(ak),3)=array(pin(ak),3)+yy 
array(pin(ak),4) = array(pin(ak),4) +zz 
end if 
do i = -6,6 
if( (i.ne.0).and.(pin(ak+i).eq.pin(ak)) ) then 
array(ak+i,2) = array(ak+i,2)+xx ; array(ak+i,3)=array(ak+i,3)+yy 
array(ak+i,4) = array(ak+i,4) +zz 
end if 
end do 
end if 
end if 
if ( pinflag(bk).eq.3 )   then 
if(bk.le.p) then 
do i = 0,6 
array(pin(bk)+i,2)=array(pin(bk)+i,2)-xx 
array(pin(bk)+i,3)=array(pin(bk)+i,3)-yy 
array(pin(bk)+i,4) = array(pin(bk)+i,4) - zz 
end do 
else 
array(pin(bk),2) = array(pin(bk),2)- xx 
array(pin(bk),3)=array(pin(bk),3)- yy 
array(pin(bk),4) = array(pin(bk),4) -zz 
end do 
end if 
end if 
end if 

!-------------Making of Conjugates Again before finding next overlap----------------
newarray =0 

newarray =0 
do ii = 1,p 
qq = (array(ii,2).gt.0).and.(array(ii,2).lt.70*compaction) 
ww = (array(ii,3).gt.0).and.(array(ii,3).lt.70) 
ece = (array(ii,4).gt.0).and.(array(ii,4).lt.70) 
if ( (.not.qq).and(.not.ww).and(.not.ee) ) then 
newarray(ii,1:5) = array(pin(ii),1:5) 
else 

newarray(ii,:) = array(ii,:)
endif
end do
array = newarray
call conjugate(p, array, mp, pin, compaction, pinflag)
endif
endif
end do
end do
write(1,*),'Number of spheres including conjugates', mp
write(2,*), counter
end do

!--------------------------------------------calculation for volume of overlap-------------
if (iteration .lt. 250 .or. counter .lt. mp*0.01) then
write(2,*), 'Compaction Step', compaction
do i = 1,mp
write(2,'(2i8,5F15.4)')pinflag(i), pin(i), array(i,1), array(i,2), array(i,3), array(i,4), array(i,5)
end do
if(compaction.gt.mincomp) go to 77
endif
write(2,*),'Compaction not possible at the stage', compaction
end program

!------------------------------- Subroutine of calculation of Conjugates ----------------
subroutine conjugate(p, array, mp, pin, compaction, pinflag)
real array(30000,5), compaction
integer p, mp, tk, pin(30000), pinflag(30000)
logical aax, aay, aaz, bbx, bby, bbz, check
real xx, yy, zz
pinflag = 0
mp = p
pin = 0
do tk = 1, p
aax = (array(tk,2)-array(tk,5)).lt.0
aay = (array(tk,3)-array(tk,5)).lt.0
aaz = (array(tk,4)-array(tk,5)).lt.0
bbx = (array(tk,2)+array(tk,5)).gt.70*compaction
bby = (array(tk,3)+array(tk,5)).gt.70
bbz = (array(tk,4)+array(tk,5)).gt.70

! Xdirection LHS
if (aax .and. (.not.aay).and.(.not.bby).and.(.not.bbz).and.(.not.aaz) )then
    mp = mp+1
    array(mp,1)= mp
    array(mp,2) = array(tk,2)+ 70*compaction
    array(mp,3) = array(tk,3)
    array(mp,4)=array(tk,4)
    array(mp,5)=array(tk,5)
    pin(tk)= mp
    pin(mp) = tk
    pinflag(tk)=1;pinflag(mp)=1
endif
!
X direction RHS
if (bbx .and.(.not.aay).and.(.not.bby).and.(.not.aaz).and. (.not. bbz) )then
    mp = mp+1
    array(mp,1) = mp
    array(mp,2) = array(tk,2)- 70*compaction
    array(mp,3) = array(tk,3)
    array(mp,4)=array(tk,4)
    array(mp,5)=array(tk,5)
    pin(tk)=mp
    pin(mp) =tk
    pinflag(tk)=1;pinflag(mp)=1
endif
!
Y direction LHS
if (aay  .and. (.not.aax) .and.(.not.bbx).and.(.not.bbz).and. (.not.aaz) )then
    mp = mp+1
    array(mp,1)= mp
    array(mp,2) = array(tk,2)
    array(mp,3) = array(tk,3)+ 70
    array(mp,4)=array(tk,4)
    array(mp,5)=array(tk,5)
    pin(tk)=mp
    pin(mp) =tk
    pinflag(tk)=1;pinflag(mp)=1
endif
!
Y direction RHS
if (bby  .and. (.not.aax).and.(.not.bbx) .and.(.not.aaz).and.(.not. bbz))then
    mp = mp+1
    array(mp,1)= mp
    array(mp,2) = array(tk,2)
    array(mp,3) = array(tk,3)- 70
    array(mp,4)=array(tk,4)
    array(mp,5)=array(tk,5)

pin(tk)= mp
pin(mp)=tk
pinflag(tk)=1;pinflag(mp)=1
endif

! Z direction LHS
    if (aaz .and. (.not.aax) .and.(.not.bbx).and. (.not.bby).and. (.not.aay) )then
        mp = mp+1
        array(mp,1) = mp
        array(mp,2) = array(tk,2)
        array(mp,3) = array(tk,3)
        array(mp,4)=array(tk,4)+ 70
        array(mp,5)=array(tk,5)
        pin(tk)=mp
        pin(mp)=tk
        pinflag(tk)=1;pinflag(mp)=1
    endif

! Z direction RHS
    if (bbz  .and. (.not.bbx) .and. (.not.aax).and. (.not.aay).and.(.not. bby) )then
        mp = mp+1
        array(mp,1)= mp
        array(mp,2) = array(tk,2)
        array(mp,3) = array(tk,3)
        array(mp,4)=array(tk,4)- 70
        array(mp,5)=array(tk,5)
        pin(tk)=mp
        pin(mp)=tk
        pinflag(tk)=1;pinflag(mp)=1
    endif

!-------------------------MAKING CONJUGATES FOR EDGES-----------------------
    ! X direction edge1
    if (aax  .and. aay .and.(.not.bbz).and. (.not.aaz) )then
        mp = mp+1
        array(mp,:)= array(tk,:); array(mp,1) = mp
        array(mp,2) = array(mp,2)+ 70*compaction ;array(mp,3) = array(mp,3)+70
        pin(tk)=mp; pin(mp) = tk
        pinflag(tk) = 2;pinflag(mp)=2
        mp = mp +1
        array(mp,:) = array(tk,)
        array(mp,1) = mp; array(mp,2) = array(mp,2)+ 70*compaction
        pin(mp) = tk ; pinflag(mp)=2
        mp = mp +1

123
array(mp,:) = array(tk,:); array(mp,1) = mp; array(mp,3) = array(mp,3)+70
pin(mp) = tk
pinflag(mp) = 2
endif

! X direction edge2
if (aax .and. (.not.bby).and. (.not.aay).and. aaz) then
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp
  array(mp,2) = array(tk,2) + 70*compaction ; array(mp,4) = array(tk,4) + 70
  pin(tk) = mp ; pin(mp) = tk; pinflag(tk) = 2; pinflag(mp) = 2
  mp = mp+1
  array(mp,:) = array(tk,:)
  array(mp,1) = mp; array(mp,2) = array(mp,2) + 70*compaction
  pin(mp) = tk ; pinflag(mp) = 2
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp; array(mp,4) = array(mp,4) + 70
  pin(mp) = tk ; pinflag(mp) = 2
endif

! X direction edge3
if (aax .and. bby .and. (.not.bbz).and. (.not.aaz)) then
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp
  array(mp,2) = array(tk,2) + 70*compaction ; array(mp,3) = array(mp,3) - 70
  pin(tk) = mp ; pin(mp) = tk; pinflag(tk) = 2; pinflag(mp) = 2
  mp = mp+1
  array(mp,:) = array(tk,:)
  array(mp,1) = mp; array(mp,2) = array(mp,2) + 70*compaction
  pin(mp) = tk ; pinflag(mp) = 2
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp; array(mp,3) = array(mp,3) - 70
  pin(mp) = tk ; pinflag(mp) = 2
endif

! X direction edge4
if (aax .and. (.not.bby).and. (.not.aay).and. bbz) then
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp
  array(mp,2) = array(tk,2) + 70*compaction; array(mp,4) = array(mp,4) - 70
  pin(tk) = mp ; pin(mp) = tk; pinflag(tk) = 2; pinflag(mp) = 2
  mp = mp+1
  array(mp,:) = array(tk,:)
  array(mp,1) = mp; array(mp,2) = array(mp,2) + 70*compaction
  pin(mp) = tk ; pinflag(mp) = 2
  mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp; array(mp,4)=array(mp,4)-70
pin(mp) = tk ; pinflag(mp)=2
endif

! X direction edge5
    if (bbx .and. aay .and.(.not.bbz).and.(.not.aaz))then
        mp = mp+1
        array(mp,:) = array(tk,:); array(mp,1) = mp
        array(mp,2) = array(tk,2)- 70*compaction ; array(mp,3) = array(tk,3)+70
        pin(tk)= mp ;pin(mp) = tk; pinflag(tk) = 2;pinflag(mp)=2
        mp = mp+1
        array(mp,:) = array(tk,)
        array(mp,1) = mp
        array(mp,2) = array(tk,2)- 70*compaction
        pin(mp) = tk ; pinflag(mp)=2
        mp = mp+1
        array(mp,:) = array(tk,);
        array(mp,1) = mp; array(mp,3) = array(tk,3)+70
        pin(mp) = tk ; pinflag(mp)=2
    endif

! X direction edge6
    if (bbx .and. (.not.aay) .and.(.not.bby).and. aaz)then
        mp = mp+1
        array(mp,:) = array(tk,);
        array(mp,1) = mp
        array(mp,2) = array(tk,2)- 70*compaction ;array(mp,4)=array(tk,4)+70
        pin(tk)= mp ;pin(mp) = tk; pinflag(tk) = 2;pinflag(mp)=2
        mp = mp+1
        array(mp,:) = array(tk,)
        array(mp,1) = mp
        array(mp,2) = array(tk,2)- 70*compaction
        pin(mp) = tk
        pinflag(mp)=2
        mp = mp+1
        array(mp,:) = array(tk,);
        array(mp,1) = mp; array(mp,4)=array(tk,4)+70
        pin(mp) = tk ; pinflag(mp)=2
    endif

! X direction edge 7
    if (bbx .and. bby .and. (.not.bb).and. (.not.aaz) ) then
        mp = mp+1
        array(mp,:) = array(tk,)
        array(mp,1) = mp
        array(mp,2) = array(tk,2)- 70*compaction
        array(mp,3) = array(tk,3)-70
        pin(tk)= mp ;pin(mp) = tk; pinflag(tk) = 2;pinflag(mp)=2
    endif

125
mp = mp+1
array(mp,:) = array(tk,:)
array(mp,1) = mp;array(mp,2) = array(tk,2) - 70*compaction
pin(mp) = tk ; pinflag(mp)=2
mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,3) = array(tk,3) - 70
pin(mp) = tk ; pinflag(mp)=2
endif
! X direction edge8
if (bbx .and. (.not.aay) .and. (.not.bby).and. bbz)then
  " 
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp
  array(mp,2) = array(tk,2) - 70*compaction ; array(mp,4)=array(tk,4)-70
  pin(tk)= mp ;pin(mp) = tk; pinflag(tk) = 2;pinflag(mp)=2
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,2) = array(tk,2) - 70*compaction
  pin(mp) = tk ; pinflag(mp)=2
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,4)=array(tk,4)-70
  pin(mp) = tk ; pinflag(mp)=2
  !write(1,*) '14'
endif

! X direction edge9
if ((.not.aax).and.(.not.bbx) .and. aay .and.aaz)then
  " 
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp
  array(mp,3) = array(mp,3) +70; array(mp,4) = array(mp,4)+70
  pin(tk)= mp ;pin(mp) = tk; pinflag(tk) = 2;pinflag(mp)=2
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,3) = array(mp,3) +70
  pin(mp) = tk ; pinflag(mp)=2
  mp = mp+1
  array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,4) = array(mp,4)+70

126
pin(mp) = tk ; pinflag(mp)=2

!write(1,*) '15'
endif

! X direction edge 10
if (not(aax).and.(not.bbx).and.aay .and. bbz)then

mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp
array(mp,3) = array(mp,3) +70; array(mp,4) = array(mp,4)-70
pin(tk)= mp ;pin(mp) = tk; pinflag(tk) = 2;pinflag(mp)=2

mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,3) = array(mp,3) +70
pin(mp) = tk ; pinflag(mp)=2

mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,4) = array(mp,4)-70
pin(mp) = tk ; pinflag(mp)=2
!write(1,*) '16'
endif

! X direction edge 11
if (not(aax).and.(not.bbx).and. bby .and. aaz)then

mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp
array(mp,3) = array(mp,3) -70; array(mp,4) = array(mp,4)+70
pin(tk)= mp ;pin(mp) = tk; pinflag(tk) = 2;pinflag(mp)=2

mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,3) = array(mp,3) -70
pin(mp) = tk ; pinflag(mp)=2

mp = mp+1
array(mp,:) = array(tk,:); array(mp,1) = mp;array(mp,4) = array(mp,4)+70
pin(mp) = tk ; pinflag(mp)=2
!write(1,*) '17'
endif
! X direction edge 12
if (.not.aax).and(.not.bbx) .and. bby.and bbwz)then
    mp = mp+1
    array(mp,:) = array(tk,:); array(mp,1) = mp
    array(mp,:3) = array(mp,:3) -70; array(mp,4) = array(mp,4) -70
    pin(tk)= mp; pin(mp)= tk; pinflag(tk) = 2; pinflag(mp) = 2
    mp = mp+1
    array(mp,:) = array(tk,:); array(mp,1) = mp; array(mp,3) = array(mp,3) -70
    pin(mp) = tk; pinflag(mp) = 2
    !write(1,*) '18'
endif

!--------------------------------MAKING CONGUGATES FOR CORNER SPHERES--------
--------------
if (aax .and. aay .and. aaz) then
    xx = 70*compaction; yy = 70 ; zz = 70
endif

if (aax .and. aay .and. bbwz)then
    xx = 70*compaction; yy = 70 ; zz = -70
endif

if (aax .and. bby .and. aaz)then
    xx = 70*compaction; yy = -70 ; zz = 70
endif

if (aax .and. bby .and. bbwz)then
    xx = 70*compaction; yy = -70 ; zz = -70
endif

if (bbx .and. aay .and. aaz)then
    xx = -70*compaction; yy = 70 ; zz = 70
endif

if (bbx .and. aay .and. bbwz)then
    xx = -70*compaction; yy = 70 ; zz = -70
endif
if (bbx .and. bby .and. aaz) then
    xx = -70*compaction; yy = -70; zz = 70
endif

if (bbx .and. bby .and. bbz) then
    xx = -70*compaction; yy = -70; zz = -70
endif

check = (aax .and. aay .and. aaz).or.(aax .and. aay .and. bbz).or. &
(aax .and. bby .and. aaz).or.(aax .and. bby .and. bbz).or. &
(bbx .and. aay .and. aaz).or.(bbx .and. aay .and. bbz).or. &
(bbx .and. bby .and. aaz).or.(bbx .and. bby .and. bbz)

if (check) then
    mp = mp+1
    array(mp,:) = array(tk,:)
    array(mp,1) = mp
    array(mp,2) = array(mp,2)+xx
    array(mp,3) = array(mp,3)+yy
    array(mp,4) = array(mp,4)+zz
    pin(tk) = mp; pin(mp) = tk
    pinflag(tk) = 3
    pinflag(mp) = 3

    mp = mp+1
    array(mp,:) = array(tk,:); array(mp,1) = mp
    array(mp,2) = array(mp,2)+xx
    array(mp,3) = array(mp,3)
    array(mp,4) = array(mp,4)
    pin(mp) = tk
    pinflag(mp) = 3

    mp = mp+1
    array(mp,:) = array(tk,:); array(mp,1) = mp
    array(mp,2) = array(mp,2)+xx
    array(mp,3) = array(mp,3)+yy
    array(mp,4) = array(mp,4)
    pin(mp) = tk; pinflag(mp) = 3

    mp = mp+1
    array(mp,:) = array(tk,:)
    array(mp,1) = mp
    array(mp,2) = array(mp,2)+xx
array(mp,3) = array(mp,3)
array(mp,4) = array(mp,4) + zz
pin(mp) = tk; pinflag(mp) = 3

mp = mp + 1
array(mp,:) = array(tk,:)
array(mp,1) = mp
array(mp,2) = array(mp,2)
array(mp,3) = array(mp,3) + yy
array(mp,4) = array(mp,4)
pin(mp) = tk; pinflag(mp) = 3

mp = mp + 1
array(mp,:) = array(tk,:)
array(mp,1) = mp
array(mp,2) = array(mp,2)
array(mp,3) = array(mp,3) + yy
array(mp,4) = array(mp,4) + zz
pin(mp) = tk; pinflag(mp) = 3
endif

end do
end
Code for volume conservation “sphregrowth.m”

new;
Vold=0;
disp('Total number of spheres')
P = input('prompt') ;
for i = 1:P
  for j = i+1:P
    x1 = M(i,4);
y1= M(i,5);
z1= M(i,6);
r1 = M(i,7);
    x2 = M(j,4);
y2= M(j,5);
z2= M(j,6);
r2 = M(j,7);
    if r1 >r2
      R=r1;
      r=r2;
    else
      R=r2;
      r=r1;
    end

    d = (( x2-x1)^2+ (y2-y1)^2+ (z2-z1)^2)^0.5;
    if d < R+r+0.1
      a = (( 4*d*R^2 -(d^2-r^2-R^2)^2)^0.5)/(2*d);
      V= 3.14*(R+r-a)^2*(a^2+2*a*r+2*a*R+6*a*R-R^2)/(12*d);
      r1new = (r1^3+(3*V/8*3.14))^0.3333;
      r2new= (r2^3+(3*V/8*3.14))^(0.33);
      %M(i,7)=r1new;
      %M(j,7)=r2new;
      Vold=Vold+V;
    end
  end
end
Vold

for i = 1:P
  rnew = ( M(i,7)^3+(Vold*3)/(P*4*3.14))^0.3333;
  N(i)= rnew;
end
NN= N';
Code for cluster ID for two component packing “connectivity_bidisperssed.m”

```matlab
new;
disp('Number of real spheres')
P = input('prompt') ;
for x = 1: size(M,1)
    ID(x) = 0;
end
tol =0.001*M(1,7);
m = 1;
for i = 1:size(M,1)
    tt(i,1)= M(i,2);
    tt(i,2) = M(i,3);
end
%for i = 1:P
%    M(i,2)=i;
%
for i = 1:size(M,1)
    M(i,3)=i;
end
for i = P+1:size(M,1)
    for j = 1:P
        if( tt(i,1) == tt(j,2))
            disp('abhi')
            M(i,2)=j;
        end
    end
end
for i = 1:P
    M(i,2)= i;
end
for i = 1:size(M,1)
    for j = i+1:size(M,1)
```
if \((M(\text{i},4)-M(\text{j},4))^2+(M(\text{i},5)-M(\text{j},5))^2+(M(\text{i},6)-M(\text{j},6))^2)^{0.5} \leq (M(\text{i},7)+M(\text{j},7)+\text{tol})\)

if \((\text{ID}(\text{i}) == 0) \& \& (\text{ID}(\text{j}) == 0))

    \text{ID}(\text{i}) = \text{m};
    \text{m} = \text{m}+1;

end

if \((\text{ID}(\text{i}) \neq 0) \& \& (\text{ID}(\text{j}) == 0))

    \text{ID}(\text{j}) = \text{ID}(\text{i});

elsif \((\text{ID}(\text{j}) \neq 0) \& \& (\text{ID}(\text{i}) == 0))

    \text{ID}(\text{i}) = \text{ID}(\text{j});

elsif \((\text{ID}(\text{i}) \neq 0) \& \& (\text{ID}(\text{j}) \neq 0))

    \text{count}_\text{merged} = 0;
    \text{merging}_\text{cluster}_\text{id} = \text{ID}(\text{j});
    \text{for} \ k = 1:\text{size}(\text{M},1)

        if \text{ID}(\text{k}) == \text{merging}_\text{cluster}_\text{id}

            \text{ID}(\text{k}) = \text{ID}(\text{i});
            \text{count}_\text{merged} = \text{count}_\text{merged} + 1;

        end

    end

end

end

end
%loop to identify the conjugate sphere and assign it in the group the same ID

for i = P+1:size(M,1)
    if ID(i)==0
        continue
    else
        if ID(i)~=ID(M(i,2))
            if ID(M(i,2))==0
                ID(M(i,2)) = ID(i);
            else
                check = ID(i);
                for j = 1: size(M,1)
                    if ID(j)==check
                        ID(j) = ID(M(i,2));
                    else
                        continue
                    end
                end
            end
        else
            continue
        end
    end
end
else
    continue
end
end

for i = 1:P
    final(i,1) = ID(i);
    final(i,2) = M(i,1);
    final(i,3) = M(i,2);
    final(i,4) = M(i,3);
    final(i,5) = M(i,4);
    final(i,6) = M(i,5);
    final(i,7) = M(i,6);
    final(i,8) = M(i,7);
end
for i = 1:size(M,1)
    finalt(i,1) = ID(i);
    finalt(i,2) = M(i,1);
    finalt(i,3) = M(i,2);
    finalt(i,4) = M(i,3);
    finalt(i,5) = M(i,4);
    finalt(i,6) = M(i,5);
    finalt(i,7) = M(i,6);
    finalt(i,8) = M(i,7);
end
AK = unique(final(:,1));
kk = transpose(ID);
Code for geometrical transformation of cluster length “think4rev.m”

new;

P = size(M,1);

r = M(1,5);

tol = 0.001*M(1,5);

for i = 1: P

%the first 9

x(i) = M(i,2) - 70;
y(i) = M(i,3) - 70;
z(i) = M(i,4) - 70;

x(i+P) = M(i,2) - 70;
y(i+P) = M(i,3) - 70;
z(i+P) = M(i,4);

x(i+(2*P)) = M(i,2) - 70;
y(i+(2*P)) = M(i,3) - 70;
z(i+(2*P)) = M(i,4) + 70;

x(i+(3*P)) = M(i,2) - 70;
y(i+(3*P)) = M(i,3);
z(i+(3*P)) = M(i,4) - 70;

x(i+(4*P)) = M(i,2) - 70;
y(i+(4*P)) = M(i,3);
z(i+(4*P)) = M(i,4);

x(i+(5*P)) = M(i,2) - 70;
y(i+(5*P)) = M(i,3);
z(i+(5*P)) = M(i,4) + 70;

x(i+(6*P)) = M(i,2) - 70;
y(i+(6*P)) = M(i,3) + 70;
z(i+(6*P)) = M(i,4) - 70;

x(i+(7*P)) = M(i,2) - 70;
y(i+(7*P)) = M(i,3) + 70;
\begin{verbatim}
z(i+(7*P)) = M(i,4);

x(i+(8*P)) = M(i,2) - 70;
y(i+(8*P)) = M(i,3) + 70;
z(i+(8*P)) = M(i,4) + 70;

%%%The second 9

x(i+(9*P)) = M(i,2);
y(i+(9*P)) = M(i,3) - 70;
z(i+(9*P)) = M(i,4) - 70;

x(i+(10*P)) = M(i,2);
y(i+(10*P)) = M(i,3) - 70;
z(i+(10*P)) = M(i,4);

x(i+(11*P)) = M(i,2);
y(i+(11*P)) = M(i,3) - 70;
z(i+(11*P)) = M(i,4) + 70;

x(i+(12*P)) = M(i,2);
y(i+(12*P)) = M(i,3);
z(i+(12*P)) = M(i,4) - 70;

x(i+(13*P)) = M(i,2);
y(i+(13*P)) = M(i,3);
z(i+(13*P)) = M(i,4);

x(i+(14*P)) = M(i,2);
y(i+(14*P)) = M(i,3);
z(i+(14*P)) = M(i,4) + 70;

x(i+(15*P)) = M(i,2);
y(i+(15*P)) = M(i,3) + 70;
z(i+(15*P)) = M(i,4) - 70;

x(i+(16*P)) = M(i,2);
y(i+(16*P)) = M(i,3) + 70;
z(i+(16*P)) = M(i,4);

x(i+(17*P)) = M(i,2);
y(i+(17*P)) = M(i,3) + 70;
z(i+(17*P)) = M(i,4) + 70;
\end{verbatim}
\[ x(i+(18*P))=M(i,2)+70; \]
\[ y(i+(18*P))=M(i,3)-70; \]
\[ z(i+(18*P))=M(i,4)-70; \]

\[ x(i+(19*P))=M(i,2)+70; \]
\[ y(i+(19*P))=M(i,3)-70; \]
\[ z(i+(19*P))=M(i,4); \]

\[ x(i+(20*P))=M(i,2)+70; \]
\[ y(i+(20*P))=M(i,3)-70; \]
\[ z(i+(20*P))=M(i,4)+70; \]

\[ x(i+(21*P))=M(i,2)+70; \]
\[ y(i+(21*P))=M(i,3); \]
\[ z(i+(21*P))=M(i,4)-70; \]

\[ x(i+(22*P))=M(i,2)+70; \]
\[ y(i+(22*P))=M(i,3); \]
\[ z(i+(22*P))=M(i,4); \]

\[ x(i+(23*P))=M(i,2)+70; \]
\[ y(i+(23*P))=M(i,3); \]
\[ z(i+(23*P))=M(i,4)+70; \]

\[ x(i+(24*P))=M(i,2)+70; \]
\[ y(i+(24*P))=M(i,3)+70; \]
\[ z(i+(24*P))=M(i,4)-70; \]

\[ x(i+(25*P))=M(i,2)+70; \]
\[ y(i+(25*P))=M(i,3)+70; \]
\[ z(i+(25*P))=M(i,4); \]

\[ x(i+(26*P))=M(i,2)+70; \]
\[ y(i+(26*P))=M(i,3)+70; \]
\[ z(i+(26*P))=M(i,4)+70; \]

end

\[ \text{for } i=1:27*P \]
\[ r(i)=M(1,5); \]
end

\[ \text{for } i = 1:27*P \]
\[ \text{if } \text{mod}(i,P)==0 \]
\[ \text{PIN}(i)=P; \]
\[ \text{else} \]
\[ \text{PIN}(i)=\text{mod}(i,P); \]
end
end

for i = 1:27*P
    info(i,1)= i;
    info(i,2)= PIN(i);
    info(i,3)=x(i);
    info(i,4)=y(i);
    info(i,5)=z(i);
    info(i,6)= r(i);
end

for x = 1:27*P
    IDNP(x) = 0;
end

m = 1;

for i = 1:27*P
    for j = i+1:27*P
        if ((info(i,3)-info(j,3))^2+(info(i,4)-info(j,4))^2+(info(i,5)-info(j,5))^2)^0.5<= (2*(r+tol))
            if ((IDNP(i) ==0) & (IDNP(j)==0))
                IDNP(i) = m;
                m = m+1;
            end

            if ((IDNP(i)~=0)&(IDNP(j)==0))
                IDNP(j) = IDNP(i);
            elseif ((IDNP(j)~=0) & (IDNP(i)==0))
                IDNP(i) = IDNP(j);
            elseif ((IDNP(i)~=0) & (IDNP(j)~=0))
                count_merged = 0;
                merging_cluster_id = IDNP(j);

                if ((IDNP(i)~==0)&(IDNP(j)==0))
                    IDNP(j) = IDNP(i);
                elseif ((IDNP(j)~=0) & (IDNP(i)==0))
                    IDNP(i) = IDNP(j);
                elseif ((IDNP(i)~==0) & (IDNP(j)~==0))
                    count_merged = 0;
                    merging_cluster_id = IDNP(j);
                end
            end
        end
    end
end
for k = 1:27*P
    if IDNP(k) == merging_cluster_id
        IDNP(k) = IDNP(i);
        count_merged = count_merged + 1;
    end
end
end
end

end

for i = 1:P
    data(i,1)= info(13*P+i,1);
data(i,2)= info(13*P+i,2);
data(i,3)=info(13*P+i,3);
data(i,4)=info(13*P+i,4);
data(i,5)= info(13*P+i,5);
data(i,6)= IDNP(13*P+i);
end

for i = 1:P
    ID14(i)= IDNP(13*P+i);
end

AB = unique(ID14);
BC = size(unique(ID14));
CD = BC(2);
m1 = 1;

for i = 2:CD
    for j = 1:27*P
        if AB(i) == IDNP(j)
            set(m1,1) = info(j,2);
            set(m1,2)= info(j,3);
            set(m1,3)= info(j,4);
            set(m1,4)= info(j,5);
            set(m1,5)= IDNP(j);
m1 = m1+1;
        else

140
IID = [];  
no = 1;  

    az1 = set(:,5);  
bz1 = unique(az1);  
cz1 = size(bz1);  
dz1 = cz1(1);  

ez1 = size(set);  
fz1 = ez1(1);  

    for i = 1:dz1  
        m = 1;  
        for j = 1:fz1  
            if set(j,5)==bz1(i)  
                Pc(m)= set(j,2);  
                m=m+1;  
            else  
                continue  
            end  
        end  
    end  

    ay= size(Pc);  
    by= ay(1);  
    cy = unique(Pc);  
    dy = size(cy);  
    ey = dy(1);  
    if by ~= ey  
        IID(no)= bz1(i);  
        no = no+1;  
    else  
    end  

end  

at = size(IID);  
btt= at(1);  
ct = size(set);  
dtt = ct(1);  

if IID ~= []  
    for i = 1:bt  
        for j = 1:dt  
            if IID(i)==set(j,5)  
                set(j:2)=[];  
            end  
        end  
    end  
end
KA = size(set);
AK = KA(1);
sset(1,:) = set(1,:);
l=1; check=0;
for i = 2:1:AK
    for k= 1:1:l
        if set(i,1) == sset(k,1)
            check=1;
        end
    end
    if check==0
        l=l+1;
        sset(l,:) = set(i,:);
    end
check=0;
end

az = sset(:,5);
bz = unique(az);
cz = size(bz);
dz = cz(1);
ez = size(sset);
fz = ez(1);

for i = 1:dz
    m = 1;
    for j = 1:fz
        if sset(j,5) == bz(i)
            xc(m) = sset(j,2);
            yc(m) = sset(j,3);
            zc(m) = sset(j,4);
            m = m+1;
        else
            continue
        end
    end
    lc(i,1) = bz(i);
    lc(i,2) = max(xc) - min(xc);
    lc(i,3) = max(yc) - min(yc);
    lc(i,4) = max(zc) - min(zc);
    xc = [];
yc = [];
zc = [];
end

for i = 1:dz
    m = 1;
    for j = 1:fz
        if sset(j,5) == bz(i)
            a_x(m) = sset(j,2);
            a_y(m) = sset(j,3);
            a_z(m) = sset(j,4);
            m = m + 1;
        else
            continue
        end
    end
end

dmax = 0;
for k = 1:m-1
    for j = k+1:m-1
        d = ((a_x(k) - a_x(j))^2 + (a_y(k) - a_y(j))^2 +
             (a_z(k) - a_z(j))^2)^0.5;
        if d > dmax
            dmax = d;
            x1 = a_x(k);
            y1 = a_y(k);
            z1 = a_z(k);
            x2 = a_x(j);
            y2 = a_y(j);
            z2 = a_z(j);
            a_p = x2 - x1;
            b_p = y2 - y1;
            c_p = z2 - z1;
        end
    end
end

for c = 1:m-1
    x_l = a_x(c) - x1;
    y_l = a_y(c) - y1;
\[ z_1 = a_z(c) - z_l; \]
\[ \theta = \text{atan}(a_p/b_p); \]
\[ x_2 = x_1 \cos(\theta) - y_1 \sin(\theta); \]
\[ y_2 = x_1 \sin(\theta) + y_1 \cos(\theta); \]
\[ z_2 = z_1; \]
\[ b_{p2} = a_p \sin(\theta) + b_p \cos(\theta); \]
\[ c_{p2} = c_p; \]
\[ \beta = \text{atan}(b_{p2}/c_{p2}); \]
\[ x_3 = x_2; \]
\[ y_3 = y_2 \cos(\beta) - z_2 \sin(\beta); \]
\[ z_3 = y_2 \sin(\beta) + z_2 \cos(\beta); \]
\[ \text{akx}(c) = x_3; \]
\[ \text{aky}(c) = y_3; \]
\[ \text{akz}(c) = z_3; \]
\[ \text{end} \]
\[ \text{ang}(1) = 0; \]
\[ \text{for } l_j = 2:18 \]
\[ \quad \text{ang}(l_j) = \text{ang}(l_j-1) + 10; \]
\[ \text{end} \]
\[ \text{for } l_k = 1:18 \]
\[ \quad \text{for } k_k = 1:m-1 \]
\[ \quad \quad \text{x}_4(k_k) = \text{akx}(k_k) \cos(\text{ang}(l_k) \cdot \pi() / 180) - \text{aky}(k_k) \sin(\text{ang}(l_k) \cdot \pi() / 180); \]
\[ \quad \quad \text{y}_4(k_k) = \text{akx}(k_k) \sin(\text{ang}(l_k) \cdot \pi() / 180) + \text{aky}(k_k) \cos(\text{ang}(l_k) \cdot \pi() / 180); \]
\[ \quad \quad \text{z}_4(k_k) = \text{akz}(k_k); \]
\[ \text{end} \]
\[ \text{lx}(l_k,i) = \text{max}(x_4) - \text{min}(x_4); \]
\[ \text{ly}(l_k,i) = \text{max}(y_4) - \text{min}(y_4); \]
\[ \text{lz}(l_k,i) = \text{max}(z_4) - \text{min}(z_4); \]
\[ \% \text{disp( lx}(l_k)); \]
end

lx_mx(i) = max(lx(:,i));
lx_mn(i) = min(lx(:,i));
ly_mx(i) = max(ly(:,i));
ly_mn(i) = min(ly(:,i));
lz_mx(i) = dmax;
lz_mn(i) = dmax;

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%% lz=[];
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aky=[];
akz=[];
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end

lengthxmax = transpose(lx_mx);
lengthxmin = transpose(lx_mn);
lengthymax = transpose(ly_mx);
lengthymin = transpose(ly_mn);
lengthzmax = transpose(lz_mx);
lengthzmin = transpose(lz_mn);
Example 1

**ALL GRAINS ARE RIGID – ONE COMPONENT SPHERE PACKING**

Example One component packing 100 spheres, initial solid volume fraction 0.10

Step-1

Input as 'new.txt' in the format

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Step-2
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Step-3
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</tbody>
</table>
and last stage at which compaction failed will be displayed in the end

Compaction not possible at the stage 0.160000

Step-4

Output file
1st column:
0 - Sphere is inside the domain
1 - Sphere is coming out of a face and will have one image
2 - Sphere is coming out of an edge and will have three images
3 - Sphere is coming out of corner and will have seven images

2nd column:
If the number is greater than number of spheres here 100 it means its a real sphere
information and this sphere have image.
zero means that the sphere is inside the box and have no image
All the image information can be found out by tracking this number in the third column

3rd column:
Serial number of spheres, all the real sphere's information will be displayed for values
from 1 to 100 in this column and rest of them corresponds to their images.

4th, 5th, 6th and 7th column:
x coordinate, y coordinate, z-coordinate and sphere radius

Step-5
Now take the data from the desired compaction stage and use "connectivity.m" for
monodispersed and "connectivity_bidispersed.m" for bidispersed packing.
For bidispersed packing, extract the information of the desired component and count the
real spheres in that component before using it.
Step-6
Enter number of spheres 100
Variable AK will give unique cluster ID
Variable kk will give the cluster ID of all the spheres
Prepare histogram of cluster frequency vs. cluster size
Example 2

**ALL GRAINS ARE DUCTILE - TWO COMPONENT SPHERE PACKING**

Example Two component packing 300 spheres, initial porosity 70%, 109 spheres are carbonaceous, ductility is 0.8R rigid radius

Step-1

input as 'new.txt' in the format

```
1  38.614   65.3685  16.5275  4.38567
2  23.9096  33.1537  46.3459  4.38567
3  39.7042  36.9746  41.5909  4.34225
4  3.84725  68.6688  28.1609  4.34225
5  25.1577  47.779  0.95618  4.38567
6  40.1337  16.9463  60.5663  4.34225
7  5.12384  1.69274  60.6869  4.34225
```

Step-2

Enter number of spheres 300
Enter compaction step 0.02
Enter ductility 0.2
At compaction 0.38

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<tr>
<td>1 308</td>
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</table>

Compaction not possible at the stage 0.360000

Step-4

Repeat step-4 of the above example

For compaction stage of 0.5 you will get:

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<tr>
<td>2 305</td>
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<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1 284 455.0000 | 38.9679  | 39.3175  | 8.1109   | 4.3857   |
Step-5

Use the "spheregrowth.m" for the volume conservation and with the new radius of the carbonaceous spheres proceed ahead. The grain volume lost is distributed evenly on every sphere.

Variable NN gives you the new radius

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Step-6

Use "connectivity_bidispersed.m" and enter the number of real spheres as 109.

Variable AK will give unique cluster ID

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Step-6

Use "connectivity_bidispersed.m" and enter the number of real spheres as 109.

Variable AK will give unique cluster ID

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</table>
Variable kk will give cluster ID of all the spheres

23
12
12
4
12
20
12
0
12
4

Step-7

Prepare histogram for cluster frequency

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Example 3

ONLY CARBONACEOUS GRAINS ARE DUCTILE- TWO COMPONENT SPHERE PACKING

Example Two component packing of 5 percent carbonaceous material 600 spheres, initial porosity 70%, 114 spheres are carbonaceous, and ductility is 0.9 R rigid radius for carbonaceous material

Step-1

Input as 'new.txt' in the format

```
1 43.3756 42.0647 5.64082 3.44644
2 9.45584 12.0812 44.73 3.44644
3 13.2906 67.8776 48.9911 3.44644
4 52.7517 16.8941 1.04113 3.44644
```

Step-2
Enter number of spheres 600
Enter compaction step 0.02
Enter ductility 0.1
Enter radius of big sphere 3.48091 (carbonaceous material)
Enter radius of small sphere 3.44644
Step-3
For compaction stage 0.54, Take the data to "ductilenonductile.m" for volume conservation and proceed ahead

Compaction Step 0.540000

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Step-4
Use the "ductilenonductile.m" for the volume conservation and with the new radius of the carbonaceous spheres proceed ahead. The grain volume lost is distributed within carbonaceous material.
Variable NN gives you the new radius.

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Step-5

Prepare histogram for cluster frequency

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Bibliography


Thane, C., Geometry and topology of model sediments and their influence in sediment properties, M.S. Thesis, The University of Texas at Austin, USA, 2006.
