Random close packing (RCP) of equal spheres: structure and implications for use as a model porous medium

Thesis

How to cite:

For guidance on citations see FAQs.

© 1989 The Author

https://creativecommons.org/licenses/by-nc-nd/4.0/

Version: Version of Record

Link(s) to article on publisher’s website:
http://dx.doi.org/doi:10.21954/ou.ro.0000dfc0

Copyright and Moral Rights for the articles on this site are retained by the individual authors and/or other copyright owners. For more information on Open Research Online’s data policy on reuse of materials please consult the policies page.

oro.open.ac.uk
RANDOM CLOSE PACKING (RCP) OF EQUAL SPHERES:
STRUCTURE AND IMPLICATIONS FOR USE AS A MODEL
POROUS MEDIUM

A thesis presented for the degree of
Doctor of Philosophy

By

David W Mellor
(B.Sc. (Hons) University of Manchester)
(M.Sc. University of Liverpool)

Department of Earth Sciences
The Open University
Walton Hall
Milton Keynes

July 1989
Volume II
ABSTRACT

The structure of the Finney Random Close Packing (RCP) of equal spheres has been analysed, together with the influence which such structure exerts over the capillary pressure characteristics of geometrically similar sphere packings.

The analysis is centred on the simplicial, or Delaunay cell, which is an irregular tetrahedron with apices defined by four immediate neighbour sphere-centres. In terms of using RCP as a model porous medium, an individual simplicial cell is equivalent to an individual pore. A number of measured pore-size distribution parameters are presented for the Finney packing, from which it is shown from first principles that drainage-imbibition hysteresis is not an intrinsic property of the individual pore.

The nature and degree of randomness which characterises the Finney packing is evaluated on two levels. First, by classifying edgelengths as either short or long, seven mutually exclusive cell classes are defined. Using the binomial theorem it is shown that cells (pores) are not random on the level of the individual cell. There are less of the extreme cells (with 6 long edges, or with 6 short edges) and more of the bland cells (with 3 short and 3 long edges) in the Finney packing than predicted on the basis of simple random expectations. Second, the distribution of cell classes within the packing is shown to be essentially homogeneously random. Evidence for extremely slight cell class clustering is found.

The drainage and imbibition processes within the packing are simulated using pore-level algorithms. The algorithms utilise both the Haines' insphere approximation and the MS-P approximation for critical drainage meniscus curvature, and the cell cavity insphere radius approximation for critical imbibition meniscus curvature. Good agreement with experimental data is obtained, and the results confirm that drainage-imbibition hysteresis is a direct consequence of the connectivity between cells (pores), and is not an intrinsic property of the individual pore. Finally, the drainage and imbibition algorithms are adapted to emulate percolation theory models. The results prove that the classical bond problem of percolation theory does not adequately describe the drainage process for RCP, and that the classical site problem does not adequately describe the imbibition process for RCP.
CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>i</td>
</tr>
<tr>
<td>LIST OF CONTENTS</td>
<td>ii</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>viii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>xxi</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>xxv</td>
</tr>
<tr>
<td><strong>VOLUME I</strong></td>
<td></td>
</tr>
<tr>
<td>CHAPTER 1: INTRODUCTION TO RANDOM CLOSE PACKING (RCP)</td>
<td></td>
</tr>
<tr>
<td>1.1 Context of the present work</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Sphere packings</td>
<td>4</td>
</tr>
<tr>
<td>1.2.1 Interdisciplinary nature of sphere packs</td>
<td>5</td>
</tr>
<tr>
<td>1.2.2 Interpretations of RCP structure</td>
<td>17</td>
</tr>
<tr>
<td>1.2.3 Physical realisations of RCP structure</td>
<td>24</td>
</tr>
<tr>
<td>1.2.4 Computer realisations of RCP structure</td>
<td>31</td>
</tr>
<tr>
<td>1.3 Objectives, approach and synopsis</td>
<td>42</td>
</tr>
<tr>
<td>CHAPTER 2: RCP SPACE DISCRETISATION</td>
<td></td>
</tr>
<tr>
<td>2.1 General considerations: Voronoi Tessellation</td>
<td>45</td>
</tr>
<tr>
<td>2.2 General considerations: Simplicial Tessellation</td>
<td>56</td>
</tr>
<tr>
<td>2.3 Mathematical theories of Voronoi statistics</td>
<td>58</td>
</tr>
<tr>
<td>2.4 Relationship between Voronoi and simplicial cells</td>
<td>60</td>
</tr>
<tr>
<td>2.4.1 Two dimensional space</td>
<td>60</td>
</tr>
<tr>
<td>2.4.2 Three dimensional space</td>
<td>63</td>
</tr>
<tr>
<td>2.5 Pore level considerations</td>
<td>67</td>
</tr>
</tbody>
</table>
2.5.1 Pore shape aspects: general .......................... 68
2.5.2 Pore shape aspects: simplicial cell
specific .............................................. 73
2.6 RCP pore network ........................................ 75
2.7 Summary of RCP space discretisation ....................... 84

CHAPTER 3: SIMPLICIAL CELL ANALYSIS OF THE FINNEY RCP MODEL

3.1 Size and shape of the RCP model ........................... 86
3.2 Analytical procedure ..................................... 90
3.3 Verification of simplicial cell sub-division ............. 93
   3.3.1 Packing density .................................. 93
   3.3.2 Simplicial and Voronoi cell relationship ......... 94
   3.3.3 Voronoi cell statistics .......................... 95
3.4 Experimental error and precision ......................... 98
   3.4.1 Estimation of E_b ................................ 101
   3.4.2 Estimation of G .................................. 105
   3.4.3 Best fit of (G*E_s + G*E_b) with S ................. 105
   3.4.4 Results .......................................... 106
3.5 Simplicial cell frequency distributions .................. 112
   3.5.1 Edgelength frequency .............................. 113
   3.5.2 Cell mean edgelength frequency ................... 116
   3.5.3 Face angle frequency ............................... 116
   3.5.4 Apex solid angle frequency ....................... 116
   3.5.5 Total solid angle frequency ...................... 117
   3.5.6 Cell total volume frequency ..................... 117
   3.5.7 Cell solid volume frequency ..................... 117
   3.5.8 Cell pore volume frequency ...................... 118
CHAPTER 4: RANDOMNESS AT THE SIMPLICIAL CELL LEVEL IN THE FINNEY MODEL

4.1 Introduction to Chapters 4 and 5........................................ 161

4.2 Some terminology and notation........................................... 163
  4.2.1 Descriptive elements.............................................. 164
  4.2.2 Definition of randomness.......................................... 165
  4.2.3 Predictive elements................................................ 166
  4.2.4 Worked example.................................................... 168

4.3 The Control Set.......................................................... 173
  4.3.1 Existence............................................................ 175
  4.3.2 Test for Existence................................................. 177
  4.3.3 Random Number Generation: AS 183................................ 178
  4.3.4 Construction of the Control Set.................................. 181

4.4 Tests of randomness..................................................... 183
| 4.4.1 | The first test | 183 |
| 4.4.2 | The second test | 187 |
| 4.4.3 | The third test | 190 |
| 4.4.4 | Consequences of non-randomness | 193 |
| 4.4.5 | Advantages conferred by non-randomness | 196 |
| 4.5 | Mason's method | 201 |
| 4.6 | Discussion and conclusions | 208 |

**CHAPTER 5: RANDOMNESS AT THE NETWORK LEVEL IN THE FINNEY MODEL**

| 5.1 | Introduction | 210 |
| 5.2 | Fundamental Concepts | 212 |
| 5.2.1 | The network | 213 |
| 5.2.2 | Finite size limitations - surface cells | 215 |
| 5.2.3 | Face Forms | 217 |
| 5.2.4 | Cell-Face Distribution [P] | 218 |
| 5.2.5 | Cell-Cell Distribution [N] | 221 |
| 5.2.6 | Isomerism | 221 |
| 5.3 | Network Data File for the Finney model | 228 |
| 5.3.1 | Construction and Format | 228 |
| 5.3.2 | Error checking and validation | 231 |
| 5.4 | Network Analysis of the Finney model | 233 |
| 5.4.1 | Surface occurring cells | 233 |
| 5.4.2 | Cell-Face Distribution [P] | 235 |
| 5.4.3 | Cell-Cell Distribution [N] | 237 |
| 5.5 | Test for Randomness of the Network Structure | 239 |
| 5.5.1 | Predicting [N] from [P] | 239 |
| 5.5.2 | Fundamental Test | 242 |
| 5.5.3 | Summary | 246 |
5.6 Isomer Distribution of the Finney model................. 248
  5.6.1 Theoretical distribution............................. 248
  5.6.2 Observed distribution................................. 250
  5.6.3 Significance of the observed distribution............. 252

5.7 Discussion: Gotoh and Finney's Most Probable Tetrahedron................................. 254

5.8 Discussion and conclusions of Chapters 4 and 5........... 257

VOLUME II

CHAPTER 6: CAPILLARY PROPERTIES OF THE FINNEY RCP MODEL

6.1 Introduction............................................. 263
  6.1.1 Fluid saturations................................. 263
  6.1.2 Capillary Pressure................................. 264
  6.1.3 Percolation theory................................. 267

6.2 The Drainage Case: General Comments...................... 269
  6.2.1 Which curvature?................................. 269
  6.2.2 Curvature distribution.............................. 271
  6.2.3 The drainage algorithm............................. 273

6.3 The Drainage Case: Haines' approximation............... 282
  6.3.1 Construction of data file.......................... 282
  6.3.2 Volume fraction or number fraction?............... 285
  6.3.3 Sample Size effects............................... 290
  6.3.4 Critical probability for the Bond Problem (1)... 299
  6.3.5 Control of non-randomness on Critical probability for the Bond problem................. 302
  6.3.6 Dis-aggregated drainage........................... 305
  6.3.7 Summary........................................... 305

6.4 The Drainage Case: M-SP Approximation.................... 308
6.4.1 Sample size effects ........................................... 311
6.4.2 Critical probability for the Bond Problem (ii) ........ 312
6.4.3 Summary ....................................................... 314

6.5 The Imbibition Case ............................................. 317
6.5.1 The imbibition algorithm .................................... 320
6.5.2 Sample size effects ......................................... 327
6.5.3 Critical probability for the Site problem ............... 328
6.5.4 Hysteresis .................................................... 330

6.6 Summary and Conclusions ........................................ 336

CHAPTER 7: APPLICATION TO SEDIMENTARY ROCKS

7.1 Aeolian Sandstone .............................................. 343
7.1.1 Particle Size analysis ...................................... 343
7.1.2 Pore Structure ............................................... 344
7.1.3 Capillary pressure characteristics ....................... 347

7.2 Recommendations for Further Research ....................... 353
7.2.1 Polydispersity ............................................... 353
7.2.2 Interpenetration ............................................. 354
7.2.3 Anisotropy .................................................... 354
7.2.4 Departures from sphericity .................................. 356
7.2.5 Decoration .................................................... 356

7.3 Concluding Remarks ............................................. 358

REFERENCES .......................................................... 359
APPENDIX 'A' .......................................................... 372
APPENDIX 'B' .......................................................... 375
| Figure 1.1 | Typical Capillary Pressure Curves | 3 |
| Figure 1.2 | Idealised 2-D element of RCP pore space | 3 |
| Figure 1.3 | Unit cells of the Graton and Fraser study | 8 |
| Figure 1.4 | Unit voids of the Graton and Fraser study | 8 |
| Figure 1.5 | Packing density as a function of co-ordination in simple sphere packings | 10 |
| Figure 1.6 | Packing density as a function of co-ordination in non-simple sphere packings | 10 |
| Figure 1.7 | Idealised 2-D neighbour distributions of the radial distribution function | 21 |
| Figure 1.8 | Voronoi division of 2-D space | 23 |
| Figure 1.9 | Geometrical and physical neighbours from Bernal's plasticene spheres | 24 |
| Figure 1.10 | Co-ordination numbers for packings of lead shot | 26 |
| Figure 1.11 | Co-ordination numbers from Bernal and Mason's paint-coated ball bearings | 26 |
| Figure 1.12 | Radial distribution function for the Scott model | 28 |
| Figure 1.13 | Voronoi statistics for the Scott model | 28 |
| Figure 1.14 | Radial distribution function for Bernal and Scott models | 29 |
| Figure 1.15 | Radial distribution function for the Scott model, enhanced using Mason's correction | 29 |
| Figure 1.16 | Cumulative neighbours for the Scott model | 30 |
| Figure 1.17 | Radial distribution function for the Finney model | 31 |
| Figure 1.18 | Voronoi polyhedron faces per cell for Scott and Finney models | 32 |
Figure 1.19 Voronoi polyhedron edges per face for Scott and Finney models.........................................................32
Figure 1.20 Comparison of Bennet's simulation with the Finney model.................................................................34
Figure 1.21 Comparison of Adams and Matheson's simulation with the Scott model.............................................35
Figure 1.22 Comparison of Matheson model with the Finney model...37
Figure 1.23 Comparison of Matheson model with the Scott model.....37
Figure 1.24 Radial distribution function for the Jodrey and Tory model.................................................................39
Figure 1.25 Comparison of Voronoi cells per face for Clark and Wiley simulation with Finney model......................40
Figure 1.26 Comparison of Voronoi edges per face for Clark and Wiley simulation with Finney model......................40
Figure 1.27 Comparison of Voronoi cell volume for Clark and Wiley simulation with Finney model......................41

CHAPTER 2

Figure 2.1 Forbidden and permitted tessera..............................46
Figure 2.2 Triangular plane tesselllation...............................47
Figure 2.3 Square plane tesselllation..................................47
Figure 2.4 Hexagonal plane tesselllation.............................47
Figure 2.5 The tetrakaidecahedron......................................48
Figure 2.6 Tessellation of the BCC lattice............................49
Figure 2.7 Hexagonal face of the tetrakaidecahedron...............50
Figure 2.8 Square face of the tetrakaidecahedron....................51
Figure 2.9 Winterfeld's expanding disc method........................55
CHAPTER 3

Figure 3.1 Isometric view of the Finney packing .................. 87
Figure 3.2 Sectional view of the Finney packing .................. 87
Figure 3.3 The standard tetrahedron geometry .................. 91
Figure 3.4 Verification of Finney model RCP discretisation
by Voronoi statistics .................................. 97
Figure 3.5 Finney model edgelength frequency, 0.992 to
1.013 sphere diameters ................................ 99
Figure 3.6 Smoothed edgelength frequency distribution ....... 103
Figure 3.7    Comparison of smoothed and unsmoothed
edgelength frequency distribution...................... 103
Figure 3.8    Boxcar models........................................ 104
Figure 3.9    Flow diagram for program VORWARD................. 107
Figure 3.10   Relationship between delta and spike for
boxcar models........................................ 108
Figure 3.11   Relationship between delta and sigma for
boxcar models........................................ 109
Figure 3.12   Convolution series (G*E_b + G*E_s) and the
observed series S........................................ 109
Figure 3.13   Convolution series G*E_s and the observed
series S............................................. 110
Figure 3.14   Convolution series G*E_b and the observed
series S............................................. 110
Figure 3.15   Finney model simplicial cell edgelength
frequency distribution.................................... 125
Figure 3.16   Finney model, detail of figure 3.15.................. 125
Figure 3.17   Finney model, mean cell edgelength frequency........ 126
Figure 3.18   Finney model, face angle frequency.......................... 126
Figure 3.19   Finney model, individual apex solid angle
frequency............................................. 127
Figure 3.20   Finney model, total cell solid angle frequency........ 127
Figure 3.21   Finney model, detail of figure 3.20.................. 128
Figure 3.22   Finney model, total cell volume frequency............. 128
Figure 3.23   Finney model, cell solid volume frequency............. 129
Figure 3.24   Finney model, cell pore volume frequency............. 129
Figure 3.25   Finney model, cell packing density frequency........... 130
Figure 3.26   Finney model, cell porosity frequency................ 130
<p>| Figure 3.27 | Finney model, cavity insphere radius frequency | Page 131 |
| Figure 3.28 | Finney model, total face insphere radius frequency | Page 131 |
| Figure 3.29 | Finney model, largest face insphere radius frequency | Page 132 |
| Figure 3.30 | Finney model, 2nd largest face insphere radius frequency | Page 132 |
| Figure 3.31 | Finney model, 3rd largest face insphere radius frequency | Page 133 |
| Figure 3.32 | Finney model, smallest face insphere radius frequency | Page 133 |
| Figure 3.33 | Finney model, equivalent pore chamber radius frequency | Page 134 |
| Figure 3.34 | Finney model, total equivalent radii of constriction frequency | Page 134 |
| Figure 3.35 | Finney model, largest eq. radius of constriction frequency | Page 135 |
| Figure 3.36 | Finney model, 2nd largest eq. radius of constriction frequency | Page 135 |
| Figure 3.37 | Finney model, 3rd largest eq. radius of constriction frequency | Page 136 |
| Figure 3.38 | Finney model, smallest eq. radius of constriction frequency | Page 136 |
| Figure 3.39 | Finney model, total hydraulic radius frequency | Page 137 |
| Figure 3.40 | Finney model, largest hydraulic radius frequency | Page 137 |
| Figure 3.41 | Finney model, 2nd largest hydraulic radius frequency | Page 138 |
| Figure 3.42 | Finney model, 3rd largest hydraulic radius frequency | Page 138 |</p>
<table>
<thead>
<tr>
<th>Figure Reference</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 3.43</td>
<td>Finney model, smallest hydraulic radius frequency</td>
<td>139</td>
</tr>
<tr>
<td>Figure 3.44</td>
<td>Cavity insphere radius/largest face insphere radius joint frequency distribution</td>
<td>144</td>
</tr>
<tr>
<td>Figure 3.45</td>
<td>Cavity insphere radius/2nd largest face insphere joint frequency distribution</td>
<td>145</td>
</tr>
<tr>
<td>Figure 3.46</td>
<td>Cavity insphere radius/3rd largest face insphere joint frequency distribution</td>
<td>146</td>
</tr>
<tr>
<td>Figure 3.47</td>
<td>Cavity insphere radius/smallest face insphere joint frequency distribution</td>
<td>147</td>
</tr>
<tr>
<td>Figure 3.48</td>
<td>Cavity insphere radius/equivalent pore chamber radius joint frequency distribution</td>
<td>148</td>
</tr>
<tr>
<td>Figure 3.49</td>
<td>Cavity insphere radius/cell pore volume joint frequency distribution</td>
<td>149</td>
</tr>
<tr>
<td>Figure 3.50</td>
<td>Largest face insphere radius/2nd largest face insphere radius joint frequency distribution</td>
<td>150</td>
</tr>
<tr>
<td>Figure 3.51</td>
<td>Largest face insphere radius/3rd largest face insphere radius joint frequency distribution</td>
<td>151</td>
</tr>
<tr>
<td>Figure 3.52</td>
<td>Largest face insphere radius/smallest face insphere radius joint frequency distribution</td>
<td>152</td>
</tr>
<tr>
<td>Figure 3.53</td>
<td>Largest face insphere radius/largest hydraulic radius joint frequency distribution</td>
<td>153</td>
</tr>
<tr>
<td>Figure 3.54</td>
<td>2nd largest face insphere radius/2nd largest hydraulic radius joint frequency distribution</td>
<td>154</td>
</tr>
<tr>
<td>Figure 3.55</td>
<td>3rd largest face insphere radius/3rd largest hydraulic radius joint frequency distribution</td>
<td>155</td>
</tr>
<tr>
<td>Figure 3.56</td>
<td>Smallest face insphere radius/smallest hydraulic radius joint frequency distribution</td>
<td>156</td>
</tr>
</tbody>
</table>
CHAPTER 4

Figure 4.1  Simplicial cells of the BCC lattice .................. 169
Figure 4.2  Relationship between number of simplicial cells
and calculated Chi-square value for simplicial cells of a perfect BCC lattice ....................... 173
Figure 4.3  Theoretical point of collapse from 3-dimensions
for a tetrahedron (case 1) ....................... 176
Figure 4.4  Theoretical point of collapse from 3-dimensions
for a tetrahedron (case 2) ....................... 176
Figure 4.5  Flow diagram for program CONTROL ..................... 182
Figure 4.6  Edgelenth frequency distribution for the control set of simplicial cells ..................... 184
Figure 4.7  Detail of figure 4.6 .................................. 184
Figure 4.8  Flow diagram for first test of randomness .......... 186
Figure 4.9  Chi-square versus fraction of state 'S' edges for the Finney model ..................... 188
Figure 4.10 Chi-square versus number of simplicial cells for the Finney model ..................... 188
Figure 4.11 Cavity insphere radius distribution function for the control set ..................... 194
Figure 4.12 Individual apex solid angle frequency distribution for the control set ..................... 195
Figure 4.13 Full cell solid angle frequency distribution for the control set ..................... 197
Figure 4.14 Detail of figure 4.13 .................................. 197
Figure 4.15 Flow diagram for Mason's method ..................... 203
Figure 4.16 Mason's method, total face insphere radius frequency distribution for $10^6$ cells ..................... 204
Figure 4.17  Mason's method, cavity insphere radius frequency distribution for $10^6$ cells ................. 204

Figure 4.18  Mason's method, largest face insphere radius frequency distribution for $10^6$ cells ................. 204

Figure 4.19  Mason's method, 2nd largest face insphere radius frequency distribution for $10^6$ cells ................. 204

Figure 4.20  Mason's method, 3rd largest face insphere radius frequency distribution for $10^6$ cells ................. 205

Figure 4.21  Mason's method, smallest face insphere radius frequency distribution for $10^6$ cells ................. 205

Figure 4.22  Mason's method, joint probability distribution for largest face insphere and cavity insphere radius ............................................... 205

Figure 4.23  Mason's method, joint probability distribution for 2nd largest face insphere and cavity insphere radius ............................................... 205

Figure 4.24  Mason's method, joint probability distribution for 3rd largest face insphere and cavity insphere radius ............................................... 206

Figure 4.25  Mason's method, joint probability distribution for smallest face insphere and cavity insphere radius ............................................... 206

CHAPTER 5

Figure 5.1  Two dimensional network models ....................... 214

Figure 5.2  Two neighbouring simplicial cells showing a common face ............................................... 216
| Figure 5.3 | The 2LS4 simplicial cell showing alpha and beta isomers | 224 |
| Figure 5.4 | Relationship between simplicial cell isomers and face forms | 225 |
| Figure 5.5 | Flow diagram for measurement of \([P]\) | 236 |
| Figure 5.6 | The Most Probable Tetrahedron of Gotoh and Finney | 256 |
| Figure 5.7 | The most frequently observed tetrahedron in the Finney packing | 258 |

**VOLUME II**

**CHAPTER 6**

| Figure 6.1 | Perfectly rectilinear distribution of 5500 face insphere radii in the range 0.15 to 0.7 | 272 |
| Figure 6.2 | Curvature frequency distribution for figure 6.1 | 272 |
| Figure 6.3 | Flow diagram for program DRAINPACK | 277 |
| Figure 6.4 | Frequency distribution for the 59840 Haines' curvatures of the Finney packing (dis-aggregated set) | 286 |
| Figure 6.5 | Frequency distribution for the 30719 Haines' curvatures of the Finney packing (network set) | 286 |
| Figure 6.6 | Volume Fraction drainage curve using Haines' Curvature Approximation | 288 |
| Figure 6.7 | Number Fraction drainage curve using Haines' Curvature Approximation | 288 |
| Figure 6.8 | Comparison of Number Fraction and Volume fraction drainage curves using Haines' Curvature Approximation | 289 |
| Figure 6.9   | Volume Fraction plotted against Number fraction for equal curvatures. | 289 |
| Figure 6.10 | Theoretical dependence of drainage curve on sample size.             | 294 |
| Figure 6.11 | Haines' approximation number fraction drainage curves for different sample size ratios. | 294 |
| Figure 6.12 | Pore Size Distribution (PSD) curve and curvature frequency distribution using the Haines' approximation. | 295 |
| Figure 6.13 | PSD curve for Sample A (Haines' approximation).                      | 295 |
| Figure 6.14 | PSD curve for Sample B (Haines' approximation).                      | 296 |
| Figure 6.15 | PSD curve for Sample C (Haines' approximation).                      | 296 |
| Figure 6.16 | PSD curve for Sample D (Haines' approximation).                      | 297 |
| Figure 6.17 | PSD curve for Sample E (Haines' approximation).                      | 297 |
| Figure 6.18 | Percolation threshold and sample size using the Haines' approximation. | 298 |
| Figure 6.19 | Relationship between Haines' curvature approximation and probability (cumulative number fraction) for Finney packing. | 298 |
| Figure 6.20 | Haines' approximation number fraction drainage curves by probability for different sample size ratios. | 301 |
| Figure 6.21 | Haines' approximation, effect of randomising bonds on critical curvature for percolation (drainage). | 304 |
| Figure 6.22 | Haines' approximation, effect of randomising bonds on critical probability for percolation (bond problem). | 304 |
Figure 6.23 Haines' approximation drainage curves, including the dis-aggregated case ......................... 306
Figure 6.24 MS-P curvature frequency distribution for the Finney RCP model ......... 309
Figure 6.25 Haines' curvature versus MS-P curvature for the Finney RCP model .......... 309
Figure 6.26 Haines' curvature minus MS-P curvature for the Finney RCP model .......... 310
Figure 6.27 MS-P approximation drainage curves for the Finney RCP model .......... 310
Figure 6.28 MS-P pore-size distribution for the Finney RCP model ................. 313
Figure 6.29 MS-P pore-size distribution for the Finney RCP model - "sample" E .......... 313
Figure 6.30 MS-P approximation, effect of randomising bonds on critical curvature for percolation (drainage) .... 315
Figure 6.31 MS-P approximation, effect of randomising bonds on critical probability for percolation (bond problem) ......................................................... 315
Figure 6.32 Imbibition curvature frequency distribution ............... 318
Figure 6.33 Relationship between imbibition curvature and probability (cumulative number fraction) for Finney packing ......................................................... 318
Figure 6.34 Capillary pressure hysteresis for the 14870 disaggregated cells of the Finney packing, showing effect of zero connectivity. Drainage curve for Haines' approximation, imbibition curve for cavity insphere curvature ................. 321
Figure 6.35  Capillary pressure hysteresis for the 14870
disaggregated cells of the Finney packing,
showing effect of zero connectivity. Drainage
curve for MS-P approximation, imbibition curve
for $C_{lab} = (2/cav)-1.6$ .................................... 321

Figure 6.36  Flow diagram for program IMBIBE.................... 322

Figure 6.37  Dependency of imbibition curve on sample size
ratio (curvature)............................................ 328

Figure 6.38  Dependency of imbibition curve on sample size
ratio (probability)............................................. 329

Figure 6.39  Effect of randomising sites on critical
curvature for percolation (imbibition)................. 331

Figure 6.40  Effect of randomising sites on critical
probability for percolation (site problem)............. 331

Figure 6.41  Capillary pressure hysteresis for approximately
infinite sample size RCP. Drainage curve for
Haines' approximation, imbibition curve for
cavity insphere curvature.................................... 334

Figure 6.42  Capillary pressure hysteresis for approximately
infinite sample size RCP. Drainage curve for
MS-P approximation, imbibition curve for
$C_{lab} = (2/cav)-1.6$ .................................... 335

Figure 6.43  Theoretical capillary pressure hysteresis curves
matched to experimental values......................... 335

CHAPTER 7

Figure 7.1  Particle size distribution for Brigham Bank
aeolian sandstone............................................. 345
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 7.2</td>
<td>Photomicrograph of Brigham Bank sand grains</td>
<td>346</td>
</tr>
<tr>
<td>Figure 7.3</td>
<td>SEM photomicrograph of Brigham Bank sandstone</td>
<td>348</td>
</tr>
<tr>
<td></td>
<td>x 129 magnification, showing occluded pore throat</td>
<td></td>
</tr>
<tr>
<td>Figure 7.4</td>
<td>SEM photomicrograph of Brigham Bank sandstone</td>
<td>348</td>
</tr>
<tr>
<td></td>
<td>x 18 magnification</td>
<td></td>
</tr>
<tr>
<td>Figure 7.5</td>
<td>SEM photomicrograph of Brigham Bank sandstone</td>
<td>349</td>
</tr>
<tr>
<td></td>
<td>x 18 magnification, showing layering</td>
<td></td>
</tr>
<tr>
<td>Figure 7.6</td>
<td>SEM photomicrograph of Brigham Bank sandstone</td>
<td>349</td>
</tr>
<tr>
<td></td>
<td>x 310 magnification, showing grain surface</td>
<td></td>
</tr>
<tr>
<td>Figure 7.7</td>
<td>Mercury injection curve for Brigham Bank sandstone</td>
<td>351</td>
</tr>
<tr>
<td>Figure 7.8</td>
<td>Mercury injection PSD for Brigham Bank sandstone</td>
<td>351</td>
</tr>
<tr>
<td>Figure 7.9</td>
<td>Example of a polydisperse simplicial cell</td>
<td>355</td>
</tr>
<tr>
<td>Figure 7.10</td>
<td>Simplicial cell with interpenetrating spheres</td>
<td>355</td>
</tr>
<tr>
<td>Figure 7.11</td>
<td>Simplicial cell formed by non-spherical, polydisperse particles</td>
<td>357</td>
</tr>
<tr>
<td>Figure 7.12</td>
<td>Simplicial cell formed by non-spherical, polydisperse particles with decoration</td>
<td>357</td>
</tr>
</tbody>
</table>
**LIST OF TABLES**

**VOLUME I**

**CHAPTER 2**

<table>
<thead>
<tr>
<th>Table 2.1</th>
<th>Comparison of theoretical and observed Voronoi statistics</th>
<th>Page 59</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 2.2</td>
<td>Comparison of topological attributes for 2-D Voronoi and simplicial cells</td>
<td>Page 62</td>
</tr>
<tr>
<td>Table 2.3</td>
<td>Comparison of topological attributes for 3-D Voronoi and simplicial cells</td>
<td>Page 67</td>
</tr>
<tr>
<td>Table 2.4</td>
<td>Range of permissible combinations of pore co-ordination and network form</td>
<td>Page 72</td>
</tr>
<tr>
<td>Table 2.5</td>
<td>Dimensionless bond magnitudes and relationship between bonds and circles</td>
<td>Page 80</td>
</tr>
<tr>
<td>Table 2.6</td>
<td>Dimensionless site magnitudes and relationship between sites and circles</td>
<td>Page 81</td>
</tr>
<tr>
<td>Table 2.7</td>
<td>Capillary properties of the 12 circle loose packing</td>
<td>Page 82</td>
</tr>
</tbody>
</table>

**CHAPTER 3**

<table>
<thead>
<tr>
<th>Table 3.1</th>
<th>The standard tetrahedron</th>
<th>Page 92</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 3.2</td>
<td>Packing density fluctuations in the Finney model</td>
<td>Page 94</td>
</tr>
<tr>
<td>Table 3.3</td>
<td>Distribution of Voronoi and ensemble polyhedra for the central 2000 spheres of the Finney model</td>
<td>Page 96</td>
</tr>
<tr>
<td>Table 3.4</td>
<td>Summary of frequency distributions presented in section 3.5</td>
<td>Page 114</td>
</tr>
<tr>
<td>Table 3.5</td>
<td>Cell parameters for unit regular tetrahedron</td>
<td>Page 115</td>
</tr>
</tbody>
</table>
CHAPTER 4

Table 4.1  Description of simplicial cell classes and notation adopted in the present work.............................165
Table 4.2  Expected random frequencies of occurrence of simplicial cell classes............................................167
Table 4.3  Edgelength values for the simplicial cells of the BCC lattice............................................................170
Table 4.4  Expected frequencies of simplicial cells in a random group, compared with observed cells for the BCC lattice............................................................171
Table 4.5  Expected frequencies of random cell types for s = 1 - 0.5..............................................................190
Table 4.6  Comparison of expected and observed simplicial cell frequencies for the Finney model.......................192
Table 4.7  Packing densities of the Finney set and the control set of simplicial cells...........................................198
Table 4.8  Total cell volumes and solid-only cell volumes for the Finney set and the control set of simplicial cells.............................................................200

CHAPTER 5

Table 5.1  Relationship between simplicial cell class and face form..............................................................218
Table 5.2  The cell-face distribution matrix [P].................................................................220
Table 5.3  The cell-cell distribution matrix [N].................................................................222
Table 5.4  Isomeric forms of the 2LS4 simplicial cell........................224
Table 5.5  Observed frequencies of surface occurring simplicial cells in the Finney model.

Table 5.6  Fully observed cell-face joint frequency distribution \([P]\) for the Finney model.

Table 5.7  Fully observed cell-cell joint frequency distribution \([N]\) for the Finney model.

Table 5.8  Prediction of \([N']\) using \([P]\).

Table 5.9  Theoretical random chance relative probabilities of occurrence of isomers of simplicial cells.

Table 5.10  Observed distribution of isomer forms within the Finney packing.

Table 5.11  Comparison of predicted and observed isomer frequencies for the Finney model.

VOLUME II

CHAPTER 6

Table 6.1  Three-step process for draining the \(i\)th simplicial cell using program DRAINPACK.

Table 6.2  Critical probabilities (\(P_{cr}\)) for the bond problem of percolation theory reported by other workers; compiled by Dullien 1979.

Table 6.3  Summary of drainage characteristics for the Finney packing using Haines' and MS-P curvature approximations.

Table 6.4  Curvatures at which percolation thresholds are reached for the Finney packing.

xxiii.
Table 6.5 Curvatures at which percolation thresholds are reached for randomised realisations of the Finney packing..........................337

Table 6.6 Critical probabilities for site and bond problems for the Finney packing..........................338

Table 6.7 Critical probabilities for site and bond problems for randomised realisations of the Finney packing....338

CHAPTER 7

Table 7.1 Sieve results for particle size analysis of Brigham Bank sandstone..........................345
Acknowledgements

This research was funded by BP. It seems to me to be fairly meaningless to express gratitude towards an organisation as vast as BP. Instead I wish to thank Mike Collett for approving my original request, and David Gair for helping to talk him into it. I would also like to thank those people at the BP Research Centre, Sunbury who have shown some interest in my work, and who have offered helpful suggestions. These people include (not in any particular order), Mervyn Grist, Nick Quirke, Jeremy Walton, Peter King, Steve Begg, David Buller, Rick Carter and Steve Bryant. Geoff Bullen performed the particle size analysis reported in Chapter 7, and Gill ter Kuile performed the mercury injection measurements of samples of Brigham Bank sandstone kindly provided by Richard Steele of BP Exploration. This thesis was skilfully deciphered and typed by Billa Davis.

Outside BP, I would like to express my thanks to Professor Geof Brown for his guidance and support. I would also like to thank Professor J L Finney for agreeing to allow me access to the sphere centre co-ordinates of his packing, without which this work could not have been completed. I extend my thanks to Adrian Wright who provided the simplicial cell sub-division of Professor J L Finney's sphere packing. I want to extend my gratitude towards my external supervisor, Geoff Mason, who provided me with not just a high level of intellectual and moral support but also his friendship. Finally, and most importantly, I wish to thank my wife Sue for bearing all this nonsense with rare good humour, and my children for suggesting that the letters Ph.D must stand for "please help Daddy!".
CHAPTER 6: CAPILLARY PROPERTIES OF THE FINNEY RCP MODEL

6.1 Introduction

The purpose of this chapter is to investigate the capillary pressure characteristics of the Finney RCP model and to relate these characteristics to attributes of pore structure described in chapters three, four and five. The view that connectivity between pores dominates capillary behaviour of porous media is frequently encountered in the literature. The conventional tool for examining connectivity issues is percolation theory, which in essence provides a rigorous mathematical analysis of networks. Percolation theory is, however, an abstract theory in that both the real network and the distribution of pore dimensions on that network are always unknown for real materials. In this Chapter, the role of connectivity, and the validity of percolation theory are evaluated for the Finney packing. Before beginning the calculation of capillary properties, it is important to review briefly some of the conventions which are used in this chapter.

6.1.1 Fluid Saturations

All practical experiments involving capillary pressure measurements on real porous media involve the measurement of two quantities - fluid volume and pressure. It is conventional to normalise the volumes of wetting and non-wetting fluid phases, by dividing the absolute volumes of both phases in the sample by the absolute total pore volume of the sample. Changes in fluid volumes are therefore
described in terms of changes in fluid saturation, ranging between 0 and 1. The convention adopted in the present work is that a saturation of 1 refers to the full occupation of the pore space by the wetting phase.

It is important to remember that saturation values are volume fractions. Thus a saturation of 0.5 means that half of the volume of the pore space of the sample is occupied by the wetting phase, whilst the non-wetting phase occupies the remaining volume of the pore space. Alternatively, it may also be useful to think in terms of number-fraction saturations. Here we are only interested in the fractional number of pores occupied by a particular phase. The significance of volume and number fraction saturations is that the former is the only result possible from a real experimental measurement, whilst the latter is the conventional result from certain percolation theory models (the so called "bond-problem" for example, discussed in section 6.1.3). In the present work it is possible to calculate capillary pressure curves in terms of both volume and number fraction saturations, enabling a direct comparison to be made. This has previously not been possible for any real disordered porous medium.

6.1.2 Capillary Pressure

Capillary pressure is conventionally measured experimentally as the difference between the pressures in the wetting and the non-wetting phases at some point of interest in the sample. It is not surprising, therefore, that there is a very wide range of experimental procedures, methods and techniques for measuring
capillary pressure in physical samples. Furthermore, capillary pressure may be quantified in units of millimetres of mercury, pounds per square inch, Pascals and inches of water gauge. Alternative terms for capillary pressure are also widely used in the literature, including capillary pressure head, piezometric head, suction head, matrix suction, negative pressure head, moisture tension and (mercury) injection pressure. In order to overcome the difficulties associated with selection of an "appropriate" system of dimensions for pressure, the present work dispenses with the concept of pressure altogether in favour of a more useful concept - that of (meniscus) curvature.

In the literature the relationship between curvature and capillary pressure is frequently attributed to Laplace (1806), though it is perhaps more appropriate to acknowledge the work of Young (1805) and refer to this relationship as the Laplace-Young equation as suggested by Pujado et al (1972). This well-known equation (neglecting gravity) is:

\[
\sigma \left[ \frac{1}{r_1} + \frac{1}{r_2} \right] = \Delta P
\]

where \( r_1 \) and \( r_2 \) are the principal radii of curvature of the meniscus surface (inner and outer radius of rotation respectively), and \( \sigma \) is the surface tension between the two fluids. The pressure difference between the two fluids is \( \Delta P \).

Introducing the now customary (e.g. Dullien 1979) mean radius of curvature, \( r_m \), defined by:
\[
\frac{1}{r_m} = \frac{1}{2} \left( \frac{1}{r_1} + \frac{1}{r_2} \right)
\]
-6.2-
gives:
\[
\Delta P = \frac{2\sigma}{r_m}
\]
-6.3-
The physical significance of \( r_m \) is that it is the mean radius of curvature of the surface (meniscus) separating two immiscible fluids at a pressure differential of \( \Delta P \). Clearly, capillary pressure is proportional to the reciprocal of meniscus radius. It has become conventional in some of the literature (e.g. Mason 1984) to eliminate the interfacial tension (\( \sigma \)) from further consideration, and to only consider the normalised or dimensionless curvature, \( C \):
\[
C = \frac{2}{(r_m/R)}
\]
-6.4-
where \( R \) is the hard sphere radius. As far as considering capillary pressure phenomena in a monodisperse random sphere packing is concerned, capillary pressure is therefore linearly proportional to the dimensionless value of curvature, \( C \):
\[
i.e. \ \Delta P \propto C
\]
-6.5-
For most of the present chapter, dimensionless curvature is used to represent capillary pressure. This approach has the advantage that the fluid-specific and sphere-size specific aspects of capillarity are eliminated. Experimentalists wishing to compare their results with the drainage or imbibition curves presented in this thesis are able to do so by using the appropriate experimental values of \( R \) and \( \sigma \) in equations 6.4 and 6.5, converting dimensionless curvature to capillary pressure.
6.1.3 Percolation Theory

Percolation theory, developed by mathematical physicists, has been applied on numerous occasions to various aspects of fluid behaviour in porous media. As pointed out by Mason (1984, 1988 (ii)), many of the mathematical analyses of percolation theory available in the literature do not relate directly to porous media. It is essential, therefore, to be completely precise in defining the percolation process of interest, specific to the porous medium of interest. The present work follows the definitions given by Mason (1984). These are reviewed briefly here, and made specific to the simplicial cell structure of the Finney RCP model.

Percolation theory deals with two classic problems - these are known as the site problem and the bond problem. In the present work a site is defined as the three dimensional volume-region (pore body) of the simplicial cell, whilst a bond is defined as the two dimensional, planar constricting-face (pore throat) of the simplicial cell. Each RCP site is therefore connected to four other sites via four bonds (faces). Percolation theory describes a process in which sites (or bonds) are switched at random from one condition to some other condition. These conditions may be "on" or "off", "full" or "empty", "available" or "unavailable" depending on the application. When the probability of a site being "empty" exceeds some critical value, defined as the critical percolation probability ($P_{cr}$), then infinite clusters of "empty" sites appear. Under this condition, for example, the network may begin to "drain" as sites which were previously "full" have direct access to "empty" sites which are infinitely connected. The two key concepts here are
the accessible fraction (the fraction connected to infinite clusters) and the probability of sites (or bonds) being available. These two key concepts can have equivalence of meaning to saturation and curvature (or capillary pressure) respectively, provided a transform between these attributes is defined. Assuming a suitable and appropriate transform is defined, then, we have:

Saturation $[0,1] = \text{Accessible Fraction } [0,1]$ and 
Curvature $[X,Y] = \text{Probability of availability } [0,1]$

- where $X$ and $Y$ are the observed minimum and maximum curvatures respectively.

The exact nature of the transforms from capillary pressure attributes (saturation, curvature) to percolation theory attributes (accessible fraction, probability) depends entirely on how the fluid-process of interest is modelled. In the present work drainage is defined as the classical bond problem, and imbibition is defined as the classical site problem. Pore volume is taken to be associated with the sites, and these two problems are treated here as follows:

DRAINAGE:

(BOND PROBLEM) Accessible Fraction of SITES controlled by probability of available BONDS.

IMBIBITION:

(SITE PROBLEM) Accessible Fraction of SITES controlled by probability of available SITES.
The transforms required by the present work are therefore straightforward. For both the bond problem and the site problem, calculating the saturation as a number fraction requires no transformation at all. The transform for the bond problem requires that the bond-curvatures are converted into bond-probabilities. Similarly, for the site problem, site-curvatures are converted into site-probabilities. Bond problem and site problem accessible fractions (saturations) are therefore directly comparable; bond-probabilities and site probabilities are not directly comparable. This is evident from the overall number of bonds and sites which represent the Finney RCP model:

\[
\text{number of sites} = \text{number of cells} = 14870 \\
\text{number of bonds} = \text{number of common faces} \gg 14870
\]

The exact number of bonds which characterise the Finney RCP model is derived in section 6.3.4.

6.2 The Drainage Case: General Comments

6.2.1 Which Curvature?

Each tetrahedral pore (simplicial cell) in the Finney packing is connected to a neighbouring pore, with which it has one face in common. If we consider one of these pores to be full of wetting liquid, and a neighbouring pore to be empty, then the pore will drain into the neighbour when the (meniscus) curvature exceeds a critical value for the face joining the pore to its neighbour. The
The key question here is - which value may be taken to define that critical curvature? The simplest and most widely used definition of the critical curvature is the face insphere, defined more than sixty years ago by Haines (1927). Figures 3.28 to 3.32 show the frequency distributions for the Haines approximation (face insphere radius) for the Finney packing. The Haines' approximation tends to overpredict experimental measurements of critical curvature by around 10% - 20% (Smith et al (ii), 1987), and is of limited practical value in accurate simulations of capillary processes. However despite its recognised shortcomings (see for example, Hackett and Strettan 1928, Mason and Morrow 1984), the Haines' approximation persists in the literature as the most readily calculated and therefore most useful preliminary estimator of critical curvature. For this reason, the Haines' approximation is adopted in section 6.3 as an initial estimate of critical curvature for the Finney packing.

A variety of other methods of calculating critical meniscus curvature exist in the literature, and many of these are reviewed by Mason and Morrow (1984). Of the methods considered by Mason and Morrow, the techniques developed by Mayer and Stowe (1965) and by Princen (1969(i), 1969(ii) and 1970) were shown to compare well with experimental results obtained by Hackett and Strettan (1928) for pores defined by spheres. Mason and Morrow were able to show that the method of Mayer and Stowe was essentially the same as that developed by Princen, and gave the name MS-P (for Mayer, Stowe-Princen) to the general technique. The MS-P method is currently the most accurate analytical technique for calculating approximate critical (drainage) curvatures for pores formed by spheres. The MS-P method is described more fully in section 6.4.
6.2.2 Curvature Distribution

In chapter 3, the structure of the Finney RCP model was extensively described in terms of insphere or equivalent radii (e.g. face-insphere radius, hydraulic radius, equivalent radius of constriction). However, in considering capillary pressure characteristics we have to deal in linear increments (or decrements) of curvature. Since curvature is twice the reciprocal of radius, it is important to bear in mind the fact that it is not an easy matter to visualise a curvature frequency distribution, given only the equivalent radius frequency distribution. For example, suppose we are given the perfectly rectilinear distribution of 5500 face insphere radii shown in figure 6.1. The corresponding curvature frequency distribution is, as shown in figure 6.2, very distinctly non-rectilinear. The frequency of small curvatures (low capillary pressures) is very much greater than the frequency of large curvatures, since the curvature interval 3.0 to 4.0 encompasses radii between 0.667 and 0.25 (a range in radius of 0.417), whilst the curvature interval 10.0 to 11.0 encompasses radii between 0.2 and 0.182 (a range in radius of only 0.02). The physical significance of this is that, although the face insphere, or MS-P radius frequency distribution may be dominated by small radii (large curvatures), as shown in figure 3.28, the corresponding curvature frequency distribution will probably be dominated by small curvatures (large radii).
Figure 6.1  Perfectly rectilinear distribution of 5500 face insphere radii in the range 0.15 to 0.7.

Figure 6.2  Curvature frequency distribution for figure 6.1.
6.2.3 The drainage algorithm

The drainage algorithm developed in the present work uses two data files as input. These input files are WRINED.DAT, described in chapter 5, and a curvature data file. The curvature data file may be for either the Haines' approximation (discussed in more detail in section 6.3) or the MS-P approximation (section 6.4). In all cases, the construction of the curvature data file must be carefully validated to preserve the exact neighbour relationship defined by WRINED.DAT.

The computer code used to simulate drainage is called DRAINPACK, and is presented in Appendix 'B'. The flow diagram for program DRAINPACK is shown in figure 6.3. Program DRAINPACK is a very robust and simple routine which uses two working arrays: FULL () and CAND (). Array FULL () registers whether or not a simplicial cell is full of wetting fluid (FULL(i) = 1) or empty of wetting fluid (FULL(i) = 0). Cell zero is the outside of the packing, as described in chapter 5, and is set to be empty of wetting fluid (FULL(0) = 0). The second working array, CAND (), registers whether or not a simplicial cell is a candidate for drainage. Thus if a cell is currently full of wetting fluid, but is directly connected to one or more neighbouring cells which are empty, the current cell is defined as a possible candidate for drainage (CAND(i) = 1). A cell which is full, but which is connected to four other neighbouring cells which are also full cannot drain into those neighbouring cells and therefore is not a candidate for possible drainage (CAND(i) = 0). Similarly, a cell which is already empty cannot drain, and is therefore also not a candidate for drainage.
The advantage of tracking candidate cells by means of array CAND() is that the beginning of drainage is marked by only a relatively small fraction of cells which are candidates. Similarly, towards the end of drainage only a few cells remain as candidates. Even during the main part of the drainage process, the vast majority of cells are not candidates for drainage. The CAND() array therefore represents an efficient way of tracking only those cells within the packing which are likely to drain.

The rules for drainage adopted by program DRAINPACK are very simple, and comprise a hierarchy of two:

rule 1 - In order to drain, a cell must be connected to at least one immediate neighbour which is already empty of wetting fluid.

rule 2 - In order to drain into an empty neighbouring cell, the current curvature must exceed the critical curvature (e.g. the Haines' curvature or the MS-P curvature) of the face which connects the cell to its empty neighbour.

Once a cell has drained, it is eliminated from further consideration as a candidate. It may, however, create new candidates in the form of neighbouring cells which can now drain into the drained cell. These new candidate cells must therefore be tested to establish whether or not they in turn are able to drain at the current curvature. Capillary pressure equilibrium is only achieved when no additional, new candidates have been generated by the drainage of cells at the current curvature. Program DRAINPACK therefore does
not attempt to increment the value of the current curvature until such equilibrium is established.

Applying rules 1 and 2 with capillary pressure equilibrium control means that each individual cell in the packing experiences three discrete steps in the process of draining. These three steps are summarised in table 6.1.

<table>
<thead>
<tr>
<th></th>
<th>Step 1</th>
<th>Step 2</th>
<th>Step 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAND(i)</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>FULL(i)</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Note that \( \text{CAND}(i) = 1 \) is prohibited \( \text{FULL}(i) = 0 \)

Table 6.1 : Three-step process for draining the \( i^{th} \) simplicial cell using program DRAINPACK.
No attempt is made in program DRAINPACK to calculate retention of wetting phase by liquid bridges or pendular rings. Although these processes could be simulated in principle, they are totally sphere-dimension and fluid-specific calculations, in contrast to the dimensionless normalised curvature calculations undertaken by DRAINPACK. Similarly, no attempt is made in program DRAINPACK to calculate drainage routes around the edges of simplicial cells as opposed to drainage routes through cell faces. Again, such calculations could be made in principle, although these are also sphere-dimension and fluid-specific calculations. Furthermore, for most practical purposes such corrections to the drainage curve are likely to be minor. Finally, program DRAINPACK makes no attempt to calculate intermediate face-filling volumes. The term face-filling refers to the phenomenon in which a small portion of the non-wetting phase protrudes into a full cell before that cell actively drains. Such face-filling corrections have been shown by Smith et al (1987 (ii)) to be essentially second order corrections to the drainage curve, and are ignored in the present work.
Identify curvature data file (e.g. HAINES or MS-P)

Input curvatures, Pore volumes

Input WRINED.DAT

Initialise

CELL ZERO
CAND (0) = 0
FULL (0) = 0

Initialise working arrays
CAND(i) = 0
FULL (i) = 1

Determine first batch of candidate cells

FOR I = 1 TO 14870

Test for cell zero neighbours (Test if A (1,2) = 3)

YES

Candidate cell identified
CAND (I) = 1

FOR J = 1 TO 200

Current curvature
C = J/10

Next I

Now begin to drain the pack

Figure 6.3: FLOW DIAGRAM FOR SIMULATED DRAINAGE SHOWING INITIALISATION LOGIC
For K = 1 to 14870

Test if CAND (K) = 1

YES

Is NEIGH #1 empty? (Test if FULL (A(K,3)) = 0)

NO

YES

Can meniscus pass face #1? (Test if A(K,4) < C)

NO

YES

Is NEIGH #2 empty? (Test if FULL (A(K,5)) = 0)

NO

YES

Can meniscus pass face #2? (Test if A(K,6) < C)

NO

YES

Is NEIGH #3 empty? (Test if FULL (A(K,7)) = 0)

NO

YES

Can meniscus pass face #3? (Test if A(K,8) < C)

NO

YES

Is NEIGH #4 empty? (Test if FULL (A(K,9)) = 0)

NO

YES

Can meniscus pass face #4? (Test if A(K,10) < C)

NO

Figure 6.3 : FLOW DIAGRAM FOR SIMULATED DRAINAGE SHOWING CELL DRAIN/NON-DRAIN DECISION LOGIC (cont.)
B Cell no. K drains

Increment total no. of drained cells
ND = ND + 1

Increment total drained volume
VD = VD + V(K)

Eliminate cell K as a candidate
CAND (K) = 0

Empty cell K
Full (K) = 0

Allocate new candidate cells from neighbours to cell K

Figure 6.3: FLOW DIAGRAM FOR SIMULATED DRAINAGE (cont.) SHOWING INDIVIDUAL CELL DRAINAGE LOGIC
Figure 6.3: FLOW DIAGRAM FOR SIMULATED DRAINAGE (cont.) SHOWING ALLOCATION OF NEW CANDIDATES LOGIC
Test for curvature/saturation equilibrium:
Test if ND > CPE

NO
Packing in equilibrium
Report data
C = ND + VD
Next J
Stop

YES
Packing not in equilibrium
Reset equilibrium check,
CPE = ND

Figure 6.3: FLOW DIAGRAM FOR SIMULATED DRAINAGE;
(cont.) SHOWING CAPILLARY PRESSURE EQUILIBRIUM LOGIC
6.3 The Drainage Case: Haines' Approximation

In this section simulated drainage of the Finney packing using the Haines' approximation (face insphere) curvature is described.

6.3.1 Construction of the data file

Calculation of the Haines' approximation curvatures for a simplicial cell is straightforward, since the mean radius, $r_m$, is identical to the face insphere radius described in chapter 3. Figure 3.28, for example, is the frequency distribution of all the Haines' mean-radii of curvatures for the Finney packing. Construction of the data file, however, is somewhat less than straightforward, since the exact structure of the network defined by datafile WRINED.DAT (described in chapter 5) must be preserved and honoured. The Haines' curvatures are calculated by program CELLFI (presented in Appendix 'B' to this thesis), which writes the output data file, CELLFI.DAT. In order to write the output file, program CELLFI requires three input data files. These input data files are:

(i) WRINED.DAT - the network structure file,
(ii) NEWFILE3.DAT - the sphere identities of each cell, and
(iii) NEWFILE5.DAT - the spatial co-ordinates of each sphere.

The working principle of program CELLFI is to use WRINED.DAT to register the identities of the four neighbouring simplicial cells to the current cell. The identities of the four spheres defining the
current cell are subsequently checked against those identities of the four defining spheres of each of the four neighbouring cells in turn. By this means, the three spheres defining the face common to the current cell and a neighbouring cell are isolated. By referring to the sphere centre co-ordinates, the three simplicial cell edgelengths forming the face defined by the three common spheres are calculated. The face insphere radius, and subsequently the normalised curvature, are then readily calculated. Each calculated curvature value therefore exactly coincides with the correct cell-face-cell connection demanded by the network structure and sphere co-ordinates.

Although the process to calculate the correct curvatures is perhaps somewhat involved, the validation procedure is a straightforward, two stage process. The most obvious step in validation is to check that the numerical values of curvature are correct. More importantly, it is essential to check that the precise structure of the network defined by WRINED.DAT has been preserved. The former check is easily completed by manual calculations. Confirming that the network structure has been correctly preserved involves checking that the same curvature value is cited by CELLFI.DAT from the i\textsuperscript{th} current cell to a neighbour (j\textsuperscript{th}) cell as from the j\textsuperscript{th} current cell to the neighbour (i\textsuperscript{th}) cell. This test was successfully completed for all 59480 curvature values in CELLFI.DAT by a dedicated checking routine.

The data file CELLFI.DAT contains four curvature values for each of the 14870 simplicial cells in the Finney packing. The frequency distribution for these 59480 Haines' curvatures is shown in figure 283.
6.4. This frequency distribution may be compared directly with that for the 59480 face insphere radii shown in figure 3.28. It is interesting to note that the face insphere radius distribution in figure 3.28 is dominated by the high frequency of small (0.15 to 0.16 sphere radii) face inspheres. The face insphere curvature distribution in figure 6.4, however, is dominated by the high frequency of relatively small (4.8 to 5.0) curvatures, corresponding to face insphere radii in the approximate range 0.4 to 0.42 sphere radii.

The frequency distribution shown in figure 6.4 is essentially that of 14870 dis-aggregated cells. However, we are interested in the distribution of curvatures characteristic of the network, not of the dis-aggregated set of cells. A discrete simplicial cell has four faces, and therefore four curvatures. In the network, each face is shared between two cells, so that there are half the number of faces (and therefore curvatures) in a packing-network than in a dis-aggregated set of cells. The outer surface of the packing complicates this simple calculation, since an "outside cell" has one face which is not shared within the pack. The exact number of curvatures for the 14870 simplicial cells of the Finney network can be derived using the information presented in chapter 5 (section 5.4.1):

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total number of cells</td>
<td>14870</td>
</tr>
<tr>
<td>- Number of &quot;outer cells&quot;</td>
<td>1958</td>
</tr>
<tr>
<td>- Number of &quot;inner cells&quot;</td>
<td>12912</td>
</tr>
</tbody>
</table>

284.
- An "inner cell" has four faces which each contribute $\frac{1}{2}$ a curvature to the network, resulting in a total of 2.0 curvatures per cell.

- An "outer cell" has three faces which each contribute $\frac{1}{2}$ a curvature to the network, together with an external face which contributes 1 curvature to the network, resulting in a total of 2.5 curvatures per cell.

The total frequency of fully shared curvatures (i.e. pore throats, or bonds) for the 14870 cells of the network is therefore:

$$(12912 \times 2) + (1958 \times 2.5) = 30719.$$  

The frequency distribution for these 30719 curvatures was obtained using program FIC, presented in Appendix 'B' to this thesis. Figure 6.5 shows the frequency distribution for the 30719 network curvatures (pore throats, or bonds) to be almost perfectly identical to the frequency distribution for the 59480 dis-aggregated curvatures of figure 6.4. This is a useful result, as it proves that there is no appreciable difference between bond frequency distributions of dis-aggregated cells and bond frequency distributions specific to the network of cells.

### 6.3.2 Volume Fraction or Number Fraction?

Program DRAINPACK was run, using datafile CELLFI.DAT as input, to simulate drainage using the Haines' (face insphere) approximation. The drainage curve is shown conventionally as volume fraction (i.e. saturation) in figure 6.6, and as number fraction in figure 6.7.
Figure 6.4 Frequency distribution for the 59840 Haines' curvatures of the Finney packing (dis-aggregated set).

Figure 6.5 Frequency distribution for the 30719 Haines' curvatures of the Finney packing (network set).
The form of these two curves is very similar indeed, as is evident from figure 6.8 which shows the two curves superimposed, and from figure 6.9 which shows volume fraction plotted against number fraction for identical curvature values. The number fraction is systematically higher than the volume fraction by an almost constant value of about 0.03.

The close correspondence between volume fraction and number fraction is an extremely useful result, especially to percolation theorists who have no physical basis for assigning pore volumes to sites. In a real, physical experiment in which a porous medium is de-saturated (or drained, or mercury-injected), the change in fluid volume resulting from change in capillary pressure is easily measured. Such an experiment will, of course, produce a volume fraction drainage curve. The number of pores drained at each pressure step, however, remains completely unknown, and so it is impossible to generate a number fraction drainage curve by experiment. The present work therefore is important in that it shows that, for the Finney RCP model, the volume fraction and number fraction drainage curves are, for all practical purposes, essentially the same.

For the remainder of this chapter, the use of volume fraction drainage curves is abandoned in favour of the number fraction drainage curve. This makes the transformation from saturation fraction to accessible fraction demanded by percolation theory unnecessary. The physical significance of the Haines' Curvature Approximation drainage curve is discussed in some detail in the following sections.
Figure 6.6  Volume Fraction drainage curve using Haines' Curvature Approximation.

Figure 6.7  Number Fraction drainage curve using Haines' Curvature Approximation.
Figure 6.8  Comparison of Number Fraction and Volume fraction drainage curves using Haines' Curvature Approximation.

Figure 6.9  Volume Fraction plotted against Number fraction for equal curvatures.
Capillary pressure curves depend to some extent on the accessibility of individual pores from the sample surface. In a small sample, the external surface area of the sample is large by comparison with the volume of the sample, resulting in a relatively large proportion of pores having almost immediate access to the sample surface. In a large sample, the majority of pores can be expected to have poor access to the surface, and therefore rely on connectivity between cells for drainage. The drainage curve of a large sample, therefore, is marked by a sharp change in saturation at the critical curvature for drainage (percolation threshold curvature, Cp). The drainage curve of a small sample, in contrast, is dominated by surface effects, and a significant volume of fluid drains at low curvatures before the percolation threshold is reached. This dependency of drainage curve characteristics was examined in a theoretical study by Larson and Morrow (1981). Larson and Morrow considered drainage of idealised samples of uniform width, but variable thickness. Their results are shown in figure 6.10 (using a different definition of curvature to the present work).

The present work affords the opportunity to study the effect of sample size on drainage characteristics, including percolation threshold and pore-size distribution (PSD) effects. As shown in the preceding section, it is perfectly valid to ignore the experimentally conventional volume fraction saturation, and use the number fraction saturation instead. In this event we are no longer concerned with surface area to volume ratios, rather, we are interested in the ratio of the number of pores in total, compared
with the number of access routes (pore throats) to the sample surface. As discussed in the preceding section, the Finney model used in the present work has 14870 cells, and 1958 access routes to the outside of the pack. The sample size number ratio \( S_R \) defined here, therefore is:

\[
S_R = \frac{14870}{1958} = 7.6
\]

- very approximately, therefore, for every pore (simplicial cell) in the Finney packing there is about 1 chance in 8 that that pore has a direct route to the packing surface. Qualitatively, this degree of access to the surface can be seen by examination of figure 3.2, which shows that the portion of the Finney packing used in the present work is roughly around 17 - 18 sphere diameters in diameter. Intuitively, therefore, it seems reasonable that the drainage curve presented in figure 6.7 is severely affected by sample size, and that a larger sample would somehow give a "better" drainage curve. Clearly, the physical size of the Finney packing cannot be arbitrarily increased from 14870 cells. The number of routes to the surface, however, can be cut down from 1958, increasing the sample size ratio, \( S_R \).

Program DRAINPACK was modified to incorporate a user defined instruction to eliminate a number of drainage routes at the pack surface. This effect was achieved by setting the critical curvature of those external cell faces selected to 999 - since all other cells drain at curvatures well below 20, such designated faces cannot subsequently drain to surface. Although the number of surface faces is a user-defined quantity, their actual positions on the pack
surface were selected at random. A total of five drainage curves were produced by this method, with the following characteristics:

"Sample" A : 1958 access faces, $S_R = 7.6$
"Sample" B : 982 access faces, $S_R = 15.1$
"Sample" C : 187 access faces, $S_R = 79.5$
"Sample" D : 22 access faces, $S_R = 675.9$
"Sample" E : 9 access faces, $S_R = 1652.2$

In effect, "Sample" E is more than 200 times larger than "Sample" A, and is equivalent to a packing of around $3.2 \times 10^6$ pores (simplicial cells). The number fraction drainage curves for these five "Samples" is shown in figure 6.11. A comparison of figure 6.10 from Larson and Morrow with figure 6.11 shows excellent qualitative correspondence between the two studies. It is evident that the sample A ($S_R = 7.6$) is roughly equivalent to Larson and Morrow's thinnest samples ($N = 1$ pore thickness and $N = 3$). Sample C ($S_R = 79.5$) is roughly equivalent to Larson and Morrow's intermediate thickness of sample ($N = 100$ pores thick), whilst Sample E ($S_R = 1652.2$) is quite close to the infinitely thick sample of Larson and Morrow.

Whilst it is possible to infer some minimum acceptable sample size from this work, it is perhaps more important to ask a different question - what are the practical consequences of attempting drainage measurements on small samples? The answer to this question is that it depends entirely upon what information one requires from the drainage curve. Perhaps the two most interesting and useful pieces of information abstracted from the drainage curve are the percolation threshold curvature ($C_p$), and the so-called pore-size distribution (PSD) for the sample. Although not apparent from the
literature, there is a simple relationship between $C_p$ and PSD for RCP and RCP-like materials. This relationship is that the "best" estimate of $C_p$ which can be obtained from a drainage curve is the curvature corresponding to the maximum gradient of the drainage curve. The definition of the PSD for the sample is the graph of drainage curve gradient versus curvature. The PSD graph, therefore, is not a distribution of pore sizes at all, but is a measure of the critical curvature (or capillary pressure or pore-throat radius) at which percolation is established within the sample. Figure 6.12 shows the PSD curve for Sample A ($S_R = 7.6$) superimposed on the real curvature distribution for the packing (i.e. figure 6.6). It is clear that the PSD curve is dominated by a prominent peak at a curvature of around 7.3 - 7.5. The PSD curve falls away from the prominent peak, both to lower curvatures, and to higher curvatures, and the overall shape of the PSD curve is roughly symmetrical. The PSD curves for all five "Samples" A to E are shown in figures 6.13 to 6.17. Detailed examination of these figures reveals two important, and related, discoveries:

(i) The position of the prominent peak in the PSD curve is essentially not affected by sample size. The drainage percolation threshold, $C_p$, can therefore be determined fairly accurately and reliably by experiment from samples, more or less independently of sample size. This is also evident from figure 6.18 which shows that the position of $C_p$ can be readily identified from all five Samples A - E.

(ii) Although the PSD curve for small samples does not correspond with the real distribution of sizes of pore throats, the PSD
Figure 6.10  Theoretical dependence of drainage curve on sample size.

Figure 6.11  Haines' approximation number fraction drainage curves for different sample size ratios.
Figure 6.12  Pore Size Distribution (PSD) curve and curvature frequency distribution using the Haines' approximation.

Figure 6.13  PSD curve for Sample A (Haines' approximation).
Figure 6.14  PSD curve for Sample B (Haines’ approximation).

Figure 6.15  PSD curve for Sample C (Haines’ approximation).
Figure 6.16  PSD curve for Sample D (Haines' approximation).

Figure 6.17  PSD curve for Sample E (Haines' approximation).
Figure 6.18 Percolation threshold and sample size using the Haines' approximation.

Figure 6.19 Relationship between Haines' curvature approximation and probability (cumulative number fraction) for Finney packing.

298.
curve does span the full range of pore throat sizes (curvatures) as is evident from figure 6.12. However, in moving to large samples, the PSD curve contains progressively less information about the occurrence of small curvatures (large pore throats). Comparison of figures 6.17 and 6.13 for example shows that there is virtually no information whatsoever regarding curvatures below the Cp value of curvature of around 7.3 for "Sample" E. In general, therefore, an experimentally derived PSD cannot detect the presence of pore throats of radii larger than (i.e. curvatures less than) the throat radius corresponding to the percolation threshold for drainage. In other words, the more the percolation process dominates the drainage of the sample, the less information there is available regarding pore sizes. It is clear from figure 6.6 that, for the Finney packing, this loss of information affects roughly half of all pore throats in the pack. The corollary of this finding is that the only condition under which a drainage curve will yield a true PSD is when only one individual pore is drained. Under this idealised condition the PSD curve is totally correct for one of the pore throats. It is completely meaningless however, to obtain an estimate of Cp under this condition. The significance of the percolation threshold itself is considered in more detail in the next section.

6.3.4 Critical Probability for the Bond Problem (i)

All of the preceding sections have dealt with the drainage curve in terms of curvatures. The percolation threshold for the Finney
packing was shown in section 6.3.3 to be associated with a dimensionless curvature of about 7.3. It is not easy to make direct comparisons of any of the results presented in the preceding chapters with existing percolation theory results unless (bond) curvatures are transformed into (bond) probabilities. The transformation of a given curvature into its equivalent probability is straightforward, and consists of generating an ordered list (array) of 30719 (bond) curvatures in ascending order, and using that list as a simple look-up conversion table. Suppose, for example, that a curvature of 6.25487 occupied element number 12103 in the ordered array. The equivalent probability of a curvature of 6.25487 is simply 12103/30719 = 0.3940. The relationship between curvature and probability (or cumulative number fraction) is shown in figure 6.19 (the integral of the curve in figure 6.5).

Using the look-up conversion table, the Haines' curvatures data file was processed to generate the equivalent Haines' curvature bond probability data file. Program DRAINPACK required a trivial modification to utilise this probability data file, and the drainage cases for "Samples" A to E were re-run. The results are shown in figure 6.20, from which it is evident that the critical probability ($P_{cr}$) for the bond problem of percolation theory, based on the Haines' approximation, is 0.51 ± 0.01. This represents a new and significant result, particularly as the critical probability is so high. Dullien (1979), for example, presented a table of results of critical probabilities for the bond problem obtained by a number of theorists for a variety of network geometries. Of all the results tabulated by Dullien (reproduced in table 6.2), only the hexagonal regular network has a higher critical probability than 0.51 ±
Figure 6.20  Haines' approximation number fraction drainage curves by probability for different sample size ratios.

<table>
<thead>
<tr>
<th>Network Geometry</th>
<th>Coordination Number, Z</th>
<th>$P_{cr}$ Monte Carlo</th>
<th>$P_{cr}$ Series Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hexagonal</td>
<td>3</td>
<td>0.640</td>
<td>0.6527 (exact)</td>
</tr>
<tr>
<td>Square</td>
<td>4</td>
<td>0.493, 0.498</td>
<td>0.5000 (exact)</td>
</tr>
<tr>
<td>Hexatriangular</td>
<td>6</td>
<td>0.341, 0.349</td>
<td>0.3473 (exact)</td>
</tr>
<tr>
<td>Tetrahedral (diamond)</td>
<td>4</td>
<td>0.390</td>
<td>0.388</td>
</tr>
<tr>
<td>Simple cubic</td>
<td>6</td>
<td>0.254</td>
<td>0.257</td>
</tr>
<tr>
<td>Base centred cubic</td>
<td>8</td>
<td>-</td>
<td>0.178</td>
</tr>
<tr>
<td>Face centred cubic</td>
<td>12</td>
<td>0.125</td>
<td>0.119</td>
</tr>
<tr>
<td>Hexagonal close packing</td>
<td>12</td>
<td>0.124</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.2: Critical Probabilities ($P_{cr}$) for the bond problem of percolation theory reported by other workers; compiled by Dullien (1979).
0.01, although the square network result is very close at 0.500. The network which is physically the most similar to the network of simplicial cells used in the present work is the tetrahedral (diamond) network, which from table 6.2 has a value of $P_c$ of 0.39.

There are two possible reasons why the present work generates a value of $P_c = 0.51 \pm 0.01$ when a value of around 0.39 is expected. The first of these is that there is some error in either program DRAINPACK or datafile CELLFI.DAT, or possibly both. The second possible reason is that the distribution of bonds (curvatures) in the Finney model is distinctly non-random, and that the value of $P_c = 0.51 \pm 0.01$ is correct. Both program DRAINPACK and data file CELLFI.DAT have been extremely carefully checked for errors, and the first of these two possible reasons for $P_c = 0.51 \pm 0.01$ can be eliminated. Furthermore, whilst chapter 5 proved that the network for the Finney packing is essentially random, chapter 4 showed that the individual simplicial cells themselves are distinctly non-random. In particular, the distribution of isomers in the Finney packing is such that it is reasonable to expect that the drainage curve is unlikely to be identical to one derived on the basis of a random bond-allocation. The suspicion that individual simplicial cell non-randomness results in the high value of $P_c = 0.51 \pm 0.01$ is therefore very strong indeed. However, the suspicion itself does not constitute proof. The proof needed is provided in the following section.

6.3.5 Control of Non-randomness on Critical Probability

The simplest method for testing whether or not non-randomness
results in the high value of $P_{cr} = 0.51 \pm 0.01$ is to drain a "randomised" version of data file CELLFI.DAT, and measure the resultant value of $P_{cr}$. This randomisation is achieved using program EXP, which is presented in appendix 'B'. Program EXP works by reading the datafile CELLFI.DAT into a working array, C(), together with the network datafile WRINED.DAT into a working array, W(). Using the VAX random number generator, EXP then picks one face of one cell at random, and finds the identity of the unique neighbouring cell which shares that face. This process is repeated a second time, resulting in two pairs of cells being selected at random. Program EXP then exchanges the curvature value shared by the first pair of cells, with that shared by the second pair of cells. This constitutes one complete random "swap". A total of 100,000 such swaps are executed by program EXP. Thus program EXP honours and preserves the total integrity of the network, but randomly allocates bonds (curvatures) to the network, in much the same fashion as a percolation theorist would. Finally, the output data file is also converted to probabilities using the same look-up conversion table described in the preceding section.

The results of draining the "randomised" bonds are presented in figures 6.21 and 6.22. It is evident from figure 6.21 that the percolation threshold from the "randomised" bonds is associated with a curvature of $6.05 \pm 0.05$, as opposed to the $7.3 \pm 0.1$ of the original curvature distribution. This reduction in curvature at the percolation threshold is consistent with a critical probability, $P_{cr}$, of $0.38 \pm 0.01$ - almost exactly consistent with the value of $P_{cr}$ calculated for the tetrahedral (diamond) lattice shown in table 6.2. This result constitutes formal proof that the critical
Figure 6.21  Haines' approximation, effect of randomising bonds on critical curvature for percolation (drainage).

Figure 6.22  Haines' approximation, effect of randomising bonds on critical probability for percolation (bond problem).
probability for bond problem for the Finney packing is strongly controlled by non-randomness at the level of the individual cell, and that the classical bond problem of percolation theory does not yield a satisfactory prediction of the critical probability for drainage for a random sphere packing.

6.3.6 Disaggregated Drainage

For the sake of completeness, it is of interest to calculate the drainage characteristics of the completely dis-aggregated set of 14870 simplicial cells of the Finney packing. The significance of the dis-aggregated drainage curve is simply that there is absolutely no connectivity whatsoever between cells. Each cell drains at its own individual smallest curvature, totally independently of the influence of other cells. The resultant drainage curve is presented in figure 6.23, together with the five drainage curves for "samples" A to E. It is interesting to note the influence of connectivity in these six curves, ranging from zero (disaggregated) to totally dominating (near infinite "Sample" E).

6.3.7 Summary

A number of important issues have been considered in section 6.3, and it is worth reviewing these briefly in order to introduce section 6.4.

Using the Haines' curvature approximation, the effects of connectivity on the drainage capillary pressure curve of the Finney RCP model were evaluated by varying the effective sample size. An
infinitely large sample depends totally on connectivity for its drainage, and the drainage curve for such a sample is characterised by a very sharp onset (percolation threshold) of drainage at some critical curvature value. At curvatures below this threshold no drainage can occur in an infinitely large sample. It is therefore physically impossible for the drainage curve of an infinitely large RCP sample to contain any information about the distribution of pore throats with curvatures less than the (percolation) threshold curvature value (roughly half of all pores in the sample). In contrast to this statement, if the objective is to use the drainage curve to obtain information about RCP pore-sizes
(as in the case of mercury injection for example), then it is necessary to choose small samples so that the surface effects dominate the drainage curve. This last statement completely contradicts the conventional wisdom of mercury-injection porosimetry in which it is deemed that surface-effects are to be avoided at all costs.

Using the Haines' curvature approximation, the critical curvature for percolation is shown to be $7.3 \pm 0.1$, and the critical probability for percolation is shown to be $0.51 \pm 0.01$. By randomising the bond distribution, the critical curvature for percolation falls to $6.05 \pm 0.05$, and the critical probability for percolation falls to that of a tetrahedrally co-ordinated (diamond) lattice, i.e. $0.38 \pm 0.01$. The percolation threshold for the Finney model is therefore shown to be strongly sensitive to non-randomness at the level of the individual cell. The exact nature of this non-randomness was discussed in chapter 4 of this thesis. This result proves that the drainage curve for the Finney RCP model cannot be well predicted by treating RCP pore space as a classical percolation theory bond problem in which the bond probabilities are randomly distributed on the network.

The aim of section 6.4 following is to repeat the work described in section 6.3 using the MS-P method (Mason and Morrow 1984) to calculate more meaningful curvatures than those afforded by the Haines' approximation. A secondary aim of section 6.4 is to compare the MS-P curvature distribution with that of the Haines' curvature distribution for a real sphere packing.
A full description of the MS-P method was presented by Mason and Morrow (1984). In that paper it is shown that the MS-P method, which is exact for calculating meniscus curvatures for rods, gives a good approximation for pores defined by spheres. The validity of the approximation arises from the close correspondence obtained for results from MS-P calculations with experimental results obtained by Hackett and Strettan (1928). The details of the MS-P method will not be given here. The computer code used by Mason and Morrow (1984) was made available to me by Mason (1989). This code was restructured and used in program CELLMSP (presented in appendix 'B') to calculate the output data file, CELLMSP.DAT. This data file is equivalent to CELLFI.DAT described in section 6.3, and contains the MS-P (bond) curvatures for the faces of all 14870 simplicial cells of the Finney packing. The MS-P curvature distribution for the Finney packing is shown in figure 6.24.

The relationship between Haines' curvature and MS-P curvature for the Finney packing is shown in figures 6.25 and 6.26. In general, the Haines' curvature is larger than the MS-P curvature by about 1.5, as noted by Mason and Morrow (1984). The exact significance of the difference between Haines and MS-P curvatures can be better deduced from the curvature at which the drainage percolation threshold arises using the MS-P approximation. This point is discussed in more detail in section 6.4.2.
Figure 6.24  MS-P curvature frequency distribution for the Finney RCP model.

Figure 6.25: HAINES CURVATURE vs MS-P CURVATURE FOR THE 30719 PORE THROATS OF THE FINNEY PACKING

309.
Figure 6.26  Haines’ curvature minus MS-P curvature for the Finney RCP model.

Figure 6.27  MS-P approximation drainage curves for the Finney RCP model.
6.4.1 Sample size effects

Using exactly the same procedure as described in section 6.3, the MS-P curvatures were used to calculate six drainage curves as follows:

Dis-aggregated: No connectivity, \( S_R = 0.25 \)

"Sample" A : 1958 access faces, \( S_R = 7.6 \)
"Sample" B : 982 access faces, \( S_R = 15.1 \)
"Sample" C : 187 access faces, \( S_R = 79.5 \)
"Sample" D : 22 access faces, \( S_R = 675.9 \)
and
"Sample" E : 9 access faces, \( S_R = 1652.2 \)

These six curves are presented in figure 6.27, which can be compared directly with their Haines' curvature counterparts shown in figure 6.23. In general, the MS-P drainage curves are displaced to lower curvatures by comparison with the Haines' approximation drainage curves. This is exactly the result expected, given the fact that the MS-P curvature is smaller by about 1.5 than the equivalent Haines' curvature. The relationship between effective sample size and drainage curve closely follows that already reported in section 6.3 for the Haines' approximation.

Differentiating the drainage curve for "Sample" A gives the so-called pore-size distribution (PSD), which is shown in figure 6.28, superimposed on the real pore size (MS-P curvature) distribution. This figure may be compared directly with that of the Haines' approximation, shown in figure 6.12. Interestingly, there appears to be slightly closer correspondence between the MS-P based PSD and
the true MS-P curvature distribution than exists between the Haines' based PSD and the true Haines' curvature distribution. However, the general conclusion drawn in section 6.3 that drainage curves for large samples contain no information regarding curvatures less than the percolation threshold applies equally well to MS-P curvatures. This is evident from figure 6.29 which shows the MS-P based PSD for "Sample" E (S_R = 1652.2).

6.4.2 Critical Probability for the Bond Problem (ii)

Using the approach developed in section 6.3, the MS-P curvature at which the percolation threshold for drainage is reached was found to be 5.25 ± 0.05. This compares with a value of 7.3 ± 0.1 for the Haines' approximation obtained in section 6.3. The main significance of the difference between Haines' and MS-P curvature approximations, therefore, is in the effect on the percolation threshold curvature. The numerical difference in the percolation threshold of 2.05 ± 0.15 is greater than expected on the basis of the value of 1.5 suggested by Mason and Morrow's (1984) work.

Again, using the approach developed in section 6.3, the MS-P curvatures were randomised by 100,000 bond-pair exchanges. Recalculating the drainage curve gives a value of 4.65 ± 0.05 for the MS-P curvature at which the percolation threshold for drainage occurs in a classical bond problem. This result is shown in figure 6.30. Finally, the critical probability for the bond problem was calculated using MS-P curvatures, and found to be 0.51 ± 0.01, identical to that obtained for the Haines' curvatures. By converting the randomised bonds (curvatures) into probabilities, the
Figure 6.28  MS-P pore-size distribution for the Finney RCP model.

Figure 6.29  MS-P pore-size distribution for the Finney RCP model - "sample" E.
critical probability for percolation for drainage in a random bond model was found to be $0.40 \pm 0.01$, virtually identical to the result obtained using the Haines' approximation in section 6.3. This result is shown in figure 6.31, confirming that percolation theory does not adequately predict the drainage process for the Finney model.

6.4.3 Summary

Using the MS-P curvature approximation given by Mason and Morrow (1984), the general conclusions regarding the effects of sample size on drainage are shown to be comparable to those obtained using the Haines' approximation. The comparison of MS-P curvature and Haines' curvature drainage characteristics are summarised in table 6.3. One extremely useful result arising from this work is that the critical probability for the bond problem is independent of the approximation used for curvature (i.e., Haines' or MS-P). This suggests that the same independence may apply to imbibition - in other words it may be possible to deduce the critical probability for the site problem (imbibition), despite the fact that very little is known regarding curvature approximations specific to the imbibition process in sphere packings. This point is addressed in more detail in section 6.5 following.
Figure 6.30 MS-P approximation, effect of randomising bonds on critical curvature for percolation (drainage).

Figure 6.31 MS-P approximation, effect of randomising bonds on critical probability for percolation (bond problem).
<table>
<thead>
<tr>
<th>Drainage Characteristic</th>
<th>Haines Curvature</th>
<th>MS-P Curvature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observed percolation threshold curvature, $C_n$</td>
<td>$7.30 + 0.1$</td>
<td>$5.25 + 0.05$</td>
</tr>
<tr>
<td>&quot;Randomised&quot; percolation threshold curvature, $C_n$</td>
<td>$6.05 + 0.05$</td>
<td>$4.65 + 0.05$</td>
</tr>
<tr>
<td>Observed critical probability for the bond problem, $P_{cr}$</td>
<td>$0.51 + 0.01$</td>
<td>$0.51 + 0.01$</td>
</tr>
<tr>
<td>&quot;Randomised&quot; critical probability for the bond problem, $P_{cr}^*$</td>
<td>$0.38 + 0.01$</td>
<td>$0.40 + 0.01$</td>
</tr>
</tbody>
</table>

$^*$ Note: $P_{cr}$ for a tetrahedral (diamond) lattice = 0.39

Table 6.3: Summary of drainage characteristics for the Finney packing using Haines' and MS-P curvature approximations.
6.5 The Imbibition Case

To complete this chapter on capillary pressure, it is necessary to consider the imbibition case. Unfortunately, there are no validated theoretical methods in the literature for calculating the meniscus curvature appropriate for imbibition into a cell formed by four spheres in contact. The default approach, therefore, is to use the imbibition curvature \( C_{imb} \) derived from the cavity insphere radius \( r_{cav} \) for the simplicial cell, as proposed by Mason (1971):

\[
C_{imb} = \frac{2}{r_{cav}}
\]

The frequency distribution for the 14870 (site) curvatures obtained using equation 6.6 is shown in figure 6.32. This frequency distribution may be compared directly with figure 3.27, to which it is equivalent. It is interesting to note that, unlike the bond frequency distributions for drainage curvatures (i.e. Haines' and MS-P shown in figures 6.5 and 6.24 respectively), the site frequency distribution shown in figure 6.32 is mono-modal and not strongly bi-modal.

As discussed in section 6.4.3, the uncertainty in the accuracy of the approximation used in equation 6.6 is probably irrelevant in terms of determining the critical probability for the site problem. This last assertion is supported by analogy with the drainage case where changing the drainage curvature approximation from Haines to MS-P had no effect on the critical probability for the bond problem.
Figure 6.32 Imbibition curvature frequency distribution.

Figure 6.33 Relationship between imbibition curvature and probability (cumulative number fraction) for Finney packing.
In simulating drainage of the Finney packing, the approach adopted was to assign individual cells to be "full" of wetting fluid, and count the number of cells which drained as the curvature (capillary pressure) was incremented from zero. An individual cell could only drain if it was connected to an already empty cell via a face which had a critical curvature less than the current incremental value of curvature (capillary pressure). The drainage algorithm therefore simulated a process in which site access is controlled by bond availability. In simulating imbibition, we are interested in almost, but not quite, the reverse process. In imbibition the starting point is a high curvature value which exceeds that curvature necessary to ensure complete drainage of the pack. All sites are therefore empty of wetting fluid. As the current value of curvature is decremented, a cell may reach the condition whereby the critical curvature of the cell \((C_{imb})\) is greater than the current curvature. At this point wetting fluid is "sucked into" the empty cell, filling it up. An empty cell imbibes from a neighbouring full cell, irrespective of the size characteristics of the face shared by these two cells. The imbibition algorithm therefore must simulate a process in which site access is controlled by site availability.

One interesting feature of the site problem considered here is that every cell has only one critical curvature \((C_{imb})\) and not the four which characterise the bond problem. The site probability/curvature graph, shown in figure 6.33, is therefore identical to the imbibition curve for the disaggregated set of 14870 cells of the Finney packing. Superimposing this figure with the disaggregated drainage curve obtained using the Haines' approximation gives an
estimation of the imbibition-drainage hysteresis of the disaggregated set of cells of the Finney packing, as shown in figure 6.34. As predicted in chapter 3, the degree of dis-aggregated cell hysteresis obtained in this manner is slight, and is most prominently developed at high curvatures. It is possible to use the result that the drainage curvature must always exceed the imbibition curvature for any given saturation on the hysteresis loop to derive a more accurate estimate of $C_{imb}$ than that given by equation 6.6. Because the MS-P curvature is more accurate than the Haines' curvature for drainage, it is reasonable to suppose that an improved estimate of $C_{imb}$ can be arrived at by shifting the disaggregated imbibition curve to lower curvatures until it just lies to the left of the MS-P disaggregated drainage curve, as shown in figure 6.35. This gives the result that the "corrected" estimation of imbibition curvature ($C_{imb}^*$) is:

$$C_{imb}^* = \frac{2}{r_{cv}} - 1.6$$

Equation 6.7 represents only a crude approximation for $C_{imb}^*$. However, it seems likely that it represents an improvement over the "uncorrected" definition given in equation 6.6.

6.5.1 The imbibition algorithm

The methodology used to develop the imbibition algorithm is comparable to that used to develop the drainage algorithm. The flow diagram used to represent program IMBIBE (presented in Appendix 'B' to this thesis) is shown in figure 6.36. As with the
Figure 6.34 Capillary pressure hysteresis for the 14870 disaggregated cells of the Finney packing, showing effect of zero connectivity. Drainage curve for Haines' approximation, imbibition curve for cavity insphere curvature.

Figure 6.35 Capillary pressure hysteresis for the 14870 disaggregated cells of the Finney packing, showing effect of zero connectivity. Drainage curve for MS-P approximation, imbibition curve for $C_{imb}^* = (2/cav) - 1.6$. 321.
Start

Input WRINED. DAT

Input pore volumes

Input cavity inspheres

Initialise cell zero
CAND (0) = 0
FULL (0) = 1

Determine first batch of candidate cells

For J = 1 to 14870

Test for cell zero numbers
(Test if A(1,2) = 3)

NO

YES

Candidate cell identified
CAND (I) = 1

Next I

For J = 1 to 200

X = (201 - J)

Now begin imbibition

Current curvature
C = X/10

A

Figure 6.36: FLOW DIAGRAM FOR SIMULATED IMBIBITION; SHOWING INITIALISATION LOGIC
For $K = 1$ to 14870

Test if $CAND(K) = 1$

YES

Is NEIGH # 1 full?
(Test if FULL $(A(K, 3)) = 1$

YES

Is current curvature less than cavity curvature?
(Test if $C < A(K, 7)$)

NO

Is NEIGH # 2 full?
(Test if FULL $(A(K, 4)) = 1$

YES

Is current curvature less than cavity curvature?
(Test if $C < A(K, 7)$)

NO

Is NEIGH # 3 full?
(Test if FULL $(A(K, 5)) = 1$

YES

Is current curvature less than cavity curvature?
(Test if $C < A(K, 7)$)

NO

Is NEIGH # 4 full?
(Test if FULL $(A(K, 6)) = 1$

YES

Is current curvature less than cavity curvature?
(Test if $C < A(K, 7)$)

NO

Figure 6.36: FLOW DIAGRAM FOR SIMULATED IMBIBITION; (cont.) SHOWING IMBIBE DECISION LOGIC BLOCK
Figure 6.36: FLOW DIAGRAM FOR SIMULATED IMBIBITION; SHOWING INDIVIDUAL CELL IMBIBITION LOGIC BLOCK
Figure 6.36: FLOW DIAGRAM FOR SIMULATED IMBIBITION; (cont.) SHOWING ALLOCATION OF NEW CANDIDATES LOGIC BLOCK
Figure 6.36: FLOW DIAGRAM FOR SIMULATED IMBIBITION; (cont.) SHOWING CAPILLARY PRESSURE EQUILIBRIUM LOGIC
drainage algorithm, the imbibition algorithm uses two working arrays, CAND() and FULL(), to register whether or not a cell is a candidate for imbibition (CAND(i) = 1), and whether or not the cell is full (FULL(i) = 1) or empty (FULL(i) = 0). Similarly, program IMBIBE uses a check on capillary pressure equilibrium to ensure that the current curvature is only decremented once equilibrium within the packing has been reached.

6.5.2 Sample Size effects

As with the drainage algorithm, program IMBIBE may be used to select the identical "sample" conditions A to E used in the drainage case. These sample sizes are:

Dis-aggregated: No connectivity, $S_R = 0.25$

"Sample" A: 1958 access cells, $S_R = 7.6$

"Sample" B: 982 access cells, $S_R = 15.1$

"Sample" C: 187 access cells, $S_R = 79.5$

"Sample" D: 22 access cells, $S_R = 675.9$

"Sample" E: 9 access cells, $S_R = 1652.2$

The results of imbibition into the above six sample conditions are shown in figure 6.37. These results were obtained using the definition of imbibition curvature given in equation 6.6, and it is clear from figure 6.37 that the percolation threshold for imbibition is associated with a curvature of $5.85 \pm 0.05$. Using the approximation given in equation 6.7, the corrected threshold curvature at which imbibition occurs in the Finney packing is equal to (or somewhat less than) $5.85 - 1.6 = 4.25 \pm 0.05$. 

327.
Figure 6.37  Dependency of imbibition curve on sample size ratio (curvature).

6.5.3 Critical Probability for the Site problem

By using exactly the same approach developed in sections 6.3 and 6.4, the 14870 values of $C_{imb}$ were converted into probabilities. It should be noted that, as a consequence of equation 6.7, the probabilities of corrected curvatures, $C_{imb}^{*}$ are precisely identical to those of $C_{imb}$. The imbibition algorithm, adapted to calculate number fraction saturations based on probabilities instead of curvatures, gave the results shown in figure 6.38 for the site problem. It is evident from figure 6.38 that the critical probability for the site problem can be estimated from the "sample" E curve to be $0.32 \pm 0.01$. Now this is a very interesting result, since Ziman (1982) gives the critical probability for the site problem on a tetrahedral (diamond) lattice as 0.43, and this value
represents the best a priori expectation for the critical probability for the tetrahedrally co-ordinated Finney packing. This is analogous to the result obtained for the critical bond problem. It appears, therefore, that the classical site problem of percolation theory fails to describe adequately the imbibition process for the Finney RCP packing just as the classical bond problem failed to describe the drainage process. As with the bond problem, it is easy to confirm this assertion by randomising the distribution of sites and re-calculating the imbibition curve.

In contrast to the bond problem, the distribution of sites may be easily randomised, as there is no network integrity to honour and preserve for the re-distributed sites. The 14870 curvature (site) values were read into an array, and two random integers in the open interval [1,14870] were generated. The curvature values
corresponding to these two array element numbers were swapped, and the process repeated 50,000 times. The resultant randomised array was used instead of the real Finney curvature values in the network, and the "Sample" E condition ($S_R = 1652.2$) was re-run. The resultant imbibition curve is shown in figure 6.39, where it is compared with the original result for "Sample" E presented in figure 6.37. The "randomised" imbibition curve has a percolation threshold for imbibition associated with a curvature of $5.38 \pm 0.05$, as opposed to the original value for the Finney packing of $5.85 \pm 0.05$. Making the correction given in equation 6.7 further reduces this value from $5.38 \pm 0.05$ to $3.78 \pm 0.05$ as opposed to the original corrected imbibition threshold value for the Finney packing of $4.25 \pm 0.05$.

Converting the randomised curvatures into probabilities and re-running program IMBIBE produces the imbibition curve shown in figure 6.40. It is evident from this graph that the critical probability for the site problem obtained from the randomised curvatures is $0.44 \pm 0.01$. This agrees rather well with the value of $0.43$ given by Ziman (1982) for the tetrahedral (diamond) lattice, and confirms that the classical site problem of percolation theory does not adequately describe the imbibition process for the Finney RCP model.

6.5.4 Hysteresis

Because of the uncertainty associated with the imbibition curvature, it is not possible to give a completely accurate description of the drainage-imbibition characteristics of the Finney packing. Furthermore, no attempt is made in the present work to estimate residual wetting and non-wetting phase saturations which both
Figure 6.39  Effect of randomising sites on critical curvature for percolation (imbibition).

Figure 6.40  Effect of randomising sites on critical probability for percolation (site problem).
shift hysteresis end points away from zero and unit saturation values. Despite these shortcomings, it is possible to present two logical hysteresis loops:

Loop 'a':  
Haines' Insphere approximation (drainage)  
Cavity Insphere approximation (imbibition)  
"Sample" E conditions ($S_r = 1652.2$)

Loop 'b':  
MS-P approximation (drainage)  
$C_{imb}$ (imbibition)  
"Sample" E conditions ($S_r = 1652.2$)

These two loops are presented in figures 6.41 and 6.42 respectively, together with experimental data from Haines' work (in Mason, 1984). It can be seen from these two figures that the approximate difference in curvature between drainage and imbibition for any given saturation on the loop is more than 2.0 throughout most of the loop (the end points are, of course, common to both segments of the loop). As discussed earlier in section 6.4, the degree of hysteresis obtained from the disaggregated set of cells is much less than 2.0, particularly at low curvatures where the two segments are essentially the same. This result confirms the assertion made in chapter three that the connectivity aspects of the Finney packing in particular, and probably RCP-like materials in general, represent a dominant factor in the origins of capillary pressure hysteresis. This view, very substantially supported by the present work, contradicts the now rather old independent domain theory of capillary pressure in which hysteresis is vested in individual cells (pores), rather than arising from the way in which the pores are connected together.
Some interesting observations can be made in comparing the results of the present work with the experimental results obtained by Haines, shown in figures 6.41 and 6.42 (note that Haines' data are volume fractions; those of this work are number fractions). In particular, the degree of hysteresis (i.e. separation between drainage and imbibition curves) obtained in the present work is very similar to that obtained by Haines. This strongly suggests that the conclusions reached by the present work regarding the origins of hysteresis are correct. The shape of the imbibition and drainage curves obtained by the present work are very similar to those obtained by Haines, again suggesting that the present work has succeeded in simulating those processes reasonably well. The absolute magnitudes (curvatures) of the drainage and imbibition curves obtained by the present work, however, are not in exact agreement with those obtained by Haines. The reasons for this inexact correspondence remain unclear. It is not too surprising that the imbibition curves obtained by the present work do not match closely with Haines' experimental data, since accurate methods for calculating imbibition curvatures do not exist for sphere packings. It is much more surprising that the experimental drainage curve is intermediate to the MS-P curve and the Haines' approximation curve obtained in the present work. The Haines' approximation is known to provide an overestimate of drainage curvature (e.g. Smith et al (11), 1987). The MS-P approximation, however, is supposed to be superior - instead it appears to underestimate drainage curvature by as much as the Haines' approximate overestimates it.

It is possible to shift the imbibition curve and the MS-P drainage curve until they both overly the experimental data obtained by
Haines. These shifts are shown in figure 6.43. In order to obtain these shifts, the "adjustments" required are + 1.0 to the MS-P curvatures, and - 1.0 to the basic cavity insphere calculation represented by equation 6.6. Without a very detailed and rigorous analysis (and possibly a repeat) of the experiments performed by Haines over fifty years ago, it is not easy to comment on the value of these "adjustments". Such analysis lies outside the scope of the present study, but may be of interest to other researchers.

Figure 6.41 Capillary pressure hysteresis for approximately infinite sample size RCP. Drainage curve for Haines' approximation, imbibition curve for cavity insphere curvature.
Figure 6.42  Capillary pressure hysteresis for approximately infinite sample size RCP. Drainage curve for MS-P approximation, imbibition curve for $C_{imb}^* = (2/cav)-1.6$

Figure 6.43  Theoretical capillary pressure hysteresis curves matched to experimental values.

335.
6.6 Summary and Conclusions

Chapter six of this thesis represents the culmination of the work developed in the preceding five chapters. This work has shown that the Finney RCP model is strongly non-random at the level of the individual simplicial cell (pore). The implications of the earlier work presented in this thesis, therefore, are that any modelling approach which randomly allocates pore sizes such as throats or bodies to a network is likely to produce estimates of capillary pressure characteristics which are significantly in error for RCP and RCP-like materials. Percolation theory is just such a modelling approach, and the work presented in chapter six demonstrates that this theory fails to predict accurately key capillary pressure characteristics of the Finney packing. Table 6.4 shows the curvatures at which the percolation threshold is reached in the Finney model for various definitions of curvature. These results may be directly compared with those of table 6.5, obtained for a randomised realisation of the Finney model. In all cases, the real Finney packing percolation threshold occurs at higher curvatures than can be arrived at by modelling the Finney packing as a random structure. Tables 6.6 and 6.7 show the critical probabilities for site and bond problems for the Finney packing: table 6.6 presents the observed response for the real Finney packing, whilst table 6.7 presents the response derived from a randomised realisation of the Finney packing. These results confirm that the classical bond and site problems of percolation theory do not adequately describe the capillary pressure characteristics of the Finney packing, as they
<table>
<thead>
<tr>
<th>Curvature Method</th>
<th>Imbibition</th>
<th>Drainage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Haines</td>
<td>-</td>
<td>7.3 ± 0.1</td>
</tr>
<tr>
<td>MS-P</td>
<td>-</td>
<td>5.25 ± 0.05</td>
</tr>
<tr>
<td>Cavity Insphere</td>
<td>5.85 ± 0.05</td>
<td>-</td>
</tr>
<tr>
<td>C^*_{ins}</td>
<td>4.25 ± 0.05</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.4: Curvatures at which percolation thresholds are reached for the Finney RCP model.

<table>
<thead>
<tr>
<th>Curvature Method</th>
<th>Imbibition</th>
<th>Drainage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Haines</td>
<td>-</td>
<td>6.05 ± 0.05</td>
</tr>
<tr>
<td>MS-P</td>
<td>-</td>
<td>4.65 ± 0.05</td>
</tr>
<tr>
<td>Cavity Insphere</td>
<td>5.38 ± 0.05</td>
<td>-</td>
</tr>
<tr>
<td>C^*_{ins}</td>
<td>3.78 ± 0.05</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.5: Curvatures at which percolation thresholds are reached in randomised realisations of the Finney RCP model.
<table>
<thead>
<tr>
<th>Curvature Method</th>
<th>Imbibition (Site Problem)</th>
<th>Drainage (Bond Problem)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Haines</td>
<td>-</td>
<td>0.51 ± 0.01</td>
</tr>
<tr>
<td>MS-P</td>
<td>-</td>
<td>0.51 ± 0.01</td>
</tr>
<tr>
<td>Cavity Insphere</td>
<td>0.32 ± 0.01</td>
<td>-</td>
</tr>
<tr>
<td>C_{i,m,n}</td>
<td>0.32 ± 0.01</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.6: Critical Probabilities for site and bond problem for the Finney packing.

<table>
<thead>
<tr>
<th>Curvature Method</th>
<th>Imbibition (Site Problem)</th>
<th>Drainage (Bond Problem)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Haines</td>
<td>-</td>
<td>0.38 ± 0.01</td>
</tr>
<tr>
<td>MS-P</td>
<td>-</td>
<td>0.40 ± 0.01</td>
</tr>
<tr>
<td>Cavity Insphere</td>
<td>0.44 ± 0.01</td>
<td>-</td>
</tr>
<tr>
<td>C_{i,m,n}</td>
<td>0.44 ± 0.01</td>
<td>-</td>
</tr>
<tr>
<td>Tetrahedral (diamond)</td>
<td>0.43</td>
<td>0.39</td>
</tr>
</tbody>
</table>

Table 6.7: Critical Probabilities for site and bond problem in randomised realisations of the Finney packing.
systematically fail to account for non-random distribution of bonds and sites.

Work presented in chapter 6 has shown that the volume fraction saturation is practically the same as the number fraction saturation for the Finney packing. This useful result confirms that this particular assumption of percolation theory is valid for RCP structure, even if the more important assumption of random bond and site allocation is invalid.

Work presented in chapter six confirms that the so called Pore Size Distribution (PSD) curve, arrived at by differentiating the drainage curve, does not represent a true pore size distribution at all. This fact is reasonably well known (though often conveniently forgotten in the oil industry). What is not well known, and what appears to be unrecorded in the literature, is that it is physically impossible for a drainage curve obtained from a large sample (> $10^6$ pores) to yield any information at all about the frequency of pores larger than (curvatures smaller than) the pore throat size associated with the percolation threshold. If the objective of the experiment is to obtain an estimate of the percolation threshold, then as large a sample as is practical is required. If, however, the objective of the experiment is to obtain an estimate of the "pore size distribution", then a number of small samples in which surface-connectivity effects dominate is preferable. By large here is meant > $10^6$ pores, and by small is meant < $10^4$ pores in roughly spherical shaped samples. This view of sample size selection completely contradicts the conventional wisdom of the oil industry, where mercury injection samples are selected to be as large as

339.
possible so as to avoid surface effects which are thought to be "undesirable". It is easy to see how this "undesirable" aspect arises, since relatively minor differences in overall sample size may introduce quite dramatic differences in the respective PSD curves. Such differences, of course, are a source of annoyance to an operator who wants the PSD curves for a set of similar samples to look similar to each other. The present work indicates that such operators are throwing away potentially useful information by labelling "small" samples as "undesirable". The work presented in chapter six proves that the major source of capillary pressure hysteresis in RCP and RCP-like materials is the connectivity between cells, and not some intrinsic property of the individual cells themselves. This result shows that the independent domain theory of capillary pressure hysteresis is wholly inadequate in accounting for the capillary properties of the Finney RCP model predicted on the basis of a detailed description of the model structure.

Finally, and perhaps most importantly, the work presented in chapter six and the preceding chapters represents the most comprehensive and detailed analysis to date of the structure of a real, disordered porous medium from which capillary properties may be predicted. The fact that this medium is a near perfectly mono-dispersed packing of near perfectly spherical particles should indicate to even the most casual reader that there are substantial difficulties associated with extending this work to natural materials such as sedimentary rocks. The philosophical approach developed in this thesis has been to discover methods and techniques for understanding pore structure on a simple material. This approach has shown that many of the key concepts in the literature pertaining to porous media (classical
bond and site problem descriptions of percolation theory, independent domain theory, pore size distribution) either cannot be applied at all to the Finney RCP model, or must be applied with extreme caution. How much more difficult, then, it may be to develop comparable techniques for use on complex systems such as sedimentary rocks.

Nevertheless, this thesis would not be complete without a discussion of how the present work may be related to the problems of understanding the influence of pore structure of real rocks on their capillary properties and fluid flow characteristics. This discussion is presented briefly in the next, and final, chapter.
CHAPTER 7: APPLICATION TO SEDIMENTARY ROCKS

The work presented in the first six Chapters is aimed almost totally at understanding the detailed structure of the Finney RCP model, and the influence that such structure exerts over capillarity within sphere packings. In many senses this work addresses an engineering/computing problem rather than a geological problem. There are, however, some general similarities between packings of spheres and detrital sedimentary rocks, as noted by Allen (1985). The purpose of this final Chapter, then, is to provide a brief excursion outside the precise confines of the Finney sphere packing into the realms of porous sedimentary rocks. Much of the value in this excursion lies in the recommendations for further research.

An important aspect of the research presented in the preceding six chapters of the present work is that RCP structure is not a direct analogue of sedimentary rocks. This is well known, and was pointed out over thirty years ago by Fatt (1958), who compared thin sections of sedimentary rocks with the type of structure expected from a sphere packing. Grains in a sphere packing are in point contact, grains in a sedimentary rock generally are not. Grains in a sphere packing are perfectly spherical and monodisperse, grains in a sedimentary rock are not. Grains in a sphere packing have no additional solid material adhering to them, grains in a sedimentary rock may have primary and secondary cements and a variety of diagenetic partially pore-filling minerals such as clays. It is clear, then, that we should not expect to be able to compare directly the Finney RCP model with a sedimentary rock.
7.1 Aeolian Sandstone

The rock type most likely to be directly comparable to the Finney RCP model is an aeolian sandstone. Such a rock is composed of highly spherical grains of roughly similar size. Steele (1981) has made a study of British aeolian sandstones, and it is clear from his work that the most suitable outcrop for study here is the Brigham Bank exposure of Penrith sandstone in the Vale of Eden, Cumbria. Samples of this material were therefore collected and analysed using the standard laboratory procedures of thin sectioning, scanning electron microscopy (SEM), particle size analysis and mercury injection. These standard analytical procedures provide a description of the Brigham Bank sandstone which may be compared with the description of the Finney RCP model presented in the preceding six chapters.

7.1.1 Particle Size Analysis

The sample of Brigham Bank sandstone used in this study was reddish brown friable coarse-grained material which is easily crumbled in the hand. To determine the particle size distribution, the sample was washed with glacial acetic acid followed by hydrochloric acid to remove calcite cement. The grains were then wash dried and the remaining loose agglomerates were lightly broken up in a hand mortar. The sample was then sieved, and particles less than 45μm were discarded. The particle size distribution was determined by sieving, and checked using a laser diffraction technique on a Malvern 2600D particle size analysis instrument (see Barth 1984 for a discussion of this technique). The results are presented in 343.
figure 7.1 and table 7.1. From these data it is evident that the median particle diameter is 645μm. The particles are clearly not mono-disperse as shown in figure 7.2, though the size distribution is quite "tight", with 43.1% of all particles contained within the range 600 - 710μm. There is little point in attempting to compute statistical data other than the median for this sample, since quite apart from questions about how representative the analysis is, we have no idea how to use such information in any practical way (i.e. related to pore structure). The most significant finding of the particle size analysis, therefore, is that the median particle size (diameter) of the Brigham Bank sandstone samples studied here is 645μm.

7.1.2 Pore Structure

Within the scope of the present work it is impractical to attempt to describe the structure of Brigham Bank sandstone samples using the simplicial cell method. Some understanding of the pore structure may be obtained using SEM photomicrographs. We are not concerned here with a detailed sedimentological description of the material. It is less important to know, for example, which particular clay species is present than it is to know which part of the pore structure is occupied by that clay. Figure 7.3 shows a pore throat formed by three grains in contact. This pore throat is largely occluded by an interstitial clay. Figure 7.4 shows a more general (lower magnification) view of the material, in which a number of pore throats formed by spheres in contact can be seen, some of which are partially blocked by clay. Figure 7.5 shows a tendency for some of the grains to line up in layers, presumably reflecting the
Figure 7.1  Particle size distribution for Brigham Bank aeolian sandstone.

Table 7.1  Sieve results for particle size analysis of Brigham Bank sandstone.
Figure 7.2 Photomicrograph of Brigham Bank sand grains.
primary deposition of the sediment. Finally, figure 7.6 shows a relatively high magnification image of the surface of an individual quartz grain. This image shows a surface which is rough, pitted and lightly coated in irregular clay platelets. From these views of the material it is possible to conclude that:

* the grains are not all the same size and shape,
* the surfaces of the grains are irregular and variable, with small pits and coatings of clay,
* pore throats may be partially blocked by clay,
* pore bodies may be partially filled with clay,
* planar layering of the grains in place suggests that structural anisotropy (a feature of RCP structure) is unlikely to characterise this material.

It is intuitively reasonable, therefore, to expect that the capillary pressure attributes of this material are likely to be very different from those of the Finney RCP model. In particular, the drainage curve is likely to be displaced to higher curvature (pressure) in order to force the invading fluid through partially occluded pore throats.

### 7.1.3 Capillary Pressure Characteristics

A sample of Brigham Bank sandstone, roughly spherical in shape and 2cm in diameter was subjected to mercury injection in an Autopore-II 9200 porosimeter. This commercial instrument provides (oil) industry standard measurements of volume of mercury injected as a function of injection pressure, and the resultant capillary
Figure 7.3  SEM photomicrograph of Brigham Bank sandstone x 129 magnification, showing occluded pore throat.

Figure 7.4  SEM photomicrograph of Brigham Bank sandstone x 18 magnification.
Figure 7.5  SEM photomicrograph of Brigham Bank sandstone x 18 magnification, showing layering.

Figure 7.6  SEM photomicrograph of Brigham Bank sandstone x 310 magnification, showing grain surface.
pressure (drainage) curve is shown in figure 7.7. It should be noted from figure 7.7 that pressure has been converted into nominal pore-diameter, by use of equation 6.3, as is industry standard practise. Differentiating the curve shown in figure 7.7 gives the so-called pore-size distribution curve, presented in figure 7.8. This latter figure has a prominent peak at a pore diameter of almost exactly 100μm. The form of this peak is very similar to the results obtained for the Finney packing, and looks qualitatively similar to figure 6.28 for example. Based on the work presented in chapter six, therefore, it must be concluded that the prominent peak at 100μm corresponds to the pore throat diameter associated with the percolation threshold for drainage in this particular sample of Brigham Bank sandstone. Now the key question is this - can this percolation threshold value be related to the sample pore structure using the Finney RCP model as an analogue?

It is possible to answer this question by setting the hard sphere diameter of the Finney model to that of the median particle diameter of the Brigham Bank sandstone. The curvature corresponding to the percolation threshold for drainage in the Finney model, using the MS-P approximation, is 5.25 ± 0.05 (table 6.4 and figure 6.28 refer). Converting this curvature gives a pore throat diameter corresponding to the percolation threshold for drainage of 0.38 hard sphere diameters.

Threshold Curvature = 5.25
Throat Radius = \( \frac{2}{5.25} = 0.38 \) sphere radii
Throat Diameter = \( 2 \times 0.38 = 0.76 \) sphere radii
Throat Diameter = \( \frac{0.76}{2} = 0.38 \) sphere diameters
Figure 7.7  Mercury injection curve for Brigham Bank sandstone.

Figure 7.8  Mercury injection PSD for Brigham Bank sandstone.
Assuming the hard sphere diameter of the Finney packing to be 645\(\mu m\), this value of 0.38 would correspond with a pore diameter of 245\(\mu m\) for the percolation threshold for drainage (using the MS-P approximation) in the Finney model. From figure 7.8 it is clear that, for Brigham Bank sandstone, this represents an over prediction by a factor of about 2.5, since the observed pore diameter associated with the percolation threshold for drainage is 100\(\mu m\) for the Brigham Bank sandstone. It is hardly surprising that the Finney model fails as a direct analogue, since the SEM photographs in figures 7.3 to 7.6 show that critical parts of the porespace of the Brigham Bank sandstone (i.e. the pore throats) are choked up by varying amounts of clay. It may be that the uncoated, clean quartz-grain pore throat diameter associated with the percolation threshold for drainage is around 245\(\mu m\), though this remains unproven. The effective pore throat diameter associated with the percolation threshold for drainage however, is reduced by secondary mineralisation to the 100\(\mu m\) observed in figure 7.8.

Whilst it is clearly impractical to use the Finney RCP model as a direct analog of the Brigham Bank (or any other) sandstone, the techniques developed in the present work could, in principle, be extended to cope with exactly the kind of complexity encountered in real sandstones. Such work lies well beyond the scope of this thesis, and constitutes the basis for further research, discussed below.
7.2 Recommendations for Further Research

The simplicial cell discretisation of space applied to the Finney packing dealt only with monodisperse spheres. However, the discretisation process itself is totally independent of the particles themselves, as the process relates only to the sphere centre co-ordinates. In principle, therefore, the particles can be polydisperse, interpenetrating (i.e. non-point contact) with secondary decoration (for example, representing cement or diagenetic mineralisation). Furthermore, the co-ordinate system can be varied anisotropically. For example, by retaining X and Y spatial relationships, but contracting the Z co-ordinates and allowing particle interpenetration may be of interest in simulating compaction. Some of the basic concepts which may prove fruitful in modelling specific porous media are now considered.

7.2.1 Polydispersity

Polydispersity is, in principle, a simple extension to the work presented in this thesis. Statistical mechanics simulators may be used to produce polydisperse sphere packings to packing densities and sphere radius compositions of interest. This approach may be of use in chemical engineering applications where packed beds are likely to be distinctly polydisperse. Provided the distribution of sphere sizes and bed (packing) density are known in advance, the fluid characteristics of the packing could be modelled by using a simplicial cell discretisation method similar to that used in the present work. A polydisperse simplicial cell is illustrated in
7.2.2 Interpenetration

The Finney RCP model was built using hard (steel) balls which did not interpenetrate. It is trivially easy to use the sphere centre co-ordinates of the Finney model as the basis of an interpenetrating sphere system. For example, keeping the sphere centre co-ordinates constant, but allowing the sphere diameters to uniformly increase produces a reduction in porosity and permeability, with attendant changes in connectivity as the pore space becomes progressively choked off. An illustration of a simplicial cell showing interpenetration is given in figure 7.10. Such an approach may be modified to simulate compaction of granular materials, and may be useful in simulating certain processes such as sintering, and may reproduce features of some sedimentary rocks such as pressure solution at grain boundaries and crystal overgrowths.

7.2.3 Anisotropy

It is possible to simulate differential compaction of a granular bed if interpretation is permitted. By contracting the magnitudes of all Z co-ordinates for example, vertical compression (compaction) of the system can be simulated. Instead of simple geometric interpenetration it may be of interest to try and simulate elastic deformation of the particles themselves. This rapidly becomes a complex problem as sphere rotation and displacement may be involved.
Figure 7.9  Example of a polydisperse simplicial cell.

Figure 7.10  Simplicial cell with interpenetrating spheres.
7.2.4 Departures from Sphericity

It may be of interest to consider granular particles which are not only polydisperse, and possibly interpenetrated, but also substantially non-spherical. Again it is possible to make simplicial cells for grains with non-spherical shapes. Minor ellipsoidal departures from sphericity may be possible; however, the problems of realistically simulating a packing of irregular shaped particles are likely to be extremely complex in practice. It may be more practical at this stage to forego any attempt at simulating the packing as a structural entity, and simply consider "decorating" simplicial cells with statistical images of the pore space which best fits the intended purpose. The pitfalls in this approach, of course, could be substantial. However, the model should be constrained to match some experimentally determined bulk properties including some or all of the following: particle size distribution, sphericity, overall porosity, permeability and capillary pressure characteristics. This degree of modelling complexity begins to resemble the problem posed in section 7.1 in which the Brigham Bank sandstone was compared with the Finney RCP model. An idealised Simplicial cell formed by non-spherical, polydisperse particles is shown in figure 7.11.

The concept of cell "decoration" may be further developed:

7.2.5 Decoration

All clastic sedimentary rocks with pore space are likely to have some degree of pore surface secondary mineralisation. This might
Figure 7.11  Simplicial cell formed by non-spherical, polydisperse particles.

Figure 7.12  Simplicial cell formed by non-spherical, polydisperse particles with decoration.
include cement, and pore-lining materials such as illite fibres or kaolinite "books" - common in some oil bearing sandstones. In principle, simplicial cells may be "decorated" to resemble the pores of a real sedimentary rock, as shown in figure 7.12. Provided the volumes of decorating material are distributed according to some preferred rule, it may be possible to model fluid flow characteristics of interest.

7.3 Concluding Remarks

The main component of the research presented in this thesis resides in the first six chapters, which are specific to the random close packing of equal spheres. These six chapters represent original research into the control which the pore structure of one specific sphere packing exerts over the capillary pressure characteristics expected from that packing. This research has generated a number of new and significant findings, all related to random close packings of equal spheres. The present chapter, on the other hand, represents initial comments on the ways in which the techniques developed so successfully for sphere packings might be applied to other porous media such as clastic rocks. Although the step from sphere packings to real rocks is large, it seems likely that significant and rapid progress could be made in pore-level modelling of rocks using an adaptation of the simplicial cell technique.
REFERENCES


361.


KELVIN, Sir W. THOMSON., 1887. On the division of space with minimum partitional area. Acta. Math. 11, 121-134.


MASON, G. 1988 (i). Personal communication.


369.


WRIGHT, A.C., 1986. Personal communication.


APPENDIX 'A'

This appendix presents the simplicial cell trigonometric calculations used in the preceding chapters.

1. Simplicial Cell Edgelengths

Given the centre coordinates of the spheres P and Q:

Point P at \((x_P, y_P, z_P)\)
Point Q at \((x_Q, y_Q, z_Q)\)

Length \(PQ = \sqrt{(x_Q-x_P)^2 + (y_Q-y_P)^2 + (z_Q-z_P)^2}\)

2. Face Angles

Using the standard tetrahedron geometry presented in figure 3.3 (page 91), for FACE 1:

\(S = \frac{1}{2} (L_1 + L_2 + L_3)\)

\[\sin \left(\frac{A_1}{2}\right) = \sqrt{\frac{(S-L_3)(S-L_2)}{L_3L_2}}\]

Alternatively,

\[\cos \left(\frac{A_1}{2}\right) = \sqrt{\frac{(S(S-L_1))}{L_2L_3}}\]

or,

\[\tan \left(\frac{A_1}{2}\right) = \sqrt{\frac{(S-L_3)(S-L_2)}{S(S-L_2)}}\]

3. Face Insphere Radius

Using the standard tetrahedron geometry presented in figure 3.3 (page 91) and the so-called LAW OF SINES for FACE 1:

\[\frac{L_1}{\sin A_1} = \frac{L_2}{\sin A_2} = \frac{L_3}{\sin A_3} = 2r\]

- given a hard sphere radius of 0.5, the radius \((R)\) of the face insphere is found from:

\[R = r - 0.5\]
4. Solid Angles

Using the standard tetrahedron geometry presented in figure 3.3 (page 91) and spherical trigonometry for APEX I:

if A, B and C are the angles of the spherical triangle opposite the three face angles A1, A4 and A7, then the apex solid angle, \( W \), is:

\[ W = (A + B + C - \pi) \text{ radian} \]

To solve for \( W \), solve for A, B and C in:

\[
\sin \left( \frac{A}{2} \right) = \sqrt{\frac{\sin(S-A4) \sin(S-A7)}{\sin A4 \sin A7}} \\
\sin \left( \frac{B}{2} \right) = \sqrt{\frac{\sin(S-A1) \sin(S-A7)}{\sin A1 \sin A7}} \\
\sin \left( \frac{C}{2} \right) = \sqrt{\frac{\sin(S-A4) \sin(S-A1)}{\sin A1 \sin A4}} \\
S = \frac{1}{2} (A1 + A4 + A7) \\
\]

-hence \( W_1, W_2, W_3 \) and \( W_4 \) for the four individual apex solid angles.

5. Total Cell (Tetrahedron) Volume

Using the standard tetrahedron geometry presented in figure 3.3 (page 91):

\[ 6V_T = L2.L3.L4 \sqrt{(1-\cos^2A1-\cos^2A4-\cos^2A7+2\cos A1\cos A4\cos A7)} \]

6. Cell Void Volume

Using the standard tetrahedron geometry presented in figure 3.3 (page 91), the solid volume, \( V_s \), associated with the individual apex solid angle, \( W_i \), is:

\[ V_s = f_i \cdot \frac{4\pi r^3}{3} \]

where \( f_i = \) fractional area of spherical triangle:

\[ f_i = \frac{W_i r^2}{4\pi r^2} = \frac{W_i}{4\pi} \]
7. Cavity Insphere Radius

Using the standard tetrahedron geometry presented in figure 3.3 (page 91), together with the total cell volume, $V_c$,

$$R_{cav} = 2x \left[ \frac{(S-(L3\cdot L4)(S-L2\cdot L6)(S-L1\cdot L5))}{V_c} \right]^{0.5}$$

$$S = 0.5(L3\cdot L4 + L2\cdot L6 + L1\cdot L5)$$
This appendix presents the computer program and subroutine listings referred to in the main text of the thesis, together with descriptions of data files used.

With the exception of subroutine WANDOM which is written in FORTRAN, all programs and subroutines are written in VAX compiled BASIC. All of the programs are short, and each normally supports an adequate level of self-documentation at the top of the listing. Where a program has little or no self-documentation, the main text of the thesis supplies relevant information.

The listings presented in this appendix fall into 3 discrete categories:

B1. Analytical subroutines
B2. Main programs
B3. Data files

Of the above three categories, the analytical subroutines are the most likely to be referred to, used or developed by other interested workers in the field. Accordingly, particular care has been taken in the self-documentation and inter-relationships of these routines. In general, most of these subroutines calculate parameters in dimensions of sphere radii. It is conventional, however, to measure cell edgelengths in sphere diameters. It is therefore worth commenting on the fact that if edgelengths are defined in sphere diameters, then subroutine DRAD should be called first in order to convert edgelengths to sphere radii.

Each of the three categories carries its own contents page, and these are presented on the following pages:

<table>
<thead>
<tr>
<th>SECTION</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>376</td>
</tr>
<tr>
<td>B2</td>
<td>393</td>
</tr>
<tr>
<td>B3</td>
<td>436</td>
</tr>
</tbody>
</table>
APENDIX ''B''

SECTION B1 - ANALYTICAL SUBROUTINES

<table>
<thead>
<tr>
<th>Routine</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANGLEA</td>
<td>378</td>
</tr>
<tr>
<td>APEX</td>
<td>378</td>
</tr>
<tr>
<td>CARE</td>
<td>379</td>
</tr>
<tr>
<td>CAVT</td>
<td>379</td>
</tr>
<tr>
<td>CONR</td>
<td>380</td>
</tr>
<tr>
<td>DIFF</td>
<td>380</td>
</tr>
<tr>
<td>DRAD</td>
<td>381</td>
</tr>
<tr>
<td>EGUR</td>
<td>381</td>
</tr>
<tr>
<td>EXIS</td>
<td>382</td>
</tr>
<tr>
<td>FARE</td>
<td>383</td>
</tr>
<tr>
<td>H020</td>
<td>383</td>
</tr>
<tr>
<td>H100</td>
<td>384</td>
</tr>
<tr>
<td>HYRA</td>
<td>384</td>
</tr>
<tr>
<td>INFA</td>
<td>385</td>
</tr>
<tr>
<td>ORD1</td>
<td>385</td>
</tr>
<tr>
<td>ORD2</td>
<td>386</td>
</tr>
<tr>
<td>MSP</td>
<td>387</td>
</tr>
<tr>
<td>PORE</td>
<td>389</td>
</tr>
<tr>
<td>SOLD</td>
<td>390</td>
</tr>
<tr>
<td>STDV</td>
<td>391</td>
</tr>
<tr>
<td>TVOL</td>
<td>391</td>
</tr>
<tr>
<td>WANDOM</td>
<td>392</td>
</tr>
</tbody>
</table>
This module calculates the 12 face angles for the standard tetrahedron geometry. This standard geometry is:

<table>
<thead>
<tr>
<th>FACE ANGLES</th>
<th>EDGES</th>
<th>APICES/SPHERES</th>
</tr>
</thead>
<tbody>
<tr>
<td>FACE 1 A1, A2, A3</td>
<td>K1, K2, K3</td>
<td>1, 2, 3</td>
</tr>
<tr>
<td>FACE 2 A4, A5, A6</td>
<td>K2, K4, K5</td>
<td>1, 3, 4</td>
</tr>
<tr>
<td>FACE 3 A7, A8, A9</td>
<td>K3, K5, K6</td>
<td>1, 2, 4</td>
</tr>
<tr>
<td>FACE 4 A10, A11, A12</td>
<td>K1, K4, K6</td>
<td>2, 3, 4</td>
</tr>
</tbody>
</table>

K() Array of 6 edgelengths as INPUT
A() Array of 12 face angles as OUTPUT

Face angles are in radians

SUB ANGL (K(), A())

20 S1 = 0.5 * (K(1) + K(2) + K(3))
S2 = 0.5 * (K(2) + K(4) + K(5))
S3 = 0.5 * (K(3) + K(5) + K(6))
S4 = 0.5 * (K(1) + K(4) + K(6))

30 A(1) = (S1 - K(2)) * (S1 - K(3)) / (S1 * (S1 - K(1)))
A(2) = (S1 - K(1)) * (S1 - K(3)) / (S1 * (S1 - K(2)))
A(3) = (S1 - K(1)) * (S1 - K(2)) / (S1 * (S1 - K(3)))
A(4) = (S2 - K(2)) * (S2 - K(5)) / (S2 * (S2 - K(4)))
A(5) = (S2 - K(4)) * (S2 - K(2)) / (S2 * (S2 - K(5)))
A(6) = (S2 - K(4)) * (S2 - K(5)) / (S2 * (S2 - K(2)))
A(7) = (S3 - K(3)) * (S3 - K(5)) / (S3 * (S3 - K(6)))
A(8) = (S3 - K(5)) * (S3 - K(6)) / (S3 * (S3 - K(3)))
A(9) = (S3 - K(3)) * (S3 - K(6)) / (S3 * (S3 - K(5)))
A(10) = (S4 - K(1)) * (S4 - K(5)) / (S4 * (S4 - K(4)))
A(11) = (S4 - K(4)) * (S4 - K(5)) / (S4 * (S4 - K(1)))
A(12) = (S4 - K(4)) * (S4 - K(1)) / (S4 * (S4 - K(6)))

40 FOR I = 1 TO 12
A(I) = SQRT(A(I))
A(I) = ATN(A(I))
A(I) = A(I) * 2
NEXT I

50 ! All 12 face angles (radians) now in array A(), in standard sequence.
! SUBEND
This module is called by EXIS

SUB ANGLEA(A, B, C, ANGA)
S = 0.5 * (A + B + C)
X = ((S - C) * (S - A)) / (S * (S - B))
Y = X^0.5
Z = ATN(Y)
ANGA = Z * 2

20 SUBEND

This module accepts four arguments:
A Apex face angle, as INPUT
B Apex face angle, as INPUT
C Apex face angle, as INPUT
W Apex solid angle, as OUTPUT

This module is called by module SOLD

SUB APEX (A, B, C, W)

S = 0.5 * (A + B + C)

AA = (SIN(S - B) * SIN(S - C)) / (SIN(B) * SIN(C))
BB = (SIN(S - A) * SIN(S - C)) / (SIN(A) * SIN(C))
CD = (SIN(S - B) * SIN(S - A)) / (SIN(B) * SIN(A))

AA = SQR(AA)
BB = SQR(BB)
CD = SQR(CD)

AA = ATN(AA / SQR(-AA * AA + 1))
BB = ATN(BB / SQR(-BB * BB + 1))
CD = ATN(CD / SQR(-CD * CD + 1))

AA = AA * 2
BB = BB * 2
CD = CD * 2

W = (AA + BB + CD - PI)

80 SUBEND
CARE

This module calculates the four constriction face areas (ie void segment only).

AF() = INPUT Array of 4 total face areas
AC() = OUTPUT Array of 4 constriction face areas

The module calculates the constriction face areas in the sequence dictated by the standard tetrahedron geometry. Thus AC(1) is the constriction face area of face 1, and so forth.

Area dimension is sphere radii squared, input array AF() MUST therefore be in units of sphere radii squared.

SUB CARE(AF(),AC())

FOR I=1 TO 4
AC(I)=AF(I)-PI/2 ! Solid area is constant & = 0.5*pi*R^2 (R^2=1)
NEXT I

30 SUBEND

CAVT

This module calculates the cavity insphere radius, R

K() Array of 6 edgelengths as INPUT
V Tetrahedron volume as INPUT
R Radius of cavity insphere as OUTPUT

Dimensions of R are sphere RADII cubed.
Input array, K(), MUST therefore be in sphere radii (ie unit edgelength=2.00000).

SUB CAVT(K(),V,R)

A=K(3)*K(4)
B=K(2)*K(6)
C=K(1)*K(5)

30 S=0.5*(A+B+C)
R=SQR(S*(S-A)*(S-B)*(S-C))
R=R/(V*6.0)
R=R-1.0

40 SUBEND
CONR

This module calculates the 4 equivalent radii of the face constriction areas, as defined by CHAN & NG (Powder Tech., 54(1988), 147-155). The module calculates the radii in the sequence dictated by the standard tetrahedron geometry. Thus RC(1) is the equivalent radius of constriction for face 1 and so forth. Dimensions of equivalent radii are sphere radii.

AC()=INPUT Array of constriction face areas
RC()=OUTPUT Array of equivalent radii of constriction

SUB CONR(AC(),RC())

20 FOR I=1 TO 4
   RC(I)=(AC(I)/PI)^0.5
NEXT I

SUBEND

*** DIFF.BAS ***

This routine accepts 5 arguments:
P() : an array as INPUT
Q() : an array as INPUT
N : the number of elements in P & Q as INPUT
L : the sample interval as INPUT
S : the sum of the difference in area between P and Q as OUTPUT

SUB DIFF(P(),Q(),N,L,S)
S=0

20 FOR I= 1 TO N-1
   IF P(I)>P(I+1) THEN MAXP=P(I) ELSE MAXP=P(I+1)
   END IF
   IF Q(I)>Q(I+1) THEN MAXQ=Q(I) ELSE MAXQ=Q(I+1)
   END IF

30 AREAP=L*(MAXP-0.5*ABS(ABS(P(I))-ABS(P(I+1))))
AREAQ=L*(MAXQ-0.5*ABS(ABS(Q(I))-ABS(Q(I+1))))
AREA=ABS(AREAP-AREAQ)

40 S=S+AREA

50 NEXT I

60 SUBEND
This module converts a preset sequence of 6 edgelengths from dimensions of sphere diameters to sphere radii. This module MUST precede all modules in which parameter dimensions are sphere radii, sphere radii squared or sphere radii cubed for edgelengths calculated as sphere diameters (eg FINEdge.DAT).

\[ K(I) = L(I) \times 2.0 \]

This module calculates the equivalent radius of the pore chamber, as defined by Chan & Ng (Powder Tech., 54(1988) 147-155). Dimensions of equivalent pore chamber radius are sphere radii.

\[ \text{RP} = \left( \frac{3.0 \times \text{VOID}}{4.0 \times \pi} \right)^{1/3} \]
This routine is called by RANCELL. The purpose of this routine is to return a value of E=1 if the (randomly selected) edgelengths happen to form a viable tetrahedral structure, or E=0 if the sequence of edgelengths is "impossible".

SUB EXIS (LSEQ(),L(),E)

Array LSEQ contains the edge length sequence for each tetrahedron (ie the standard reference tetrahedron sequence). Thus although LSEQ(1) to (6) contain a sequence of edge lengths in the correct order, there are five other (different) sequences. In order to test for an "impossible" configuration, all sequences are examined.

20 ! Test loop:
   R=0

LOOPTOP:F=L(LSEQ(R+1))
   A=L(LSEQ(R+2))
   B=L(LSEQ(R+3))
   C=L(LSEQ(R+4))
   D=L(LSEQ(R+5))
   E=L(LSEQ(R+6))

30 CALL ANGLEA(A,B,C,ANGA)
   CALL ANGLEA(C,D,E,ANGD)

40 T=((C-(A*COS(ANGA)+E*COS(ANGD)))^2+(A*SIN(ANGA)+E*SIN(ANGD))-2)^0.5

50 IF T > F THEN GOTO EXIST ELSE GOTO NONEXIST

EXIST:IF R=>30 THEN GOTO XOUT ELSE GOTO INCREMENT

END IF

INCREMENT:R=R+6
GOTO LOOPTOP

XOUT:E=1
GOTO 60

NONEXIST:E=0
GOTO 60

60 SUBEND
FARE

This module calculates the total four total face areas (ie both solid segment and void segment).

K()= INPUT Array of 6 edgelengths
AF()=OUTPUT Array of 4 total face areas

The module calculates the total face areas in the sequence dictated by the standard tetrahedron geometry. Thus AF(1) is the total face area of face 1, and so forth.

Area dimension is sphere radii squared, input array K() MUST therefore be in units of sphere radii.

SUB FARE(K(), AF())

20 S1=0.5*(K(1)+K(2)+K(3))
S2=0.5*(K(2)+K(4)+K(5))
S3=0.5*(K(3)+K(5)+K(6))
S4=0.5*(K(1)+K(4)+K(6))

30 AF(1)=(S1*(S1-K(1))*(S1-K(2))*(S1-K(3)))^0.5
AF(2)=(S2*(S2-K(2))*(S2-K(4))*(S2-K(5)))^0.5
AF(3)=(S3*(S3-K(3))*(S3-K(5))*(S3-K(6)))^0.5
AF(4)=(S4*(S4-K(1))*(S4-K(4))*(S4-K(6)))^0.5

40 SUBEND

H020

This module accepts a fractional number in the interval 0<X<1 and returns an integer in the interval 1<Y<20

SUB H020(X, Y)

20 Y=20*X
Y=Y+1
Y=FIX(Y)

30 SUBEND
This module accepts a fractional number in the interval \(0 < X < 1\) and returns an integer in the interval \(1 < Y < 100\).

```plaintext
SUB H100(X,Y)
  Y=100*X
  Y=Y+1
  Y=FIX(Y)
SUBEND
```

This module calculates the hydraulic radii of 4 face constictions. The module calculates the radii in the sequence dictated by the standard tetrahedron geometry. Thus \(HY(1)\) is the hydraulic radius for face 1 and so forth. Dimensions of hydraulic radius are sphere radii.

```
AC()=INPUT Array of face constriction areas
HY()=OUTPUT Array of face hydraulic radii

SUB HYRA(AC(),HY())
20 FOR I=1 TO 4
   HY(I)=AC(I)/PI ! Wetted perimeter is constant & = pi
NEXT I
SUBEND
```
This module calculates the four face insphere radii. The dimensions of the insphere radii are sphere radii.

K0 Array of 6 edgelengths as INPUT
A0 Array of 12 face angles as INPUT
RF0 Array of 4 face insphere radii as OUTPUT

The module calculates the face inspheres in the sequence dictated by the standard tetrahedron geometry. Thus RF(1) is the insphere radius for face 1, and so forth.

SUB INFA(K(),A(),RF())

20 RF(1)=K(1)/SIN(A(1))
    RF(2)=K(4)/SIN(A(4))
    RF(3)=K(5)/SIN(A(9))
    RF(4)=K(6)/SIN(A(12))

30 FOR I=1 TO 4
    RF(I)=RF(I)/2.0
    RF(I)=RF(I)-1.0
NEXT I

40 SUBEND

This module orders a sequence of 4 numbers, from highest to lowest.

IN=INPUT array
OU=OUTPUT array

SUB ORD1(IN(),OU())

20 FOR I=1 TO 4
    OU(I)=IN(I)
NEXT I
B=3

30 C=0

50 FOR L=1 TO B
    IF OU(L)>=OU(L+1) THEN GOTO 70 ELSE GOTO 60

60 T=OU(L)
    OU(L)=OU(L+1)
    OU(L+1)=T
    C=L

70 NEXT L
    B=C-1
    IF B>0 THEN GOTO 30

80 SUBEND
This module orders a sequence of 4 numbers, from highest to lowest, and returns the positions of the newly ordered numbers in the original input array.

IN=INPUT array
OU=OUTPUT array
OC=OUTPUT array containing new element sequence

SUB ORD2(IN(), OU(), OC())

20 FOR I=1 TO 4
    OU(I)=IN(I)
NEXT I
B=3

30 C=0

50 FOR L=1 TO B
    IF OU(L)>=OU(L+1) THEN GOTO 70 ELSE GOTO 60

60 T=OU(L)
    OU(L)=OU(L+1)
    OU(L+1)=T
    C=L

70 NEXT L
    B=C-1
    IF B>0 THEN GOTO 30

80 FOR J=1 TO 4
    FOR K=1 TO 4
        IF OU(K)=IN(J) THEN GOTO 90 ELSE GOTO 100

90 OO(J)=K
100 NEXT K
    NEXT J

110 SUBEND
This routine calculates MS-P curvatures. The output values are identical to those obtained by Mason & Morrow in J. Coll. Int. Sci. Vol. 100, No. 2 pp 519-535.

```fortran
SUB MSP(xx, yy, zz, MS)
14 x(1)=xx
15 x(2)=yy
16 x(3)=zz
30 RD=0.5
40 for j=1 to 2
50 for i=1 to 2
60 if x(i)>x(i+1) then goto 100 else goto 70
70 m=x(i)
80 x(i)=x(i+1)
90 x(i+1)=m
100 next i
110 next j
120 eps=10^-8
130 s=0
140 rroot=0
150 s=0.5*(x(1)+x(2)+x(3))
160 atri=(s*(s-x(1))*(s-x(2))*(s-x(3)))^0.5
170 atot=atri-0.5*pi*RD^2
180 pto=pi*RD
190 rstart=atot/pto
200 rinc=(x(1)*x(2)*x(3))/(4*atri)-RD
210 for i=1 to 4
220 ct=0
230 fx=i
240 if fx=4 then goto 250 else goto 270
250 r=rstart
260 goto 530
270 rmin=(x(i)-2*RD)/2
280 r=rmin
290 gosub 590
300 if f<0 then goto 560 else goto 310
310 r2=rinc
320 r2=r2
330 gosub 590
340 f2=f
350 r1=rmin
360 r=r1
370 gosub 590
380 f1=f
390 if abs(f1)<(10^-10) then goto 530 else goto 400
400 if abs(f1-f2)<(10^-10) then goto 410 else goto 430
410 kk=40
420 goto 440
430 kk=f1/(f1-f2)
440 if abs(kk)>40 then goto 450 else goto 460
450 kk=sgn(kk)*40
460 r3=r1-kk*(r1-r2)
470 if abs((r3-r1)/r3)<eps then goto 530 else goto 480
```

387.
480 f2=f1
490 r2=r1
500 r1=r3
510 ct=ct+1
520 if ct>100 then goto 710 else goto 360
530 if r>rroot then goto 540 else goto 560
540 rroot=r
550 sif=fx
560 next i
570 MS=RD/rroot
580 goto 720
590 p=ptot
600 a=atot
610 for j=fx to 3
620 talp=(((RD+r)^2-(x(j)/2)^2)^0.5)/(x(j)/2)
630 alp=atn(talp)
640 delp=2*(alp*RD-r*(pi/2-alp))
650 dela=(RD+r)^2*sin(alp)*cos(alp)-(RD^2*alp+r^2*(pi/2-alp))
660 p=p-delp
670 a=a-dela
680 next j
690 f=a/p-r
700 return
710 MS=999
720 END SUB
This module accepts four arguments:

- S() An array of 5 solid angles, of which only the first four are used: INPUT
- V The tetrahedron volume: INPUT
- PO The tetrahedron porosity
- PD The tetrahedron packing density

- PO & PD OUTPUT -

V MUST previously have been calculated in dimensions of sphere radii cubed.

SUB PORE(S(), V, PO, PD)

20 \( F_1 = S(1)/(4\pi) \)
\( F_2 = S(2)/(4\pi) \)
\( F_3 = S(3)/(4\pi) \)
\( F_4 = S(4)/(4\pi) \)

30 \( \text{SUM} = F_1 + F_2 + F_3 + F_4 \)

40 \( \text{SOLIDVOL} = 4\pi \times \text{SUM}/3 \)
\( \text{VOIDVOL} = V - \text{SOLIDVOL} \)

50 \( \text{PO} = \text{VOIDVOL}/V \)
\( \text{PD} = \text{SOLIDVOL}/V \)

60 SUBEND
This module calculates the 4 tetrahedral solid angles, and sums these to produce a 5th solid angle for the entire cell.

A() An array of 12 face angles as INPUT
S() An array of 5 solid angles (1 to 4 for apices 1 to 4; 5 for the total tetrahedral solid angle)

The face angles are input in RADIANS

~~~~~~~~~ This routine calls module APEX ~~~~~~~~~~

SUB SOLD (A(), S())

20 ! For apex number 1 :-
   A=A(1)
   B=A(4)
   C=A(7)
   CALL APEX (A, B, C, W1)

30 ! For apex number 2 :-
   A=A(2)
   B=A(9)
   C=A(10)
   CALL APEX (A, B, C, W2)

40 ! For apex number 3 :-
   A=A(3)
   B=A(5)
   C=A(12)
   CALL APEX (A, B, C, W3)

50 ! For apex number 4 :-
   A=A(6)
   B=A(8)
   C=A(11)
   CALL APEX (A, B, C, W4)

60 W5=W1+W2+W3+W4
   S(1)=W1
   S(2)=W2
   S(3)=W3
   S(4)=W4
   S(5)=W5

70 SUBEND
This module calculates the standard deviation and mean of an array.

\[
X()=\text{Input array}
\]
\[
N=\text{Number of elements in } X()
\]
\[
\text{MN}=\text{Calculated mean value}
\]
\[
\text{ST}=\text{Standard deviation}
\]

```
SUB STDV(XO, N, MN, ST)
20 SUM=0
         SUMSQ=0
30 FOR I=1 TO N
    SUM=SUM+X(I)
    SUMSQ=SUMSQ+X(I)^2.0
NEXT I
40 MN=SUM/N
    ST=SUMSQ/N
    ST=ST-(SUM^2.0)/(N^2.0)
    ST=ST^0.5
SUBEND
```

This module calculates the total simplicial cell volume, \( V \).

\[
K()=\text{Array of 6 edgelengths as INPUT}
\]
\[
A()=\text{Array of 12 face angles as INPUT}
\]
\[
VT=\text{The tetrahedron volume as OUTPUT}
\]

\( V \) has dimensions of sphere radii cubed.
Input array, \( K() \), MUST therefore be in sphere radii (ie unit edgelength =2.0000).

```
SUB TVOL(K(), A(), V)
20 X=K(2)
    Y=K(3)
    Z=K(5)
    A=A(1)
    B=A(4)
    C=A(7)
30 V=X*Y*Z
    V=V*SQR(1-COS(A)*COS(A)-COS(B)*COS(B)-COS(C)*COS(C)+2*COS(A)*COS(B)*COS(C))
    V=V/6.00
SUBEND
```
FUNCTION WANDOM(IX, IY, IZ)
C
C by Wichmann B.A. and Hill I.D.
C
C Returns a psuedo-random number rectangularly distributed
C between 0 and 1.
C
C IX, IY and IZ should be set to integer values between 1 and
C 3000 before first entry.
C
C Integer arithmetic up to 30323 is required
C
 IX = 171*MOD(IX, 177) - 2*(IX/177)
 IY = 172*MOD(IY, 176) - 35*(IY/176)
 IZ = 170*MOD(IZ, 178) - 63*(IZ/178)
C
 IF (IX .LT. 0) IX=IX+30269
 IF (IY .LT. 0) IY=IY+30307
 IF (IZ .LT. 0) IZ=IZ+30323
 WANDOM=AMOD(FLOAT(IX) / 30269.0 +
 1 FLOAT(IY) / 30307.0 +
 1 FLOAT(IZ) / 30323.0, 1.0)
C
C Following statements are modifications to Algorithm
C AS 183, as provided by Remark AS R58, due to
C
C These modifications preserve the original performance
C of AS 183, but prevent the occurrence of perfectly zero
C values which may arise as a consequence of using
C rounded arithmetic with 24 bits for the fractional part
C of a single precision variable. Expected frequency of
C such zero "artifacts" is about 1 in 7.4x10^-6 calls.
C
 IF (WANDOM .GT. 0.0) RETURN
 WANDOM=DBMOD(DBLE(FLOAT(IX)) /
 1 30269.0D0 +
 1 DBLE(FLOAT(IY))/30307.0D0 +
 1 DBLE(FLOAT(IZ))/30323.0D0, 1.0D0)
 IF (WANDOM .GE. 1.0) WANDOM=0.999999
RETURN
END

392.
APPENDIX 'B'

SECTION B2 - MAIN PROGRAM LISTINGS

CELLFI ................... 394
CELLMSP .................. 397
CONTROL .................. 401
DRAINPACK ................ 403
EXP ...................... 407
FOLD ..................... 409
HISTOGRAM ................. 410
IMBIBE .................... 411
ISOCOUNT .................. 414
ISOMER .................... 415
LENGTHS ................... 417
NEIGH-0 ................... 418
NEIGH-1 ................... 419
NEIGH-2 ................... 420
NEIGH-3 ................... 421
NEIGH-4 ................... 422
NEIGH-5 ................... 423
NEIGH-6 ................... 424
NET1 ...................... 425
PMATRIX ................... 427
P ........................ 429
TYPE ...................... 430
VORONHIST .................. 431
VORONOI ................... 432
VORWARD ................... 433
VSMOOTH ................... 435

393.
This program provides the FACE INSPHERE RADII for the entire network contained in WRINED.DAT. The output from this program is called CELLFI.DAT, and is used as an input data file in constructing capillary pressure curves for the Finney packing.

```plaintext
DIM S(14870,4), X(4021), Y(4021), Z(4021)
DIM N(4), P(4), Q(4), R(3), W(12), G(12), FA(4), RF(4)

OPEN "NEWFILE3.DAT" FOR INPUT AS FILE #3
OPEN "NEWFILE5.DAT" FOR INPUT AS FILE #5
OPEN "WRINED.DAT" FOR INPUT AS FILE #6
OPEN "CELLFI.DAT" FOR OUTPUT AS FILE #7

FOR I = 1 TO 14870
    INPUT #3, S(I,1), S(I,2), S(I,3), S(I,4)
NEXT I

FOR J = 1 TO 4021
    INPUT #5, D1, X(J), Y(J), Z(J), D2
NEXT J

FOR K = 1 TO 14870
    INPUT #6, A, B, N(1), N(2), N(3), N(4)
    N(1) TO N(4) are the identities of the 4 cells which connect directly with cell K
    P(1) = S(K,1)
P(2) = S(K,2)
P(3) = S(K,3)
P(4) = S(K,4)
    P() contains the identities of the 4 spheres defining the reference cell.
    SC=0

FOR L = 1 TO B
    Q(1) = S(N(L),1)
    Q(2) = S(N(L),2)
    Q(3) = S(N(L),3)
    Q(4) = S(N(L),4)
    Q() contains the identities of the 4 spheres defining one of the neighbouring cells.
```

. 394.
70 CALL PICK(P(),Q(),R(),SS)
!
! the 3 element array R() contains the identities of the spheres
! which form the face between cell 'K' and cell 'N(L)'.
! Now perform error check. SS must equal 4, otherwise error
! in cell-neighbour relationship exists.
!
80 IF SS=4 THEN GOTO 100 ELSE GOTO 90

90 PRINT"ERROR CONDITION : NO COMMON FACE ON CELL";K

100 W(SC+1)=R(1)
    W(SC+2)=R(2)
    W(SC+3)=R(3)
    SC=SC+3

110 NEXT L

120 ! determine 4th face identity if reference cell neighbours
! with cell zero (pack surface)
! IF B=3 THEN GOTO 130 ELSE GOTO 170

130 CALL FRTH(W(),P(),F1,F2,F3,EF)

140 ! error check, EF must equal zero, otherwise an error in the
! cell-neighbour relationship exists
! IF EF=0 THEN GOTO 160 ELSE GOTO 150

150 PRINT"ERROR CONDITION : NO COMMON FACE ON CELL";K

160 W(10)=F1
    W(11)=F2
    W(12)=F3

170 CALL DIST(X(),Y(),Z(),W(),G())

180 ! Convert edgelengths from sphere diams. to sphere radii:
! FOR Q=1 TO 12
    G(Q)=G(Q)*2.0
    NEXT Q

190 ! Find a face angle (in radians) for each of the 4 faces:
! S1=0.5*(G(1)+G(2)+G(3))
    S2=0.5*(G(4)+G(5)+G(6))
    S3=0.5*(G(7)+G(8)+G(9))
    S4=0.5*(G(10)+G(11)+G(12))
200 $\text{FA}(Q) = \frac{(S_l-G(2)) \times (S_l-G(3))}{S_l \times (S_l-G(l))}$
$\text{FA}(Q) = \frac{(S_2-G(5)) \times (S_2-G(6))}{S_2 \times (S_2-G(4))}$
$\text{FA}(Q) = \frac{(S_3-G(8)) \times (S_3-G(9))}{S_3 \times (S_3-G(7))}$
$\text{FA}(Q) = \frac{(S_4-G(11)) \times (S_4-G(12))}{S_4 \times (S_4-G(10))}$

210 FOR $Q=1$ TO 4
\begin{align*}
\text{FA}(Q) &= \text{SQR}(\text{FA}(Q)) \\
\text{FA}(Q) &= \text{ARIN}(\text{FA}(Q)) \\
\text{FA}(Q) &= \text{FA}(Q) \times 2.0
\end{align*}
NEXT $Q$

220 ! Now calculate face insphere radii
\begin{align*}
\text{RF}(1) &= \frac{G(1)}{\sin(\text{FA}(1))} \\
\text{RF}(2) &= \frac{G(4)}{\sin(\text{FA}(2))} \\
\text{RF}(3) &= \frac{G(7)}{\sin(\text{FA}(3))} \\
\text{RF}(4) &= \frac{G(10)}{\sin(\text{FA}(4))}
\end{align*}

230 FOR $Q=1$ TO 4
\begin{align*}
\text{RF}(Q) &= \text{RF}(Q) / 2.0 \\
\text{RF}(Q) &= \text{RF}(Q) - 1.0
\end{align*}
NEXT $Q$

! -and convert to curvatures:

FOR $Q=1$ TO 4
\begin{align*}
\text{RF}(Q) &= 2.0 / \text{RF}(Q)
\end{align*}
NEXT $Q$

240 PRINT #7, K; "", \text{RF}(1); "", \text{RF}(2); "", \text{RF}(3); "", \text{RF}(4)

250 NEXT K
This program provides the MS-P curvatures for the entire network contained in WRINED.DAT. The output from this program is called CELLMSP.DAT, and is used as an input data file in constructing capillary pressure curves for the Finney packing.

DIM S(14870,4), X(4021), Y(4021), Z(4021)
DIM N(4), P(4), Q(4), R(3), W(12), G(12), FA(4), RF(4), MS(4)

OPEN "NEWFILE3.DAT" FOR INPUT AS FILE #3
OPEN "NEWFILE5.DAT" FOR INPUT AS FILE #5
OPEN "WRINED.DAT" FOR INPUT AS FILE #6
OPEN "CELLMSP.DAT" FOR OUTPUT AS FILE #7

FOR I = 1 TO 14870
  INPUT #3, S(I,1), S(I,2), S(I,3), S(I,4)
  NEXT I

FOR J = 1 TO 4021
  INPUT #5, X(J), Y(J), Z(J), D2
  NEXT J

MSUM = 0

FOR K = 1 TO 14870
  INPUT #6, A, B, N(1), N(2), N(3), N(4)
  P(1) = S(K,1)
  P(2) = S(K,2)
  P(3) = S(K,3)
  P(4) = S(K,4)
  ! P() contains the identities of the 4 spheres defining the reference cell.
  SC = 0

FOR L = 1 TO B
  Q(1) = S(N(L),1)
  Q(2) = S(N(L),2)
  Q(3) = S(N(L),3)
  Q(4) = S(N(L),4)
  ! Q() contains the identities of the 4 spheres defining one of the neighbouring cells.
CALL PICK(P(),Q(),R(),SS)
!
! the 3 element array R() contains the identities of the spheres
! which form the face between cell 'K' and cell 'N(L)'.
! Now perform error check. SS must equal 4, otherwise error
! in cell-neighbour relationship exists.
!
IF SS=4 THEN GOTO 100 ELSE GOTO 90

PRINT "ERROR CONDITION : NO COMMON FACE ON CELL";K

W(SC+1)=R(1)
W(SC+2)=R(2)
W(SC+3)=R(3)
SC=SC+3

NEXT L

! determine 4th face identity if reference cell neighbours
! with cell zero (pack surface)
!
IF B=3 THEN GOTO 130 ELSE GOTO 170

CALL FRTH(Wo, Po, Fl, F2, F3, EF)

! error check, EF must equal zero, otherwise an error in the
! cell-neighbour relationship exists
!
IF EF=0 THEN GOTO 160 ELSE GOTO 150

PRINT "ERROR CONDITION : NO COMMON FACE ON CELL";K

W(10)=Fl
W(11)=F2
W(12)=F3

CALL DIST(Xo, Yo, Zo#Wo, Go)

1 Convert edgelengths from sphere dias. to sphere radii:
FOR Q=1 TO 12
G(Q)=G(Q)*2.0
NEXT Q

1 Find a face angle (in radians) for each of the 4 faces:
S1=0.5*(G(1)+G(2)+G(3))
S2=0.5*(G(4)+G(5)+G(6))
S3=0.5*(G(7)+G(8)+G(9))
S4=0.5*(G(10)+G(11)+G(12))
200 FA(1)=(S1-G(2))*(S1-G(3))/(S1*(S1-G(1)))
FA(2)=(S2-G(5))*(S2-G(6))/(S2*(S2-G(4)))
FA(3)=(S3-G(8))*(S3-G(9))/(S3*(S3-G(7)))
FA(4)=(S4-G(11))*(S4-G(12))/(S4*(S4-G(10)))

210 FOR Q=1 TO 4
FA(Q)=SQR(FA(Q))
FA(Q)=ATN(FA(Q))
FA(Q)=FA(Q)*2.0
NEXT Q

220 ! Now calculate face insphere radii
RF(1)=G(1)/SIN(FA(1))
RF(2)=G(4)/SIN(FA(2))
RF(3)=G(7)/SIN(FA(3))
RF(4)=G(10)/SIN(FA(4))

230 FOR Q=1 TO 4
RF(Q)=RF(Q)/2.0
RF(Q)=RF(Q)-1.0
NEXT Q
!
! -and convert to curvatures:
FOR Q=1 TO 4
RF(Q)=2.0/RF(Q)
NEXT Q
!
!
Haines' curvatures stored in array RF()
!
!
250 !
! convert edgelengths back to sphere diameters
!
FOR Q=1 TO 12
G(Q)=G(Q)/2.0
NEXT Q

260 XX=G(1)
YY=G(2)
ZZ=G(3)
CALL MSP(XX, YY, ZZ, MSP)
IF MSP>500 THEN GOTO 270 ELSE GOTO 280

270 MSP=RF(1)-1.5
MSUM=MSUM+1

280 MS(1)=MSP
XX=G(4)
YY=G(5)
ZZ=G(6)
CALL MSP(XX, YY, ZZ, MSP)
IF MSP>500 THEN GOTO 290 ELSE GOTO 300

399.
290 MSP=RF(2)-1.5
  MSUM=MSUM+1

300 MS(2)=MSP
  XX=G(7)
  YY=G(8)
  ZZ=G(9)
  CALL MSP(XX, YY, ZZ, MSP)
  IF MSP>500 THEN GOTO 310 ELSE GOTO 320

310 MSP=RF(3)-1.5
  MSUM=MSUM+1

320 MS(3)=MSP
  XX=G(10)
  YY=G(11)
  ZZ=G(12)
  CALL MSP(XX, YY, ZZ, MSP)
  IF MSP>500 THEN GOTO 330 ELSE GOTO 340

330 MSP=RF(4)-1.5
  MSUM=MSUM+1

340 MS(4)=MSP

350 PRINT #7, K;",", MS(1);",", MS(2);",", MS(3);",", MS(4)

355 PRINT K, MSUM

360 NEXT K
This program generates a control file, in which random tetrahedra are generated using the observed simplicial cell edgelength distribution for the central 2000 spheres of the Finney model.

```
DIM F(89220), L(6), K(6), LSEQ(36)
20 DECLARE INTEGER IX, IY, IZ
   IX=23154
   IY=12569
   IZ=27981
EXTERNAL REAL FUNCTION WANDOM(INTEGER, INTEGER, INTEGER)
   MP=0
25 !
   Read in sequences for testing 3-D validity
   FOR M=1 TO 36
      READ LSEQ(M)
   NEXT M
30 OPEN "FINEDGE.DAT" FOR INPUT AS FILE #3
   OPEN "CONTROL.DAT" FOR OUTPUT AS FILE #4
   OPEN "CONTROL_REJ.DAT" FOR OUTPUT AS FILE #5
40 INPUT #3, DUMMY1
50 !
   Input the observed edgelength distribution for the Finney model
   FOR I=0 TO 89214 STEP 6
      INPUT #3, DUMMY2, F(I+1), F(I+2), F(I+3), F(I+4), F(I+5), F(I+6)
   NEXT I
60 !
   Create 100000 random cells
   FOR I=1 TO 100000
      Assign 6 values at random to form a potential cell
      FOR G=1 TO 6
         Z = WANDOM(IX, IY, IZ)
         X = FIX(Z*89220+1)
         K(G) = F(X)
      NEXT G
      ! Test to confirm that the cell can exist in 3 dimensions
      CALL EXIS(LSEQ(0), K(0), E)
      IF E=1 THEN GOTO 70 ELSE GOTO 68
   MP=MP+1
   GOTO 62
68
70 PRINT #4, K(1); ","; K(2); ","; K(3); ","; K(4); ","; K(5); ","; K(6)
80 NEXT I
90 !
```
! Sequence data for 3-D validity test
!
DATA 1,6,3,5,4,2
DATA 2,3,5,6,1,4
DATA 3,2,5,4,1,6
DATA 4,2,1,3,5,6
DATA 5,3,2,1,6,4
DATA 6,1,3,2,4,5

95 !
! Report diagnostics
!
PRINT #5, " In creating file CONTROL.DAT,";MP;"cells were rejected"
PRINT #5, " as having no 3-dimensional validity."

100 CLOSE #3,#4,#5
END
This program simulates drainage of wetting fluid from the Finney packing, and calculates the capillary pressure curve for the packing.

Three methods of estimating meniscus curvature are available:
(i) Face Insphere,
(ii) Mason's approximated MSP curvature,
(iii) MSP curvature.

Before the program runs, one of these methods is selected by the user.

WORKING PRINCIPLE
2 working arrays are used to keep track of the fluid status within each simplicial cell. These arrays are FULL() and CAND(). All cells are initialised to be full, except cell zero which is empty. All cells are initialised NOT as candidates for drainage, except for those cells with cell zero as an immediate neighbour. Cell zero is the outer pack surface.

```
DIM A(14870,10),FULL(14870),CAND(14870),V(14870)
```

20 OPEN "DRAIN.DAT" FOR OUTPUT AS FILE #6
OPEN "WRINED.DAT" FOR INPUT AS FILE #5
OPEN "POREVOL.DAT" FOR INPUT AS FILE #3

Porevol contains the pore volume for each simplicial cell.

30 INPUT"Enter name of curvature file (CELLFI,CELLAMS,CELLMSP)";A$
OPEN A$ FOR INPUT AS FILE #4

A$ is the network file, together with the critical meniscus curvature values from cell to cell.

```
PRINT #6," FOR INPUT FILE";A$
```

40 ND=0 I running sum of number of drained cells
VD=0 I running sum of total volume of drained fluid
TV=0 I running sum of total pore volume
CPE=0 I capillary pressure equilibrium test

50 FOR I=1 TO 14870
 INPUT #3,DUMMY,V(I)
 TV=TV+V(I)
 NEXT I
55 FOR I=1 TO 14870
    INPUT #5, A(I,1), A(I,2), A(I,3), A(I,5), A(I,7), A(I,9)
    INPUT #4, DUMKY, A(I,4), A(I,6), A(I,8), A(I,10)
    !
    ! Initialise working arrays:
    !
    57 FULL(I)=1 ! All cells are full
    CAND(I)=0 ! All cells are NOT candidates for drainage

60 NEXT I

70 FULL(0)=0 ! Cell zero is empty, and can not therefore be
    CAND(0)=0 ! a candidate to drain.

80 ! All cells which have cell zero as an immediate neighbour are
    ! candidates for drainage. These candidates are identified as
    ! having 3 simplicial cell neighbours, not 4:
    ! i.e. A(i,2)=3
    ! This is the basis for initialisation.
    !
    ! Set the fraction (ZQ) of surface occurring cells which are allowed
    ! free access to drain into cell zero. This can be all the surface
    ! occurring cells (ZQ=1), or none of them (ZQ=0 - in which case the pack
    ! cannot drain at all).
    !
    PRINT"By setting a threshold fraction in the range 0 to 1, the number"
    PRINT11"of surface occurring cells connected to cell zero is restricted"
    INPUT"Enter threshold (1=all surface cells connected; 0=None)"; ZQ
    !
    FOR I=1 TO 14870
      IF A(I,2)=3 THEN GOTO 90 ELSE GOTO 100
    90 WE=RND
      IF WE<ZQ THEN GOTO 95 ELSE GOTO 99
    95 CAND(I)=1 ! This cell is now a candidate for drainage.
      GOTO 100
    99 CAND(I)=0 ! Despite being a potential candidate, this cell is blocked.
      A(I,10)=999.9 ! Curvature set so face cannot drain to cell zero

100 NEXT I

110 ! Initialisation of arrays is now complete.
    !
120 FOR J=1 TO 200
    ! This gives 200 steps in curvature from just below the known
    ! minimum curvature for the packing.
    !
    C=J/10
    !
    ! C is the current value of meniscus curvature.
    !

404.
130 FOR K=1 TO 14870
  IF CAND(K)=1 THEN GOTO 200 ELSE GOTO 370
  ! This conditional branch identifies which cells are needed
  ! to be considered for possible drainage.
  ! Having found a candidate cell, it is necessary to establish
  ! whether or not it will drain at the current meniscus curvature
  ! value (C). Thus a face connecting a candidate cell to an EMPTY
  ! neighbouring cell will allow the candidate cell to drain only
  ! if the current meniscus curvature (C) is greater than the
  ! critical value for that face.

200 !*******************************
!Cell drain/non-drain logic:
*******************************
  IF FULL(A(K,3))=0 THEN GOTO 210 ELSE GOTO 220
210 IF A(K,4)<C THEN GOTO 280 ELSE GOTO 220
220 IF FULL(A(K,5))=0 THEN GOTO 230 ELSE GOTO 240
230 IF A(K,6)<C THEN GOTO 280 ELSE GOTO 240
240 IF FULL(A(K,7))=0 THEN GOTO 250 ELSE GOTO 260
250 IF A(K,8)<C THEN GOTO 280 ELSE GOTO 260
260 IF FULL(A(K,9))=0 THEN GOTO 270 ELSE GOTO 370
270 IF A(K,10)<C THEN GOTO 280 ELSE GOTO 370
280 !*******************************
!Individual cell drainage:
*******************************
  ND=ND+1
  VD=VD+V(K)
  CAND(K)="O
  FULL(K)=O

290 !*******************************
!Allocation of new candidates:
*******************************
  IF FULL(A(K,3))=1 THEN GOTO 300 ELSE GOTO 310
300 CAND(A(K,3))=1
310 IF FULL(A(K,5))=1 THEN GOTO 320 ELSE GOTO 330
320 CAND(A(K,5))=1
330 IF FULL(A(K,7))=1 THEN GOTO 340 ELSE GOTO 350
340 CAND(A(K,7))=1
350 IF FULL(A(K,9))=1 THEN GOTO 360 ELSE GOTO 370
360 CAND(A(K,9))=1
370 ***************
   Capillary pressure equilibrium logic:
   ***************
   NEXT K
380 IF ND>CPE THEN GOTO 390 ELSE GOTO 400
390 CPE=ND
   GOTO 130
400 SX=0
   FOR PP=1 TO 14870
   IF CAND(PP)=1 THEN GOTO 402 ELSE GOTO 404
402 SX=SX+1
404 NEXT PP
   NF=((14870-ND)/14870)
   VF=(1.0-(VD/TV))
   PRINT C;ND;VD;NF;VF;SX
   PRINT #6,C",";ND",";VD",";NF",";VF",";SX
   CPE=0
410 NEXT J
420 CLOSE #6
END
10 ! EXP

1
DIM W(14870,6),C(14870,5)

20 OPEN "WRINED.DAT" FOR INPUT AS FILE #3
OPEN "CELLFI.DAT" FOR INPUT AS FILE #4
OPEN "MIXFI.DAT" FOR INPUT AS FILE #5

30 FOR I=1 TO 14870
   INPUT #3,W(I,1),W(I,2),W(I,3),W(I,4),W(I,5),W(I,6)
   INPUT #4,C(I,1),C(I,2),C(I,3),C(I,4),C(I,5)
NEXT I
CLOSE #3,#4

40 FOR J=1 TO 100000
   PRINT J

50 X=FIX(1+RND*14870)

60 Y=FIX(3+RND*4)

70 P=W(X,Y)

80 IF P<1 THEN GOTO 60

90 IF W(P,3)=X THEN GOTO 100 ELSE GOTO 110
100 Q=2
   GOTO 200

110 IF W(P,4)=X THEN GOTO 120 ELSE GOTO 130
120 Q=3
   GOTO 200

130 IF W(P,5)=X THEN GOTO 140 ELSE GOTO 150
140 Q=4
   GOTO 200

150 IF W(P,6)=X THEN GOTO 160 ELSE GOTO 170
160 Q=5
   GOTO 200

170 PRINT "***FATAL ERROR***"
   GOTO 999

200 IF C(X,Y-1)=C(P,Q) THEN GOTO 300 ELSE GOTO 250

250 PRINT"***FACE FATAL ERROR***"
   GOTO 999

300 CURV1=C(X,Y-1)

310 A=FIX(1+RND*14870)

320 B=FIX(3+RND*4)

330 C=W(A,B)

340 IF C<1 THEN GOTO 320
350 IF W(C, 3)=A THEN GOTO 360 ELSE GOTO 370
360 D=2
   GOTO 500
370 IF W(C, 4)=A THEN GOTO 380 ELSE GOTO 390
380 D=3
   GOTO 500
390 IF W(C, 5)=A THEN GOTO 400 ELSE GOTO 410
400 D=4
   GOTO 500
410 IF W(C, 6)=A THEN GOTO 420 ELSE GOTO 430
420 D=5
   GOTO 500
430 PRINT"****FATAL ERROR****"
   GOTO 999

500 IF C(A, B-1)=C(C, D) THEN GOTO 600 ELSE GOTO 550
550 PRINT"****FACE FATAL ERROR****"
   GOTO 999

600 CURV2=C(A, B-1)

610 !PRINT C(X, Y-1), C(P, Q), CURV1
   !PRINT C(A, B-1), C(C, D), CURV2
   !PRINT"

620 C(X, Y-1)=CURV2
   C(P, Q)=CURV2
   C(A, B-1)=CURV1
   C(C, D)=CURV1

650 NEXT J

660 FOR I=1 TO 14870
   PRINT #5, I; ","; C(I, 2); ","; C(I, 3); ","; C(I, 4); ","; C(I, 5)
NEXT I
   CLOSE #5

999 END
10 ! *** FOLD.BAS ***
! Author: D.W. Mellor
! Created: August 1986
! Documentation: This program uses data in VSMOOTHEDGE.DAT as input,
! and prompts for a starting point in the input array. The program
! then subtracts elements on the LH side of the starting point from
! elements on the RH side. This is a crude step in deducing the
! approximate form of the structure away from the 1.00000 diameter
! spike. Data is output to VMODEL1.DAT

DIM L(800), IN(800), OUT(800)

20 OPEN "VSMOOTHEDGE.DAT" FOR INPUT AS FILE #6
30 OPEN "VMODEL1.DAT" FOR OUTPUT AS FILE #7
40 FOR I = 1 TO 750
50 INPUT #6, L(I), IN(I)
60 NEXT I
70 INPUT "Enter starting position"; X
80 PRINT "That corresponds with "; L(X); IN(X)
90 INPUT "Is this correct"; A$
100 IF A$ = "Y" THEN GOTO 110 ELSE GOTO 70
110 FOR I = 1 TO X
120 OUT(I+X) = IN(I+X) - IN(X-I)
130 PRINT #7, L(I+X), OUT(I+X)
140 NEXT I
150 CLOSE #6
160 CLOSE #7
170 END
10 ! ** HISTOGRAM.BAS **

! Author : D.W. Mellor
! Created : July 1986
! Documentation : This program examines the edge lengths from FINNEY's
! data. The input file is FINEDGE.DAT created by LENGTHS.DAT, the output
! file is called HISTEDGE.DAT.
20 DIM L(6), EDGE(800)
30 OPEN "FINEDGE.DAT" FOR INPUT AS FILE #6
40 OPEN "HISTEDGE.DAT" FOR OUTPUT AS FILE #7
50 FOR I=1 TO 14870
60 INPUT #6,DUMMY,L(1),L(2),L(3),L(4),L(5),L(6)
70 FOR K=1 TO 6
80 L(K)=L(K)+0.0005
90 A%=FIX((L(K)*1000)-900)
100 EDGE(A%)=EDGE(A%)+1
110 NEXT K
120 NEXT I
130 FOR J=0 TO 800
140 PRINT #7,((J+900)/1000),",",EDGE(J)
150 NEXT J
160 CLOSE #6
170 CLOSE #7
180 END
IMBIBE

This program simulates imbibition of wetting fluid into the Finney packing, and calculates the capillary pressure curve for the packing.

The critical meniscus curvature is taken to be the cavity insphere radius.

WORKING PRINCIPLE

2 working arrays are used to keep track of the fluid status within each simplicial cell. These arrays are FULL() and CAND(). All cells are initialised to be empty, except cell zero which is full. All cells are initialised NOT as candidates for imbibition, except for those cells with cell zero as an immediate neighbour. Cell zero is the outer pack surface.

DIM A(14870,7), FULL(14870), CAND(14870), V(14870)

OPEN "IMBIBE.DAT" FOR OUTPUT AS FILE #6
OPEN "WRINED.DAT" FOR INPUT AS FILE #5
OPEN "POREVOL.DAT" FOR INPUT AS FILE #3
OPEN "IMBMIX.DAT" FOR INPUT AS FILE #4

Porevol contains the pore volume for each simplicial cell.
Cavity contains the cavity insphere radius for each cell.

PRINT #6," FOR CAVERY INSPHERE RADIUS CURVATURES"

NI=0 ! running sum of number of imbibed cells
VI=0 ! running sum of total volume of imbibed fluid
TV=0 ! running sum of total pore volume
CPE=0 ! capillary pressure equilibrium test

FOR I=1 TO 14870
INPUT #3,DUMMY,V(I)
TV=TV+V(I)
NEXT I

FOR I=1 TO 14870
INPUT #5,A(I,1),A(I,2),A(I,3),A(I,4),A(I,5),A(I,6)
INPUT #4,DUMMY,A(I,7)

**initialise working arrays:**

FULL(I)=0 ! All cells are empty
CAND(I)=0 ! All cells are NOT candidates for imbibition

NEXT I
70 FULL(0)=1  ! Cell zero is full, and can not therefore be CAND(0)=0  ! a candidate to imbibe.

80 ! All cells which have cell zero as an immediate neighbour are candidates for imbibition. These candidates are identified as having 3 simplicial cell neighbours, not 4: i.e. A(i,2)=3 ! This is the basis for initialisation.

! Set the fraction (ZQ) of surface occurring cells which are allowed free access to drain into cell zero. This can be all the surface occurring cells (ZQ=1), or none of them (ZQ=0 - in which case the pack cannot drain at all).

PRINT"By setting a threshold fraction in the range 0 to 1, the number" PRINT"of surface occurring cells connected to cell zero is restricted" INPUT"Enter threshold (1=all surface cells connected; 0=none)";ZQ

FOR I=1 TO 14870 IF A(I,2)=3 THEN GOTO 90 ELSE GOTO 100

90 WE=RND IF WE<ZQ THEN GOTO 95 ELSE GOM 99

95 CAND(I)=1  ! This cell is now a candidate for imbibition. GOTO 100

99 CAND(I)=0  ! Despite being a potential candidate, this cell is blocked.

100 NEXT I

110 ! Initialisation of arrays is now complete.

120 FOR J=1 TO 200

! This gives 200 steps in curvature

XCC=(201-J)
C=XCC/10

! C is the current value of meniscus curvature.

130 FOR K=1 TO 14870 IF CAND(K)=1 THEN GOTO 200 ELSE GOTO 370

! This conditional branch identifies which cells are needed to be considered for possible imbibition.

! Having found a candidate cell, it is necessary to establish whether or not it will imbibe at the current meniscus curvature value (C). Thus a connection of a candidate cell to a FULL neighbouring cell will allow the candidate cell to imbibe only if the current meniscus curvature (C) is greater than the critical value (cavity insphere radius) for that cell.

200 !******************************************************************************
!Cell imbibe/non-imbibe logic: !******************************************************************************
! IF FULL(A(K,3))=1 THEN GOTO 210 ELSE GOTO 220
210 IF A(K,7)>C THEN GOTO 280 ELSE GOTO 220
220 IF FULL(A(K,4))=1 THEN GOTO 230 ELSE GOTO 240
230 IF A(K,7)>C THEN GOTO 280 ELSE GOTO 240
240 IF FULL(A(K,5))=1 THEN GOTO 250 ELSE GOTO 260
250 IF A(K,7)>C THEN GOTO 280 ELSE GOTO 260
260 IF FULL(A(K,6))=1 THEN GOTO 270 ELSE GOTO 370
270 IF A(K,7)>C THEN GOTO 280 ELSE GOTO 370
280 !******************************************************************************
    !Individual cell imbibition:                                                   
    !******************************************************************************
    NI=NI+1
    VI=VI+V(K)
    CAND(K)=0
    FULL(K)=1

290 !******************************************************************************
    !Allocation of new candidates:                                               
    !******************************************************************************
    IF FULL(A(K,3))=0 THEN GOTO 300 ELSE GOTO 310
300 CAND(A(K,3))=1
310 IF FULL(A(K,4))=0 THEN GOTO 320 ELSE GOTO 330
320 CAND(A(K,4))=1
330 IF FULL(A(K,5))=0 THEN GOTO 340 ELSE GOTO 350
340 CAND(A(K,5))=1
350 IF FULL(A(K,6))=0 THEN GOTO 360 ELSE GOTO 370
360 CAND(A(K,6))=1
370 !******************************************************************************
    !Capillary pressure equilibrium logic:                                      
    !******************************************************************************
    ! NEXT K
380 IF NI>CPE THEN GOTO 390 ELSE GOTO 400
390 CPE=NI
        GOTO 130
400 SX=0
FOR PP=1 TO 14870
IF CAND(PP)=1 THEN GOTO 402 ELSE GOTO 404
402 SX=SX+1
404 NEXT PP
NF=(NI/14870)
VF=(VI-TV)
PRINT C;NI;VI;NF;VF;SX
PRINT #6, C;"", NI;"", VI;"", NF;"", VF;"", SX
CPE=0
410 NEXT J
420 CLOSE #6
END

10 ! *** ISOCOUNT ***
! Author : D.W. Mellor
! Created: February 1988
! Documentation: This program analyses the output from
! program ISOMER, and counts the frequency of all isomeric
! forms of tetrahedra for the 50% pack definition (i.e.
! LONG>1.0229).
! DIM T(6,3)
20 OPEN "ISOMER.DAT" FOR INPUT AS FILE #3
30 FOR I=1 TO 14870
    INPUT #3, D, TPE, ISO
40 T(TPE,ISO)=T(TPE,ISO)+1
50 NEXT I
60 CLOSE #3
70 FOR I=6 TO 0 STEP -1
    PRINT"TYPE ";I;"LS";(6-I);" = ";T(I,0);T(I,1);T(I,2);T(I,3)
NEXT I

414.
**ISOMER.BAS**

Author: D.W. Mellor
Created: February 1988

Documentation: This program finds the isomeric forms of tetrahedra at the 50% pack definition (i.e. long > 1.01229).

The identities of isomers are:

0 = no isomer (6LS0, 5LS1, 1LS5, 0LS6)
1 = alpha (4LS2, 3LS3, 2LS4)
2 = beta (4LS2, 3LS3, 2LS4)
3 = gamma (3LS3)

Dim L(14870,6), TPE(14870), ISO(14870)
C = 1.01229

20 OPEN "FINEDGE.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "ISOMER.DAT" FOR OUTPUT AS FILE #5

30 INPUT #3, TET

40 FOR I = 1 TO 14870
   INPUT #3, D1, L(I,1), L(I,2), L(I,3), L(I,4), L(I,5), L(I,6)
   INPUT #4, D2, TPE(I)
   NEXT I

50 CLOSE #3, #4

60 FOR I = 1 TO 14870
   IF TPE(I) = 6 OR TPE(I) = 5 OR TPE(I) = 1 OR TPE(I) = 0 THEN GOTO 70 ELSE GO:

70 ! Types with no isomers, ISO = 0
   ISO(I) = 0
   GOTO 400

80 ! Type with isomers,
   IF TPE(I) = 4 THEN GOTO 100 ELSE GOTO 90

90 ! Either a 3LS3 or a 2LS4 structure,
   IF TPE(I) = 3 THEN GOTO 200 ELSE GOTO 95

95 ! Either a 2LS4 structure or a fatal error,
   IF TPE(I) = 2 THEN GOTO 300 ELSE GOTO 99

99 PRINT "~~~~~~~~~FATAL ERROR DETECTED FOR TET. #";I;"~~~~~~~~~"
   GOTO 400

100 IF L(I,1) <= C AND L(I,5) <= C OR L(I,2) <= C AND L(I,6) <= C OR L(I,3) <= C AND L(I,4) <= C THEN GOTO 110 ELSE GOTO 120

110 ISO(I) = 2
   GOTO 400
120 ISO(I) = 1
GOTO 400

200 IF L(I, 1) > C AND L(I, 2) > C AND L(I, 3) > C THEN GOTO 240 ELSE GOTO 210

210 IF L(I, 1) > C AND L(I, 4) > C AND L(I, 6) > C THEN GOTO 240 ELSE GOTO 220

220 IF L(I, 2) > C AND L(I, 4) > C AND L(I, 5) > C THEN GOTO 240 ELSE GOTO 230

230 IF L(I, 3) > C AND L(I, 5) > C AND L(I, 6) > C THEN GOTO 240 ELSE GOTO 250

240 ISO(I) = 2
GOTO 400

250 IF L(I, 1) <= C AND L(I, 2) <= C AND L(I, 3) <= C THEN GOTO 290 ELSE GOTO 26

260 IF L(I, 1) <= C AND L(I, 4) <= C AND L(I, 6) <= C THEN GOTO 290 ELSE GOTO 27

270 IF L(I, 2) <= C AND L(I, 4) <= C AND L(I, 5) <= C THEN GOTO 290 ELSE GOTO 28

280 IF L(I, 3) <= C AND L(I, 5) <= C AND L(I, 6) <= C THEN GOTO 290 ELSE GOTO 29

290 ISO(I) = 3
GOTO 400

295 ISO(I) = 1
GOTO 400

300 IF L(I, 1) > C AND L(I, 5) > C OR L(I, 2) > C AND L(I, 6) > C OR L(I, 3) > C AND L(I, 4) > C THEN GOTO 310 ELSE GOTO 320

310 ISO(I) = 2
GOTO 400

320 ISO(I) = 1

400 .EXT I

500 FOR I = 1 TO 14870

510 PRINT #5, I, ";", TPE(I), ";", ";ISO(I)
NEXT I

520 CLOSE #5
**LENGTHS.BAS**

Created: July 1986
Author: D.W. Mellor
Documentation: This program calculates tetrahedron edge lengths from FINNEY's sphere coordinates. The inputs are:
(i) FILES.DAT which holds x, y, z coords for 4021 spheres
(ii) FILE3.DAT which contains the sequence of spheres in terahedra. There are 14870 terahedra. The output file is FINEDGE.DAT which contains the 89220 tetrahedron edge lengths.

20 DIM L(6), X(4021), Y(4021), Z(4021)
30 OPEN "NEWFILE3.DAT" FOR INPUT AS FILE #3
40 OPEN "NEWFILE5.DAT" FOR INPUT AS FILE #5
50 OPEN "FINEDGE.DAT" FOR OUTPUT AS FILE #6
60 FOR I= 1 TO 4021
70 INPUT #5, DUMMY1, X(I), Y(I), Z(I), DUMMY2
80 NEXT I
90 TET=0
100 IF TET => 14870 THEN GOTO 999
110 INPUT #3, B1, B2, B3, B4
120 TET = TET+1
130 L(1) = (X(B2)-X(B3))*(X(B2)-X(B3))
140 L(1) = L(1)+(Y(B2)-Y(B3))*(Y(B2)-Y(B3))
150 L(1) = L(1)+(Z(B2)-Z(B3))*(Z(B2)-Z(B3))
160 L(2) = (X(B1)-X(B3))*(X(B1)-X(B3))
170 L(2) = L(2)+(Y(B1)-Y(B3))*(Y(B1)-Y(B3))
180 L(2) = L(2)+(Z(B1)-Z(B3))*(Z(B1)-Z(B3))
190 L(3) = (X(B1)-X(B2))*(X(B1)-X(B2))
200 L(3) = L(3)+(Y(B1)-Y(B2))*(Y(B1)-Y(B2))
210 L(3) = L(3)+(Z(B1)-Z(B2))*(Z(B1)-Z(B2))
220 L(4) = (X(B3)-X(B4))*(X(B3)-X(B4))
230 L(4) = L(4)+(Y(B3)-Y(B4))*(Y(B3)-Y(B4))
240 L(4) = L(4)+(Z(B3)-Z(B4))*(Z(B3)-Z(B4))
250 L(5) = (X(B1)-X(B4))*(X(B1)-X(B4))
260 L(5) = L(5)+(Y(B1)-Y(B4))*(Y(B1)-Y(B4))
270 L(5) = L(5)+(Z(B1)-Z(B4))*(Z(B1)-Z(B4))
280 L(6) = (X(B2)-X(B4))*(X(B2)-X(B4))
290 L(6) = L(6)+(Y(B2)-Y(B4))*(Y(B2)-Y(B4))
300 L(6) = L(6)+(Z(B2)-Z(B4))*(Z(B2)-Z(B4))
310 FOR I= 1 TO 6
320 L(I) = SQR(L(I))
330 NEXT I
340 PRINT #6, TET; "", "; L(1); "", "; L(2); "", "; L(3); "", "; L(4); "", "; L(5); "", "; L(6)"
390 GOTO 100
999 CLOSE #3
1000 CLOSE #5
1100 CLOSE #6
1111 END
**NEIGH_0.BAS**

**Author:** D.W. Mellor  
**Created:** February 1988  
**Documentation:** This program finds the distribution of tetrahedral types which are common to (i.e. share one face with) the OLS6 type of tetrahedra.

```plaintext
DIM TPE(14870), NEI(6)
OPEN "WRINEI.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "NEIGH_O.DAT" FOR OUTPUT AS FILE #5

FOR I=1 TO 14870
   INPUT #4, DUMMY, TPE(I)
NEXT I
CLOSE #4

TOT3=0
TOT4=0

FOR J=1 TO 14870
   INPUT #3, DUMMY, X, T1, T2, T3, T4
   IF TPE(J)=0 THEN GOTO 100 ELSE GOTO 130
   NEI(TPE(T1))=NEI(TPE(T1))+1
   NEI(TPE(T2))=NEI(TPE(T2))+1
   NEI(TPE(T3))=NEI(TPE(T3))+1
   IF X=4 THEN GOTO 110 ELSE GOTO 120
   NEI(TPE(T4))=NEI(TPE(T4))+1
   TOT4=TOT4+1
   GOTO 130
   TOT3=TOT3+1
100
120 TOT3=TOT3+1
130 NEXT J

CLOSE #3

PRINT #5, "For all OLS6 reference tetrahedra,"  
PRINT #5, "a total of " ;TOT3+TOT4 ; " were found, of which"  
PRINT #5, " ;TOT3 ; " were surface occurring,"  
PRINT #5, " and ;TOT4 ; " were entirely in the pack."  
PRINT #5, " Distributions of tetrahedral types found are:"  
PRINT #5, " 6LS0 ;NEI(6)  
PRINT #5, " 5LS1 ;NEI(5)  
PRINT #5, " 4LS2 ;NEI(4)  
PRINT #5, " 3LS3 ;NEI(3)  
PRINT #5, " 2LS4 ;NEI(2)  
PRINT #5, " 1LS5 ;NEI(1)  
PRINT #5, " 0LS6 ;NEI(0)
```

**418.**
**NEIGH_1.BAS**

Author: D.W. Mellor

Created: February 1988

Documentation: This program finds the distribution of tetrahedral types which are common to (i.e. share one face with) the 1LS5 type of tetrahedra.

DIM TPE(14870), NEI(6)

OPEN "WRINEI.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "NEIGH_1.DAT" FOR OUTPUT AS FILE #5

FOR I = 1 TO 14870
  INPUT #4, DUMMY, TPE(I)
NEXT I
CLOSE #4

TOT3 = 0
TOT4 = 0

FOR J = 1 TO 14870
  INPUT #3, DUMMY, X, T1, T2, T3, T4
  IF TPE(J) = 1 THEN GOTO 100 ELSE GOTO 130
  NEI(TPE(T1)) = NEI(TPE(T1)) + 1
  NEI(TPE(T2)) = NEI(TPE(T2)) + 1
  NEI(TPE(T3)) = NEI(TPE(T3)) + 1
  IF X = 4 THEN GOTO 110 ELSE GOTO 120
  NEI(TPE(T4)) = NEI(TPE(T4)) + 1
  TOT4 = TOT4 + 1
  GOTO 130

  TOT3 = TOT3 + 1

GOTO 130

CLOSE #3

PRINT #5, "For all 1LS5 reference tetrahedra,",
PRINT #5, "a total of "; TOT3 + TOT4; "; were found, of which"
PRINT #5, ";TOT3; "; were surface occurring,",
PRINT #5, "and "; TOT4; "; were entirely in the pack.",
PRINT #5, "Distributions of tetrahedral types found are:
PRINT #5, "6LS0 "; NEI(6)
PRINT #5, "5LS1 "; NEI(5)
PRINT #5, "4LS2 "; NEI(4)
PRINT #5, "3LS3 "; NEI(3)
PRINT #5, "2LS4 "; NEI(2)
PRINT #5, "1LS5 "; NEI(1)
PRINT #5, "0LS6 "; NEI(0)

CLOSE #5
10 ! *** NEIGH_2.BAS ***
! Author : D.W. Mellor
! Created : February 1988
! Documentation : This program finds the distribution of
! tetrahedral types which are common to (i.e. share one
! face with) the 2LS4 type of tetrahedra.
! DIM TPE(14870), NEI(6)

20 OPEN "WRINEI.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "NEIGH_2.DAT" FOR OUTPUT AS FILE #5

30 FOR I=1 TO 14870
   INPUT #4, DUMMY, TPE(I)
   NEXT I
   CLOSE #4

40 TOT3=0
   TOT4=0

50 FOR J=1 TO 14870
   INPUT #3, DUMMY, X, T1, T2, T3, T4
   IF TPE(J)=2 THEN GOTO 100 ELSE GOTO 130
   NEI(TPE(T1))=NEI(TPE(T1))+1
   NEI(TPE(T2))=NEI(TPE(T2))+1
   NEI(TPE(T3))=NEI(TPE(T3))+1
   IF X=4 THEN GOTO 110 ELSE GOTO 120
110 NEI(TPE(T4))=NEI(TPE(T4))+1
   TOT4=TOT4+1
   GOTO 130
120 TOT3=TOT3+1
130 NEXT J

140 CLOSE #3

150 PRINT #5, "For all 2LS4 reference tetrahedra,"
   PRINT #5, "a total of ";TOT3+TOT4," were found, of which"
   PRINT #5, "TOT3," were surface occurring,"
   PRINT #5, "TOT4," were entirely in the pack."
   PRINT #5, "Distributions of tetrahedral types found are:-"
   PRINT #5, "NEI(6) ";NEI(6)
   PRINT #5, "NEI(5) ";NEI(5)
   PRINT #5, "NEI(4) ";NEI(4)
   PRINT #5, "NEI(3) ";NEI(3)
   PRINT #5, "NEI(2) ";NEI(2)
   PRINT #5, "NEI(1) ";NEI(1)
   PRINT #5, "NEI(0) ";NEI(0)

160 CLOSE #5
10 ! *** NEIGH_3.BAS ***
! Author: D.W. Mellor
! Created: February 1988
! Documentation: This program finds the distribution of
! tetrahedral types which are common to (i.e. share one
! face with) the 3LS3 type of tetrahedra.
! DIM TPE(14870), NEI(6)

20 OPEN "WRINEI.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "NEIGH_3.DAT" FOR OUTPUT AS FILE #5

30 FOR I=1 TO 14870
   INPUT #4, DUMMY, TPE(I)
NEXT I
CLOSE #4

40 TOT3=0
TOT4=0

50 FOR J=1 TO 14870
   INPUT #3, DUMMY, X, T1, T2, T3, T4
   IF TPE(J)=3 THEN GOTO 100 ELSE GOTO 130
   NEI(TPE(T1))=NEI(TPE(T1))+1
   NEI(TPE(T2))=NEI(TPE(T2))+1
   NEI(TPE(T3))=NEI(TPE(T3))+1
   IF X=4 THEN GOTO 110 ELSE GOTO 120
   TOT4=TOT4+1
   GOTO 130
   TOT3=TOT3+1
120 TOT3=TOT3+1

130 NEXT J

140 CLOSE #3

150 PRINT #5, "For all 3LS3 reference tetrahedra,"
PRINT #5, "a total of "#;TOT3+TOT4; " were found, of which"
PRINT #5, "TOT3; " were surface occurring,"
PRINT #5, " and "#;TOT4; " were entirely in the pack."
PRINT #5, " Distributions of tetrahedral types found are:-""n
PRINT #5, "6LS0 "#;NEI(6)
PRINT #5, "5LS1 "#;NEI(5)
PRINT #5, "4LS2 "#;NEI(4)
PRINT #5, "3LS3 "#;NEI(3)
PRINT #5, "2LS4 "#;NEI(2)
PRINT #5, "1LS5 "#;NEI(1)
PRINT #5, "0LS6 "#;NEI(0)

160 CLOSE #5

421.
10 ! *** NEIGH_4.BAS ***
! Author: D.W. Mellor
! Created: February 1988
! Documentation: This program finds the distribution of
tetrahedral types which are common to (i.e. share one
face with) the 4LS2 type of tetrahedra.
! DIM TPE(14870), NEI(6)

20 OPEN "WRINEI.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "NEIGH_4.DAT" FOR OUTPUT AS FILE #5

30 FOR I=1 TO 14870
   INPUT #4, DUMMY, TPE(I)
NEXT I
CLOSE #4

40 TOT3=0
TOT4=0

50 FOR J=1 TO 14870
   INPUT #3, DUMMY, X, T1, T2, T3, T4
   IF TPE(J)=4 THEN GOTO 100 ELSE GOTO 130
   NEI(TPE(T1))=NEI(TPE(T1))+1
   NEI(TPE(T2))=NEI(TPE(T2))+1
   NEI(TPE(T3))=NEI(TPE(T3))+1
   IF X=4 THEN GOTO 110 ELSE GOTO 120
   NEI(TPE(T4))=NEI(TPE(T4))+1
   TOT4=TOT4+1
   GOTO 130
   TOT3=TOT3+1
130 NEXT J

140 CLOSE #3

150 PRINT #5, "For all 4LS2 reference tetrahedra,"
PRINT #5, "a total of "; TOT3+TOT4; " were found, of which"
PRINT #5, "TOT3; " were surface occurring,"
PRINT #5, "and "; TOT4; " were entirely in the pack."
PRINT #5, "Distributions of tetrahedral types found are:-"
PRINT #5, "6LS0 "; NEI(6)
PRINT #5, "5LS1 "; NEI(5)
PRINT #5, "4LS2 "; NEI(4)
PRINT #5, "3LS3 "; NEI(3)
PRINT #5, "2LS4 "; NEI(2)
PRINT #5, "1LS5 "; NEI(1)
PRINT #5, "0LS6 "; NEI(0)

160 CLOSE #5

422.
A
10 ! *** NEIGH_5.BAS ***
! Author : D.W.Mellor
! Created : February 1988
! Documentation : This program finds the distribution of
! tetrahedral types which are common to (i.e. share one
! face with) the 5LS1 type of tetrahedra.
! DIM TPE(14870),NEI(6)

20 OPEN "WRINEI.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "NEIGH_5.DAT" FOR OUTPUT AS FILE #5

30 FOR I=1 TO 14870
   INPUT #4,DUMMY,TPE(I)
NEXT I
CLOSE #4

40 TOT3=0
TOT4=0

50 FOR J=1 TO 14870
   INPUT #3,DUMMY,X,T1,T2,T3,T4
   IF TPE(J)=5 THEN GOTO 100 ELSE GOTO 130
100 NEI(TPE(T1))=NEI(TPE(T1))+1
   NEI(TPE(T2))=NEI(TPE(T2))+1
   NEI(TPE(T3))=NEI(TPE(T3))+1
   IF X=4 THEN GOTO 110 ELSE GOTO 120
110 NEI(TPE(T4))=NEI(TPE(T4))+1
   TOT4=TOT4+1
   GOTO 130
120 TOT3=TOT3+1
130 NEXT J

140 CLOSE #3

150 PRINT #5,"For all 5LS1 reference tetrahedra,"
PRINT #5,"a total of ";TOT3+TOT4," were found, of which"
PRINT #5," ";TOT3," were surface occurring,"
PRINT #5," ";TOT4," were entirely in the pack."
PRINT #5," Distributions of tetrahedral types found are:-"
PRINT #5," 6LS0 ";NEI(6)
PRINT #5," 5LS1 ";NEI(5)
PRINT #5," 4LS2 ";NEI(4)
PRINT #5," 3LS3 ";NEI(3)
PRINT #5," 2LS4 ";NEI(2)
PRINT #5," 1LS5 ";NEI(1)
PRINT #5," 0LS6 ";NEI(0)

160 CLOSE #5

423.
**NEIGH_6.BAS**

*Author: D. W. Mellor*

*Created: February 1988*

*Documentation: This program finds the distribution of tetrahedral types which are common to (i.e. share one face with) the 6LS0 type of tetrahedra.*

```basic
DIM TPE(14870), NEI(6)

20 OPEN "WRINEI.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR INPUT AS FILE #4
OPEN "NEIGH_6.DAT" FOR OUTPUT AS FILE #5

30 FOR I=1 TO 14870
   INPUT #4, DUMMY, TPE(I)
   NEXT I
   CLOSE #4

40 TOT3=0
   TOT4=0

50 FOR J=1 TO 14870
   INPUT #3, DUMMY, X, T1, T2, T3, T4
   IF TPE(J)=6 THEN GOTO 100 ELSE GOTO 130
   NEI(TPE(T1))=NEI(TPE(T1))+1
   NEI(TPE(T2))=NEI(TPE(T2))+1
   NEI(TPE(T3))=NEI(TPE(T3))+1
   IF X=4 THEN GOTO 110 ELSE GOTO 120
   NEI(TPE(T4))=NEI(TPE(T4))+1
   TOT4=TOT4+1
   GOTO 130
   TOT3=TOT3+1

100 NEI(TPE(T2))=NEI(TPE(T2))+1
   GOTO 130

110 NEI(TPE(T4))=NEI(TPE(T4))+1
   TOT4=TOT4+1
   GOTO 130

120 TOT3=TOT3+1

130 NEXT J

140 CLOSE #3

150 PRINT #5,"For all 6LS0 reference tetrahedra,"
   PRINT #5,"a total of ";TOT3+TOT4," were found, of which"
   PRINT #5," ";TOT3," were surface occurring,"
   PRINT #5," and ";TOT4," were entirely in the pack."
   PRINT #5," Distributions of tetrahedral types found are:-"
   PRINT #5," 6LS0 ";NEI(6)
   PRINT #5," 5LS1 ";NEI(5)
   PRINT #5," 4LS2 ";NEI(4)
   PRINT #5," 3LS3 ";NEI(3)
   PRINT #5," 2LS4 ";NEI(2)
   PRINT #5," 1LS5 ";NEI(1)
   PRINT #5," 0LS6 ";NEI(0)

160 CLOSE #5
```

424.
Author: D.W. Mellor
Created: February 1988
Documentation: This program finds the identity of neighbouring tetrahedra. By definition, such tetrahedra share a face with the reference tetrahedron, so there are a maximum of 4 neighbours (tetrahedron not at pack surface), and a minimum of 3 (tetrahedron at pack surface)

The output format is:
A, X, T1, T2, T3, T4
Where, A=(reference) tetrahedron number
X=number of neighbours
T1-T4=identity of neighbours (consistent with sequence used in FINEDGE.dat)

DIM X(14870,12), TET(4), SCAN(14870)

20 OPEN "NEWFILE3.DAT" FOR INPUT AS FILE #3
OPEN "NET1.DAT" FOR OUTPUT AS FILE #6

30 FOR I=1 TO 14870
INPUT #3, A, B, C, D
X(I,1)=A
(I,2)=B
(I,3)=C
X(I,4)=A
X(I,5)=B
X(I,6)=D
X(I,7)=A
X(I,8)=C
X(I,9)=D
X(I,10)=B
X(I,11)=C
X(I,12)=D
NEXT I
CLOSE #3

40 FOR J=1 TO 14870
K=0
TOT=0
FOR Z=1 TO 4
TET(Z)=0
NEXT Z

45 K=K+1
IF SCAN(K)=4 THEN GOTO 45 ELSE GOTO 50

50 IF J=K THEN GOTO 45 ELSE GOTO 60

60 FOR A=0 TO 9 STEP 3
FOR B=0 TO 9 STEP 3

70 IF X(J,A+1)=X(K,B+1) AND X(J,A+2)=X(K,B+2) AND X(J,A+3)=X(K,B+3) THEN:
ELSE GOTO 90

425.
80 TOT=TOT+1
    TET(TOT)=K

90 NEXT B

100 NEXT A

110 IF TOT=4 OR K=14870 THEN GOTO 120 ELSE GOTO 45

120 PRINT #6,J;"",";TOT;",";TET(1);",";TET(2);",";TET(3);",";TET(4)
    SCAN(TET(1))=SCAN(TET(1)+1)
    SCAN(TET(2))=SCAN(TET(2)+1)
    SCAN(TET(3))=SCAN(TET(3)+1)
    SCAN(TET(4))=SCAN(TET(4)+1)
    PRINT J

130 NEXT J

140 CLOSE #6

END
10 ! *** PMATRIX ***
!
! This program uses the cell-face matrix [P] output by program P in
! order to calculate the cell-cell matrix [N']. This estimate of [N']
! may then be compared with the fully observed matrix [N] for the
! Finney model.
!
! DIM S(3), P(6,3), X(6,6)
OPEN "PMATRIX.DAT" FOR OUTPUT AS FILE #3
PRINT #3," *** PMATRIX.DAT ***

20 PRINT #3,"
PRINT #3," INPUT DATA: CELL-FACE MATRIX [P] FOR FINNEY MODEL"
PRINT #3," DATA FROM PROGRAM P"
PRINT #3,"
PRINT #3,"
FOR I=0 TO 6
FOR J=0 TO 3
READ P(I,J)
NEXT J
NEXT I
PRINT #3," J=0 J=1 J=2 J=3"
PRINT #3,"
FOR I=0 TO 6
PRINT #3," I=":I,P(I,0),P(I,1),P(I,2),P(I,3)
NEXT I
PRINT #3,"
PRINT #3,""

30 DATA 216,0,0,0
DATA 1511,1523,0,0
DATA 2252,8982,2286,0
DATA 627,11356,10736,915
DATA 0,2379,9330,2418
DATA 0,0,1378,1402
DATA 0,0,0,211

40 PRINT #3," CALCULATE Sj"
PRINT #3,""
FOR J=0 TO 3
FOR I=0 TO 6
S(J)=S(J)+P(I,J)
NEXT I
PRINT #3," S(J)=S(J)+P(I,J)"
NEXT J
PRINT #3,""
PRINT #3,""
PRINT #3," NOW CALCULATE CELL-CELL MATRIX, [X]"
PRINT #3,""

427.
50 FOR Q=0 TO 6
   FOR I=0 TO 6
   FOR J=0 TO 3
      X(Q,I)=X(Q,I)+(P(I,J)/S(J))*P(Q,J)
   NEXT J
   NEXT I
   NEXT Q

55 FOR I=0 TO 6
   FOR J=0 TO 6
      X(I,J)=FIX(X(I,J)+0.5)
   NEXT J
   NEXT I

60 !PRINT #3," I J X(I,J)"
!FOR J=0 TO 6
!FOR I=0 TO 6
!PRINT #3,I,J,FIX(X(I,J)+0.5)
!NEXT I
!NEXT J

70 FOR I=0 TO 6
   PRINT #3,X(I,0);TAB(10);X(I,1);TAB(20);X(I,2);TAB(30);X(I,3);TAB(40)
   B(60);X(I,6)
   NEXT I
This program finds the observed cell-face matrix \([P]\) for the 14870 simplicial cells of the Finney packing.

\[
\begin{align*}
\text{DIM } & C(4), N1(4), N2(4), S(3) \\
\text{DIM } & P(6,3), CELSPH(14870,4), X(4021), Y(4021), Z(4021) \\
\text{XT}=1.01229
\end{align*}
\]

20 OPEN "WRINED.DAT" FOR INPUT AS FILE #4
OPEN "NEWFILE3.DAT" FOR INPUT AS FILE #3
OPEN "NEWFILE5.DAT" FOR INPUT AS FILE #5
OPEN "TYPE.DAT" FOR INPUT AS FILE #6
OPEN "P.DAT" FOR OUTPUT AS FILE #7

30 FOR K=1 TO 14870
   INPUT #3, CELSPH(K,1), CELSPH(K,2), CELSPH(K,3), CELSPH(K,4)
   NEXT K

40 FOR M=1 TO 4021
   INPUT #5, DUMMY1, X(M), Y(M), Z(M), DUMMY2
   NEXT M

50 FOR II=1 TO 14870
   INPUT #6, DUMMY3, TT
   INPUT #4, A, B, C(1), C(2), C(3), C(4)

60 FOR JJ=1 TO 4
   IF C(JJ) > 0 THEN GOTO 70 ELSE GOTO 100

70 N1(1)=CELSPH(A,1)
   N1(2)=CELSPH(A,2)
   N1(3)=CELSPH(A,3)
   N1(4)=CELSPH(A,4)
   N2(1)=CELSPH(C(JJ),1)
   N2(2)=CELSPH(C(JJ),2)
   N2(3)=CELSPH(C(JJ),3)
   N2(4)=CELSPH(C(JJ),4)

80 CALL SHAR(N1(), N2(), S())
   CALL THRS(XT, X(), Y(), Z(), S(), QQ)

90 P(TT,QQ)=P(TT,QQ)+1

100 NEXT JJ

110 NEXT II

120 SUMP=0
   FOR I=0 TO 6
      SUMP=SUMP+P(I,0)+P(I,1)+P(I,2)+P(I,3)
   PRINT #7, P(I,0);",";P(I,1);",";P(I,2);",";P(I,3)
   NEXT I

130 PRINT "MATRIX TOTAL=";SUMP

140 CLOSE #3, #4, #5, #6, #7
10 ! *** TYPE.BAS ***
! Author : D.W. Mellor
! Created : February 1988
! Documentation: This program finds the number of long
! edges in each tetrahedron for a fixed definition of
! edgelength. The 50% pack definition of long>1.01229
! is used.
!
DIM L(14870,6), T(14870)

20 OPEN "FINEDGE.DAT" FOR INPUT AS FILE #3
OPEN "TYPE.DAT" FOR OUTPUT AS FILE #4

30 C=1.01229
INPUT #3, TET

40 FOR I=1 TO 14870
   INPUT #3, D, L(I,1), L(I,2), L(I,3), L(I,4), L(I,5), L(I,6)
   T=0

50 FOR J=1 TO 6
   IF L(I,J)>C THEN GOTO 60 ELSE GOTO 70

60 T=T+1

70 NEXT J

80 PRINT #4, I;",", T

90 NEXT I

100 CLOSE #3, #4
10 ! *** VORONHIST.BAS ***
19 ! Author: D.W. Mellor
20 ! Created: September 1987
21 ! Documentation: This program produces a histogram of
22 ! the types of Voronoi polyhedra for the central 2000
23 ! spheres in Finney's pack. The types are distinguished
24 ! on the basis of the number of component tetrahedra.
25 !
26 ! DIM X(100)
27 !
28 20 OPEN "VORONOI.DAT" FOR INPUT AS FILE #3
29 !
30 30 FOR I=1 TO 2000
31 31 INPUT #3, D, Z
32 32 X(Z)=X(Z)+1
33 33 NEXT I
34 !
35 40 CLOSE #3
36 !
37 50 OPEN "VORONHIST.DAT" FOR OUTPUT AS FILE #4
38 !
39 51 FOR J=1 TO 100
40 52 PRINT #4, J; ""; X(J)
41 53 NEXT J
42 54 CLOSE #4
43 END
**VORONOI.BAS**

Author: D.W. Mellor

Created: September 1987

Documentation: This program counts the number of times that each of the central 2000 spheres in Finney's pack occurs in a tetrahedron. This number, for each individual sphere, defines that sphere's Voronoi polyhedron.

DIM X(14871,4), Y(2000)

20 OPEN "NEWFILE3.DAT" FOR INPUT AS FILE#3
OPEN "VORONOI.DAT" FOR OUTPUT AS FILE #4

30 FOR I=1 TO 14871
   INPUT #3,X(I,1),X(I,2),X(I,3),X(I,4)
   NEXT I

40 FOR J=1 TO 2000
   FOR K=1 TO 14871
      50 IF X(K,1)=J OR X(K,2)=J OR X(K,3)=J OR X(K,4)=J THEN GOTO 60 ELSE GOTO 70
      60 Y(J)=Y(J)+1
      NEXT K
   NEXT J

90 FOR J=1 TO 2000
   PRINT #4,J;",";Y(J)
   NEXT J

100 CLOSE #3
CLOSE #4
END
**FORWARD**

```basic
INPUT "ENTER NAME OF INPUT FILE"; A$
DIM X(200), G(200), L(800), IN(800), OUT(800), HIST(800), DELTA(5,5)
A$ is the boxcar model, eg EB2.dat

20 OPEN A$ FOR INPUT AS FILE #6
25 OPEN "HISTEDGE3.DAT" FOR INPUT AS FILE #7
30 FOR I=1 TO 800
40 INPUT #6, L(I), IN(I)
45 INPUT #7, DUMMY, HIST(I)
50 NEXT I
60 INPUT "ENTER MINIMUM AMPLITUDE OF SPIKE"; Z
70 INPUT "ENTER SPIKE INCREMENT"; ZI
75 INPUT "ENTER MINIMUM VALUE FOR SIGMA"; M
80 INPUT "ENTER SIGMA INCREMENT"; MI
R=1
C=1
90 FOR SPI=Z TO (Z+4*ZI) STEP ZI
100 FOR SG=M TO (M+4*MI) STEP MI
110 IN(201)=SPI
120 SIG=SG
130 TOT=0
140 SUM=0
150 FOR I=1 TO 200
160 X(I)=((I-9900)/10000+0.00005)
170 G(I)=EXP(-0.5*((X(I)-1.00005)**2)/SIG**2)
180 SUM=SUM+G(I)
190 NEXT I
200 FOR I=1 TO 200
210 G(I)=G(I)/SUM
220 TOT=TOT+G(I)
228 NEXT I
250 CLOSE #6
255 CLOSE #7
260 FOR I=100 TO 700
270 VA=0
272 VA=IN(I)*G(100)
280 FOR J=1 TO 99
290 VA=VA+IN(I+J)*G(100+J)
292 VA=VA+IN(I-J)*G(100-J)
300 NEXT J
310 OUT(I)=VA
330 NEXT I
350 FOR I=1 TO 120
360 OUT(I)=0
370 HIST(I)=0
380 NEXT I
390 FOR I=320 TO 800
400 OUT(I)=0
410 HIST(I)=0
420 NEXT I
430 N=800
440 L=0.0001
450 CALL DIFF(HIST(), OUT(), N, L, SSUM)
DELTA(R, C)=SSUM
R=R+1
IF R=>6 THEN R=1 ELSE R=R
```

433.
470 NEXT SG
C=C+1
480 NEXT SPI
PRINT"SPIKE AMPLITUDE"
PRINT"
PRINT Z, (Z+ZI), (Z+2*ZI), (Z+3*ZI), (Z+4*ZI)
PRINT"
PRINT"
500 FOR R=1 TO 5
PRINT DELTA(R,1), DELTA(R,2), DELTA(R,3), DELTA(R,4), DELTA(R,5), M+(R-1)*MI
PRINT"
NEXT R
PRINT"
PRINT"
PRINT"
PRINT"
PRINT"
PRINT"
PRINT"
PRINT"TABLE"
PRINT"
PRINT"
PRINT"MODEL=";As
**VSMOOTH.BAS**

Author: D.W. Mellor  
Created: August 1986  
Documentation: This program accesses file HISTOGRAM3.DAT as input and passes a 9-point moving average over the data. This is written to file VSMOOTHEdge.DAT. The sampling interval of the data is 0.0001 hard sphere diameters. The width of the smoothing filter is therefore 0.0005 diameters. Since the current best estimate for sigma is 0.00221, the smoothing process is under the experimental error, and I will not, therefore, smooth real structure in the data.

```basic
DIM L(800), IN(800), OUT(800)

20 OPEN "HISTEDGE3.DAT" FOR INPUT AS FILE #6
30 OPEN "VSMOOTHEdge.DAT" FOR OUTPUT AS FILE #7
40 FOR I=1 TO 800
50 INPUT #6, L(I), IN(I)
60 NEXT I
70 FOR I=5 TO 795
80 OUT(I)=(IN(I)+IN(I-1)+IN(I-2)+IN(I+1)+IN(I+2))
   OUT(I)=(OUT(I)+IN(I-3)+IN(I+3)+IN(I-4)+IN(I+4))
   OUT(I)=OUT(I)/9
90 PRINT #7, L(I), ",", FIX(OUT(I)+0.5)
100 NEXT I
110 CLOSE #6
120 CLOSE #7
130 END
```
APPENDIX 'B'

SECTION B3 - DATA FILES

BOXCAR MODELS .................. 437
FINEDGE.DAT ..................... 439
NEWFILE3.DAT .................... 440
NEWFILES.DAT .................... 441
TYPE.DAT ......................... 442
WRINED.DAT ....................... 443

436.
The following data sets are the boxcar models of the idealised edgelength distribution (ie excluding the hard sphere contact "spike") used to derive an estimate of sigma (standard deviation) of normally distributed experimental error specific to simplicial cell edgelength measurements of the Finney model described in Chapter 3.

<table>
<thead>
<tr>
<th>EDGE LENGTH</th>
<th>FREQUENCY</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTERVAL</td>
<td>EB1</td>
</tr>
<tr>
<td>.99975</td>
<td>0</td>
</tr>
<tr>
<td>.99995</td>
<td>0</td>
</tr>
<tr>
<td>1.00005</td>
<td>135</td>
</tr>
<tr>
<td>1.00025</td>
<td>132</td>
</tr>
<tr>
<td>1.00035</td>
<td>130</td>
</tr>
<tr>
<td>1.00045</td>
<td>128</td>
</tr>
<tr>
<td>1.00055</td>
<td>127</td>
</tr>
<tr>
<td>1.00065</td>
<td>125</td>
</tr>
<tr>
<td>1.00075</td>
<td>123</td>
</tr>
<tr>
<td>1.00085</td>
<td>122</td>
</tr>
<tr>
<td>1.00095</td>
<td>120</td>
</tr>
<tr>
<td>1.00105</td>
<td>118</td>
</tr>
<tr>
<td>1.00115</td>
<td>116</td>
</tr>
<tr>
<td>1.00125</td>
<td>114</td>
</tr>
<tr>
<td>1.00135</td>
<td>112</td>
</tr>
<tr>
<td>1.00145</td>
<td>110</td>
</tr>
<tr>
<td>1.00155</td>
<td>109</td>
</tr>
<tr>
<td>1.00165</td>
<td>108</td>
</tr>
<tr>
<td>1.00175</td>
<td>107</td>
</tr>
<tr>
<td>1.00185</td>
<td>105</td>
</tr>
<tr>
<td>1.00195</td>
<td>104</td>
</tr>
<tr>
<td>1.00205</td>
<td>102</td>
</tr>
<tr>
<td>1.00215</td>
<td>100</td>
</tr>
<tr>
<td>1.00225</td>
<td>99</td>
</tr>
<tr>
<td>1.00235</td>
<td>97</td>
</tr>
<tr>
<td>1.00245</td>
<td>96</td>
</tr>
<tr>
<td>1.00255</td>
<td>95</td>
</tr>
<tr>
<td>1.00265</td>
<td>93</td>
</tr>
<tr>
<td>1.00275</td>
<td>92</td>
</tr>
<tr>
<td>1.00285</td>
<td>91</td>
</tr>
<tr>
<td>1.00295</td>
<td>90</td>
</tr>
<tr>
<td>1.00305</td>
<td>88</td>
</tr>
<tr>
<td>1.00315</td>
<td>87</td>
</tr>
<tr>
<td>1.00325</td>
<td>86</td>
</tr>
<tr>
<td>1.00335</td>
<td>85</td>
</tr>
<tr>
<td>1.00345</td>
<td>84</td>
</tr>
<tr>
<td>1.00355</td>
<td>83</td>
</tr>
<tr>
<td>1.00365</td>
<td>82</td>
</tr>
<tr>
<td>1.00375</td>
<td>81</td>
</tr>
<tr>
<td>1.00385</td>
<td>80</td>
</tr>
<tr>
<td>1.00395</td>
<td>79</td>
</tr>
<tr>
<td>1.00405</td>
<td>78</td>
</tr>
<tr>
<td>1.00415</td>
<td>77</td>
</tr>
<tr>
<td>1.00425</td>
<td>76</td>
</tr>
<tr>
<td>1.00435</td>
<td>75</td>
</tr>
<tr>
<td>1.00445</td>
<td>75</td>
</tr>
<tr>
<td>1.00455</td>
<td>74</td>
</tr>
<tr>
<td>1.00465</td>
<td>73</td>
</tr>
<tr>
<td>1.00475</td>
<td>72</td>
</tr>
<tr>
<td>1.00485</td>
<td>72</td>
</tr>
<tr>
<td>1.00495</td>
<td>71</td>
</tr>
<tr>
<td>BOXCAR MODELS (CONTINUED)</td>
<td></td>
</tr>
<tr>
<td>---------------------------</td>
<td></td>
</tr>
<tr>
<td>1.00505</td>
<td>71 84 98 98 98 98 98 98</td>
</tr>
<tr>
<td>1.00515</td>
<td>70 83 97 97 97 97 97 97</td>
</tr>
<tr>
<td>1.00525</td>
<td>70 82 95 95 95 95 95 95</td>
</tr>
<tr>
<td>1.00535</td>
<td>69 81 93 93 93 93 93 93</td>
</tr>
<tr>
<td>1.00545</td>
<td>69 80 92 92 92 92 92 92</td>
</tr>
<tr>
<td>1.00555</td>
<td>68 79 90 90 90 90 90 90</td>
</tr>
<tr>
<td>1.00565</td>
<td>68 78 89 89 89 89 89 89</td>
</tr>
<tr>
<td>1.00575</td>
<td>67 77 87 87 87 87 87 87</td>
</tr>
<tr>
<td>1.00585</td>
<td>67 76 86 86 86 86 86 86</td>
</tr>
<tr>
<td>1.00595</td>
<td>66 75 85 85 85 85 85 85</td>
</tr>
<tr>
<td>1.00605</td>
<td>66 74 83 83 83 83 83 83</td>
</tr>
<tr>
<td>1.00615</td>
<td>65 73 82 82 82 82 82 82</td>
</tr>
<tr>
<td>1.00625</td>
<td>65 73 81 81 81 81 81 81</td>
</tr>
<tr>
<td>1.00635</td>
<td>64 72 80 80 80 80 80 80</td>
</tr>
<tr>
<td>1.00645</td>
<td>64 71 78 78 78 78 78 78</td>
</tr>
<tr>
<td>1.00655</td>
<td>63 71 77 77 77 77 77 77</td>
</tr>
<tr>
<td>1.00665</td>
<td>63 70 76 76 76 76 76 76</td>
</tr>
<tr>
<td>1.00675</td>
<td>63 69 75 75 75 75 75 75</td>
</tr>
<tr>
<td>1.00685</td>
<td>62 68 73 73 73 73 73 73</td>
</tr>
<tr>
<td>1.00695</td>
<td>62 68 72 72 72 72 72 72</td>
</tr>
<tr>
<td>1.00705</td>
<td>62 67 71 71 71 71 71 71</td>
</tr>
<tr>
<td>1.00715</td>
<td>62 66 70 70 70 70 70 70</td>
</tr>
<tr>
<td>1.00725</td>
<td>61 65 69 69 69 69 69 69</td>
</tr>
<tr>
<td>1.00735</td>
<td>61 65 68 68 68 68 68 68</td>
</tr>
<tr>
<td>1.00745</td>
<td>61 64 67 67 67 67 67 67</td>
</tr>
<tr>
<td>1.00755</td>
<td>61 63 66 66 66 66 66 66</td>
</tr>
<tr>
<td>1.00765</td>
<td>60 63 65 65 65 65 65 65</td>
</tr>
<tr>
<td>1.00775</td>
<td>60 62 64 64 64 64 64 64</td>
</tr>
<tr>
<td>1.00785</td>
<td>60 61 63 63 63 63 63 63</td>
</tr>
<tr>
<td>1.00795</td>
<td>60 61 63 63 63 63 63 63</td>
</tr>
<tr>
<td>1.00805</td>
<td>59 60 62 62 62 62 62 62</td>
</tr>
<tr>
<td>1.00815</td>
<td>59 59 61 61 61 61 61 61</td>
</tr>
<tr>
<td>1.00825</td>
<td>59 59 60 60 60 60 60 60</td>
</tr>
<tr>
<td>1.00835</td>
<td>58 58 59 59 59 59 59 59</td>
</tr>
<tr>
<td>1.00845</td>
<td>57 57 58 58 58 58 58 58</td>
</tr>
<tr>
<td>1.00855</td>
<td>57 57 58 58 58 58 58 58</td>
</tr>
<tr>
<td>1.00865</td>
<td>57 57 57 57 57 57 57 57</td>
</tr>
<tr>
<td>1.00875</td>
<td>56 56 57 57 57 57 57 57</td>
</tr>
<tr>
<td>1.00885</td>
<td>56 56 56 56 56 56 56 56</td>
</tr>
<tr>
<td>1.00895</td>
<td>56 56 56 56 56 56 56 56</td>
</tr>
<tr>
<td>1.00905</td>
<td>55 55 55 55 55 55 55 55</td>
</tr>
<tr>
<td>1.00915</td>
<td>55 55 55 55 55 55 55 55</td>
</tr>
<tr>
<td>1.00925</td>
<td>54 54 54 54 54 54 54 54</td>
</tr>
<tr>
<td>1.00935</td>
<td>54 54 54 54 54 54 54 54</td>
</tr>
<tr>
<td>1.00945</td>
<td>54 54 54 54 54 54 54 54</td>
</tr>
<tr>
<td>1.00955</td>
<td>54 54 54 54 54 54 54 54</td>
</tr>
<tr>
<td>1.00965</td>
<td>53 53 53 53 53 53 53 53</td>
</tr>
<tr>
<td>1.00975</td>
<td>53 53 53 53 53 53 53 53</td>
</tr>
<tr>
<td>1.00985</td>
<td>53 53 53 53 53 53 53 53</td>
</tr>
<tr>
<td>1.00995</td>
<td>52 52 52 52 52 52 52 52</td>
</tr>
<tr>
<td>1.01005</td>
<td>52 52 52 52 52 52 52 52</td>
</tr>
<tr>
<td>1.01015</td>
<td>52 52 52 52 52 52 52 52</td>
</tr>
<tr>
<td>1.01025</td>
<td>52 52 52 52 52 52 52 52</td>
</tr>
<tr>
<td>1.01035</td>
<td>52 52 52 52 52 52 52 52</td>
</tr>
<tr>
<td>1.01045</td>
<td>51 51 51 51 51 51 51 51</td>
</tr>
<tr>
<td>1.01055</td>
<td>51 51 51 51 51 51 51 51</td>
</tr>
<tr>
<td>1.01065</td>
<td>51 51 51 51 51 51 51 51</td>
</tr>
<tr>
<td>1.01075</td>
<td>51 51 51 51 51 51 51 51</td>
</tr>
<tr>
<td>1.01085</td>
<td>50 50 50 50 50 50 50 50</td>
</tr>
<tr>
<td>1.01095</td>
<td>50 50 50 50 50 50 50 50</td>
</tr>
<tr>
<td>1.01105</td>
<td>50 50 50 50 50 50 50 50</td>
</tr>
<tr>
<td>1.01115</td>
<td>50 50 50 50 50 50 50 50</td>
</tr>
<tr>
<td>1.01125</td>
<td>49 49 49 49 49 49 49 49</td>
</tr>
<tr>
<td>1.01135</td>
<td>49 49 49 49 49 49 49 49</td>
</tr>
<tr>
<td>1.01145</td>
<td>49 49 49 49 49 49 49 49</td>
</tr>
</tbody>
</table>
Structure of data file FINEDGE.DAT

<table>
<thead>
<tr>
<th>COLUMN</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
</tr>
<tr>
<td>--------</td>
</tr>
<tr>
<td>14870</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

Column A of the first line is the number of following lines (14870). Column A is the simplicial cell identity, columns B to G are the cell edgelength values in sphere diameters. The sequence of edgelengths is as given in figure 3.3 in the main text of this thesis.
Structure of data file NEWFILE3.DAT

<table>
<thead>
<tr>
<th>COLUMN</th>
</tr>
</thead>
<tbody>
<tr>
<td>A  B  C  D</td>
</tr>
<tr>
<td>1, 2, 3, 5</td>
</tr>
<tr>
<td>1, 2, 3, 9</td>
</tr>
<tr>
<td>1, 2, 4, 6</td>
</tr>
<tr>
<td>1, 2, 4, 8</td>
</tr>
<tr>
<td>. . . .</td>
</tr>
<tr>
<td>. . . .</td>
</tr>
<tr>
<td>2000, 2317, 2433, 3149</td>
</tr>
<tr>
<td>2000, 2317, 2639, 3149</td>
</tr>
<tr>
<td>2000, 2433, 2899, 3149</td>
</tr>
<tr>
<td>2000, 2639, 2899, 3149</td>
</tr>
</tbody>
</table>

| A  B  C  D |
| 1 -------- COLUMN -------- |

Column A, B, C & D are the four sphere identities of the individual simplicial cells. Note that cell number is not explicitly declared, so that cell number must be identified by counting as the file is read. For example, the identities of the four spheres which define simplicial cell number 1 are 1,2,3,5. Similarly, the identities of the four spheres which define simplicial cell number 14869 are 2000,2433,2899,3149.
### Structure of data file NEWFILE5.DAT

<table>
<thead>
<tr>
<th>COLUMN</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>4018</td>
</tr>
<tr>
<td>4019</td>
</tr>
<tr>
<td>4020</td>
</tr>
<tr>
<td>4021</td>
</tr>
</tbody>
</table>

Column A is the sphere identity, columns B, C and D are the x, y, z coordinates (respectively) for the sphere identified in column A. Column E is not used in the present work.
Structure of data file TYPE.DAT

COLUMN

A  B

1 , 3..............................[FIRST LINE]
2 , 4
3 , 3
4 , 4
...
...
...
...
14867 , 2
14868 , 2
14869 , 4
14870 , 4..............................[LAST LINE]

A  B

COLUMN

Column A is the simplicial cell identity, and column B is the number (x) of state 'L' edges in that cell. This enables cell class to be immediately recognised as xLS(6-x). The edgelength threshold value used is Xt=1.01229. For example, simplicial cell number 14869 has 4 edges in state 'L' and is therefore belongs to the 4LS2 class.
Structure of data file WRINED.DAT

<table>
<thead>
<tr>
<th>COLUMN</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
</tr>
<tr>
<td>B</td>
</tr>
<tr>
<td>C</td>
</tr>
<tr>
<td>D</td>
</tr>
<tr>
<td>E</td>
</tr>
<tr>
<td>F</td>
</tr>
</tbody>
</table>

1, 4, 2, 5, 8, 25                       [FIRST LINE]
2, 4, 1, 7, 10, 26
3, 4, 4, 6, 11, 29
4, 4, 3, 5, 12, 27

...........................

A B C D E F

14867, 3, 12881, 14868, 14869, 0
14868, 3, 13205, 14867, 14870, 0
14869, 3, 14866, 14867, 14870, 0
14870, 3, 14865, 14868, 14869, 0       [LAST LINE]

Column A = Identity of reference cell
Column B = Number of immediate neighbour cells to A
Column C to F = Identities of neighbour cells
Note: When column B = 3, one of the columns C to F must identify cell zero as a neighbour. Cell zero is the sphere packing outer surface.