

ANALYSIS OF THE POROSITY VARIATIONS IN A PEBBLE-BED REACTOR CORE

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I thank God for the talents I have received. I thank Him for opportunities, and courage to take them. I thank Him for what He has given me.

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ABSTRACT

The variation in porosity of a packed column is an important parameter in its design. The flow patterns, mass transfer, heat transfer, and other transfer phenomena are dependent on the porosity variations in the column.

Physical experiments are normally employed to study the porosity characteristics of packed columns. Only a few numerical investigations into the porosity of packed columns have been performed.

The objective of this study is to develop numerical procedures to analyse the porosity of numerically generated packed columns (axial distribution, radial distribution, and representative elementary volume). Numerical procedures have the advantage of better accuracy and are easier and faster (than experimental studies) to conduct.

The development of the models is discussed in detail, and the algorithms and implementation of the codes are explained. Validation tests that were conducted show that the implementation of the models is correct.

Four data sets were analysed with these procedures. These preliminary results show the general trends discussed in the literature. The results suggest that the numerical models were correctly derived and implemented. The results also indicate that the numerically generated packed beds are (relatively) good representations of physical packed beds.

OPSOMMING

Die variasie in porositeit is 'n belangrike faktor in die ontwerp van 'n gepakte bed. Die vloeipatrone, massa-oordrag, hitte-oordrag, en ander oordragsverskynsels is afhanklik van die variasie in die porositeit van die bed.

Die porositeitskenmerke van gepakte beddens word normaalweg bestudeer deur middel van eksperimentele studies. Slegs enkele numeriese ondersoeke van die porositeit van gepakte beddens is al uitgevoer.

Die doel van hierdie studie is om numeriese metodes te ontwikkel om die porositeit van numeries gegenereerde gepakte beddens te analiseer (aksiale verspreiding, radiale verspreiding, en kleinste verteenwoordigende volume). Numeriese prosedures besit die voordeel van beter akkuraatheid, en is makliker en vinniger (as eksperimentele studies) om uit te voer.

Die ontwikkeling van die modelle word in detail bespreek, en die algoritmes en implementering van die kodes word uiteengesit in die verslag. Validasie toetse is gedoen om te bevestig dat die modelle korrek geïmplementeer is.

Vier stelle data is geanaliseer met behulp van die prosedures. Die voorlopige resultate voorspel die algemene verskynsels wat in die literatuur beskryf word. Die resultate dui daarop dat die numeriese metodes korrek afgelei en geïmplementeer is. Die resultate dui ook aan dat die numeries gegenereerde gepakte beddens 'n (redelike) goeie voorstelling is van fisiese gepakte beddens.

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NOMENCLATURE

a	Pore cross-sectional area
a_1, a_2, a_3, a_4	Constants for porosity distribution function (Cohen & Metzner (1981)).
$a(0)$	The total cross sectional area of all pores.
$a(A)$	The total cross-sectional area of all pores with cross-sectional area greater than A .
A	Area of cross-section of sphere.
A_T	Total area of cross-section.
A_v	Cross-sectional area of voids.
$A_T(r)$	Total area at radial position r .
$binratio$	The ratio of the height, or thickness of a bin, to the diameter of a particle d_p .
B	Proportionality constant (Sodré & Parise (1998))
B_c	Proportionality constant for capillary model (Cohen & Metzner (1981))
c_1, c_2	Constants for exponential porosity distribution (Cheng & Hsu (1986)).
C^*	Defined by the ratio of L_e/L (Tri-regional model)
$distance$	Distance between grid point and sphere centre.
d_p	Particle diameter.
D	Column diameter.
D_h	Hydraulic diameter used in flow calculations.
D_e	Equivalent diameter of the tubes, capillary model (Carman (1937) and Kozeny (1927))
f_m	Solid fraction (or Füllfactor) defined by Bedenig (1966).
g	Gravitational acceleration.
G	Mass flux.
h	Fill height of bulk void fraction experiment (Gordon (2001)).
h_b	Height of axial bin.
K	Rheological power law parameter (consistency index)

	used in capillary model (Cohen & Metzner (1981)).
K_1, K_2, K_3	Constants of proportionality (Carman (1937) and Kozeny (1927)).
K_0	Constant to account for the inadequacy in the choice of a proper effective diameter, used in capillary model.
<i>length</i>	The length of the sides of grid cell.
ℓ	Characteristic length scale for the REV (Kaviany (1991)).
L	Height of the machined annulus. Height of the column.
L_e	The equivalent length of a packed column is the length of the tortuous path that a fluid particle will follow through the packed column.
Δm	Difference in mass of samples.
M	Correction factor defined by Mehta and Hawley (1969).
n	The total number of cells in a Cartesian coordinate direction.
N	Number of pores.
N_{U_i}	Number of grid points that lie in spheres, in the i 'th and smaller, grid bins.
$N(A)$	Number of pores with cross sectional area greater than A .
$N(0)$	Total number of pores on slice.
<i>overlap</i>	The overlap between spheres.
o	Origin of local coordinate system.
O	Origin of global coordinate system.
Δp	Pressure drop.
P	Point in a fluid or porous domain.
P'	Point near P in a fluid or porous domain.
Q	Volume flow rate.
$Q(A)$	The volume flow rate through the pores with cross-sectional area greater than A .
$Q(0)$	The total volume flow rate through the column.
r	Local radial coordinate direction.
r'	Radius of the area A , formed by an axial plane cutting

Nomenclature

	a sphere.
r_e	Outer radius of an annular column.
r_i	Inner radius of an annular column.
r_t	The thickness of a radial bin.
Δr	The thickness of an annular ring, used to determine the radial porosity distribution.
Re	Reynolds number
R_{max}	The radius of the largest spherical bin U_n .
R	Global radial coordinate. The radial position of the radial cutting plane used to determine the radial porosity variation.
R_0	Radial position of a sphere in a column (global coordinates).
R_h	Hydraulic radius.
S_v	Surface area per unit volume of the particles.
S_{sphere}	Surface area of a sphere
U	Volume.
U_0	The Representative Elementary Volume (REV).
U_1	The first spherical volume about the point P .
U_{cell}	The volume of a cell in the cubic grid.
U_i	The i 'th spherical volume about the point P .
U_n	The largest spherical volume about the point P .
U_s	Volume occupied by the solids.
$(U_s)_i$	Volume occupied by solids in the i 'th spherical volume.
U_{sphere}	Volume of a spherical particle.
U_T	Total volume.
ΔU_T	Total volume of an annular cut from the column sample.
$\Delta U_T(r)$	Total volume of an annular cut from the column sample, at radial position r .
U_v	Volume occupied by voids.

$(U_v)_i$	Volume occupied by voids in the $i'th$ spherical volume.
ΔU_v	The volume of an annular cut from the column sample, occupied by voids.
$\Delta U_v(r)$	The volume of an annular cut, at radial position r from the column sample, occupied by voids.
$\bar{V}$	Superficial velocity of the fluid.
V_i	The interstitial velocity of the fluid through the porous media.
(x, y, z)	The local Cartesian coordinate system.
(x_a, y_a, z_a)	The intersection point (as viewed from above) of the radial cutting plane with the sphere (in the local coordinate system).
(x_i, y_i, z_i)	The Cartesian coordinates of the centre of the $i'th$ sphere.
(x_j, y_j, z_j)	The Cartesian coordinates of the centre of the $j'th$ sphere.
(x_s, y_s, z_s)	The Cartesian coordinates of the cutting line (local coordinates).
(X, Y, Z)	The global Cartesian coordinate system.
(X_a, Y_a, Z_a)	The intersection point (as viewed from above) of the radial cutting plane with the sphere (in the global coordinates).
(X_i, Y_i, Z_i)	The Cartesian coordinates of the $i'th$ grid point (global coordinates).
(X_p, Y_p, Z_p)	The Cartesian coordinates of point P (global coordinates).
(X_s, Y_s, Z_s)	The Cartesian coordinates of the cutting line (global coordinates).
Δz	Axial distance between planes cutting the packed column.
z_{ti}	The height of the cutting line (local coordinates).
z_{bi}	The height of the cutting line (local coordinates).
Z_{low}	The lower cut-off plane for the radial porosity distribution procedure.

Z_{high}	The upper cut-off plane for the radial porosity distribution procedure.
Z_0	The axial position of a sphere (global coordinates).
Z_i	Horizontal plane cutting the packed column at height Z_i .

GREEK SYMBOLS

ε	Porosity.
ε_{∞}	The bulk porosity of an infinite column. (Cheng & Hsu (1986))
ε_b	Bulk porosity. (Cohen & Metzner (1981))
ε_{ave}	The average porosity of a packed column. Sato <i>et al.</i> (1973)
θ	Angle.
θ_i	Angular positions at integration intervals.
$\Delta\theta$	Size of angular increments for integration intervals.
θ_a	The angular position of the intersection point (as viewed from above) of the radial cutting plane with the sphere (local coordinates).
μ	Fluid viscosity.
ρ	Fluid density.
ρ_T	Total density of annular ring.
ρ_s	Density of spherical particles.
ρ_M	Density of epoxy matrix

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1.1 Background to study

Packed column devices are used extensively in industry and research facilities. Many industrial processes and other applications are supported by this equipment. Examples of packed column devices are amongst others, packed filters, catalytic chemical reactors, thermal storage systems and petroleum reservoirs.

Packed column reactors are used in new generation nuclear power generators, to supply heat to the thermo-fluid cycle. In the Pebble Bed Modular Reactor (PBMR, currently under development) the reactor will (probably) be an annular column packed with spherical particles. The spherical particles contain the (nuclear) fuel to generate the heat needed to maintain the thermo-fluid cycle.

The design of the PBMR reactor, like that of any packed column, is dependent on the fluid velocity, pressure drop of the fluid through the packed column and the mechanisms of heat transfer. All these mechanisms are sensitive to the packing density and structure of the pores (between the particles). A measure of the packing density is the void fraction (porosity). The void fraction is defined as the ratio of volume occupied by voids to the total volume of the packing.

Heat transfer is dependent on the interface area between the fluid and the solid phase, where the transfer takes place. Packed columns are ideal for transfer processes. Substantial contact area for transfer is exposed per unit volume of the column. The transfer is thus optimised in terms of space available.

The flow of fluids through packed columns has been investigated extensively. For these complex geometries it is impossible to obtain analytic solutions for heat- and mass transfer, and other phenomena. Because of the complexity of the problem it is very difficult to understand the mechanisms and dependence of the different phenomena involved. In order to understand the problem more completely, the void fraction variations in packed columns must be investigated.

In a packed column the void fraction varies locally. In the region close to the wall of the column the packing of particles are highly ordered. This leads to radial variations in the void fraction. The structure of the packing in the wall region approaches a simple cubic packing. In the central part of the column, where the

packing is more random, the void fraction approaches the bulk value of a totally random packing.

In this text the *bulk void fraction* (or any *bulk* property) is defined as the value in an infinite packed column (no bounding surfaces present). There is a clear difference between the bulk void fraction and the average void fraction for a finite sized column. The average void fraction for any specific volume follows directly from the definition.

It is important to note that void fraction is not rigorously defined for volumes smaller than the representative elementary volume (REV). The REV is defined in Chapter 2.

The local flow velocity in a packed column is related to the local void fraction of the column. As the void fraction increases, the flow resistance decreases. This leads to an increase in volume flow. As a result, the velocity profile inside packed columns is severely distorted near the wall. The mean local flow velocity reaches a maximum in the near-wall region. This phenomenon is known as flow- or wall channelling. Wall channelling can influence the heat transfer and mass flow rate through the reactor.

From the discussion above it is clear that the void fraction, flow velocity, mass flow and other phenomena that are present in packed columns are important to the operation of packed column devices. This study is concerned with the development and implementation of numerical methods to analyse the void fraction variations in packed columns.

1.2 Problem Statement

The importance of the void fraction of packed columns has been highlighted in the previous section. To improve our understanding of the problem it is suggested that packed columns be investigated with numerical models.

Packed columns have been studied extensively. There are only a few accounts in the literature of numerical studies done on the void fraction of packed columns. Many models predict the flow velocity and the resultant mass flow through packed

columns. Yet the packing structure of these columns has not been investigated more thoroughly by means of numerical studies.

In most fields of research, numerical analysis and simulations are used to predict the behaviour of systems of interest. It is therefore interesting to note that there have not been much numerical work done on the structure, and void fraction of packed columns.

1.3 Objective of Study

It is believed that numerical analysis of the structure of packed columns can make a major contribution to the understanding of the effects of the porosity on the performance and operation of packed columns.

It is generally accepted that the porosity variations in packed columns has an important effect on the operation of the device. These porosity variations have been investigated by means of physical experiments. This study will now concentrate on the development of numerical tools to investigate the porosity effects in cylindrical (and annular) columns packed with spherical particles of uniform size.

Numerical models that can simulate the packing of spherical particles in packed columns are available. Physical experiments that can also be used to obtain the positions of particles in packed columns. With this data available, numerical investigation into the structure of the column is possible.

1.4 Contribution of Study

The primary outcome of this study is to provide numerical tools to accurately analyse the porosity variations in packed columns. These tools can be used to investigate packed columns more thoroughly. This will contribute to the understanding of the packing structure in packed columns. It will also lay the foundation for further numerical work to study the pore structure, heat transfer coefficients, and other effects in packed columns.

1.5 Overview of Report

Chapter one gives the background to the problem addressed by this study. This includes the problem statement, the objective, and the contribution that this study will make to the understanding of packed column devices.

Chapter 2 is an account of the literature relating to the subject. Here the investigations by other authors into the porosity variations in packed columns are examined. The most important flow models implemented in the literature are also discussed. This will lead to a thorough understanding of the current state of this field of study.

In Chapter 3 the numerical techniques developed in this study are described. The models developed are; overlap analysis procedure, axial porosity distribution procedure, radial porosity distribution procedure, and a procedure to calculate the porosity distribution about a point in the column (this model can be used to determine the size of the REV).

The implementation of the models is discussed in Chapter 4. In this chapter the algorithms are explained, and the codes are validated with special test cases. This chapter provides the reader with thorough insight into the functioning of the codes. In Chapter 5, a complete analysis of four data sets is discussed.

In Chapter 6, a brief summary of this report is provided, and the most important conclusions that can be drawn are discussed. Recommendations for further research are also suggested.

Chapter 2

Literature Survey

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2.1 Introduction

In the introductory chapter the importance of packed column devices was discussed. The void fraction of these columns has a significant influence on their operation. In this chapter the information that is available in the literature is examined.

First the continuum approach to the fluid domain and the porous domain is discussed. Then experimental methods, from the literature, to investigate packed columns are explained and the results are shown.

The flow of fluids through packed columns is also considered. The velocity distribution in a packed column is distorted due to the variations in porosity near the wall of the column. This discussion will highlight the dependence of the flow through the porous domain on the void fraction.

2.2 The Continuum Approach to Porous Media

2.2.1 Fluid domain

Fluids are composed of a very large number of molecules. To describe the behaviour of the fluid, it is required that the individual molecules and their interactions with all other molecules be described. The molecules move about in space (container) and collide with each other and with the wall of the container. It is possible to describe the movement and interactions of a small number of these molecules by means of classical mechanics theory. However, when dealing with any significant volume (containing a significant mass) of the fluid, it is impossible to solve this problem.

To reduce the problem to manageable proportions a fluid particle is defined. "A particle is an ensemble of many molecules contained in a small volume" (Bear, 1972). By averaging the fluid and flow properties of the molecules contained in a particle, the bulk properties of the fluid are obtained. The bulk property values are assigned to some centroid (P) of the fluid particle. The bulk properties used regularly, for example temperature, pressure and density, are only measures of the average value of some attribute of the individual molecules in the sample.

The particle size is much larger than the *mean free path* of a fluid molecule. The property values assigned to a point (P) must be representative of that point. Thus, the fluid particle must be much smaller than the fluid domain.

Fluid particles are defined about every mathematical point in the fluid domain. Bulk properties are therefore defined at every point in the fluid domain. This is the fluid continuum. This level of approximation is referred to as the microscopic approach. Bear (1972) present a clear account of the microscopic view of fluids.

Porous media bound the fluid domain. In principle, it is possible to solve the flow field by means of fluid mechanics. Again, an accurate description of the flow through the porous medium is not viable. This is due to the geometrical complexity of the porous domain. To overcome this difficulty, it is useful to move to a coarser (higher) level of approximation.

2.2.2 Porous domain

As explained in the introductory chapter, the void fraction is a measure of the volume (or area) available for fluid flow.

At the next, higher, level of modelling the porous medium is approximated as a continuum. The representative elementary volume, REV, (similar to the fluid particle) is now defined. Kaviany (1991) defines this as follows. "The smallest differential volume that results in statistically meaningful local average properties such as local void fraction, saturation, and capillary pressure. When the representative elementary volume is appropriately chosen, the limited addition of extra pores around this local volume will not change the values of the local properties."

Kaviany (1991) states that for the REV $\ell \gg d_p$. Here ℓ is a characteristic length scale for the REV and d_p is a particle diameter. The REV must be much smaller than the porous domain for the bulk properties to represent the point P . In the REV the average void fraction (and other properties) can be calculated and assigned to P . REV's are constructed about every point P in the domain (continuum approximation). This view is called the macroscopic approach.

A mathematical definition of REV will now be presented (Bear, 1972). Let P be a mathematical point in the domain occupied by a porous medium. Consider a volume U_i (say having the shape of a sphere, for $i = 1, 2, \dots, n$) of which P is the centroid. The volume of U_1 is much larger than the volume of the REV centred about P . The void fraction in the region of P , as a function of U_i , is calculated as follows:

$$\varepsilon(U_i) = \frac{(U_v)_i}{U_i} \quad (2.1)$$

Where U_v is the volume of the voids in the volume U . Accordingly $(U_v)_i$ is the volume of the voids in the volume U_i .

Take consecutively smaller U_i and calculate the void fraction each time. For large volumes U_i , gradual changes in void fraction will be seen for *inhomogeneous* media. *Homogeneous* media will not display any significant changes in void fraction for large U_i . As U_i slowly tends to zero a limiting volume U_0 , will be reached. For a volume U_i smaller than U_0 the void fraction calculated varies significantly. This happens because U_i is in the order of the pore size of the porous medium. As U_i converge to the point P the value of the void fraction will approach either one or zero. The REV is defined as the volume U_0 .

With the above definition in mind the void fraction at the point P in the porous domain is:

$$\varepsilon(P) = \lim_{U_i \rightarrow U_0} \varepsilon(U_i(P)) = \lim_{U_i \rightarrow U_0} \frac{(U_v)_i}{U_i} \quad (2.2)$$

It is clear that the void fraction will not change significantly when adding (or taking away) several pores to the REV. This agrees with the definition of the REV given by Kaviani (1991). It is further assumed that $(U_v)_i$ and U_0 varies smoothly in the region of P .

Thus from eq.(2.2) follows:

$$\varepsilon(P) = \lim_{P' \rightarrow P} \varepsilon(P') \quad (2.3)$$

Where P' is a point near P . This equation states that the void fraction is a continuous function of position in the porous domain.

It is clear that void fraction is not rigorously defined for U_i smaller than U_0 . Kaviany (1991) states that various approximations are used in dealing with (bulk) void fraction. Some of these are rather contradictory. Further, when dealing with wall channelling (and similar phenomena) different approximations are used. The length scale over which wall channelling occurs is much smaller than the characteristic length of the REV. To account for this the description (or geometric interpretation) of the void fraction needed to account for wall channelling has to be on the scale of the phenomena described.

It follows that the use of void fraction in these investigations (scale much smaller than the REV) are not rigorously defined.

2.3 The Discrete Approach to Porous Media

The void fraction at a point is defined as:

$$\varepsilon(P) = 1 \text{ or } \varepsilon(P) = 0 \quad (2.4)$$

There is either a void or a solid at a point P . This method to describe the flow field is used in Direct Numerical Simulation (DNS) and Lattice Boltzmann methods. In these methods the particles are modelled explicitly. The flow is modelled at a level much smaller than the size of the packing particles. These studies result in a detailed description of the flow field through the porous domain.

2.4 Void fraction distribution

As explained in the introductory chapter, there are void fraction variations in packed columns. These variations are ascribed to the discontinuities that are present in the column.

There are several factors that have been identified by investigators that can influence the packing structure of particles in columns. In this section the main factors that are highlighted in the literature are discussed. These factors include the wall effect, the influence of the particle shape and size, the axial void fraction variation and the aspect ratio (ratio of cylinder to particle diameter) of the packing.

2.4.1 Effect of wall on void fraction for uniform spherical particles

Goodling *et al.* (1980) conducted experiments for cylindrical packed columns with uniform sized spheres. It was found that the void fraction near the wall oscillates through various maxima and minima in a strongly damped fashion. These oscillations were detected up to a distance of 5-particle diameters from the cylinder wall. The maximum void fraction equals unity, and was encountered at the restraining wall. The void fraction decreases sharply to a minimum value at approximately $\frac{1}{2}$ -particle diameter from the cylinder wall. In the region further than 5-particle diameters away from the wall the void fraction takes on the bulk value of the randomly packed undisturbed column.

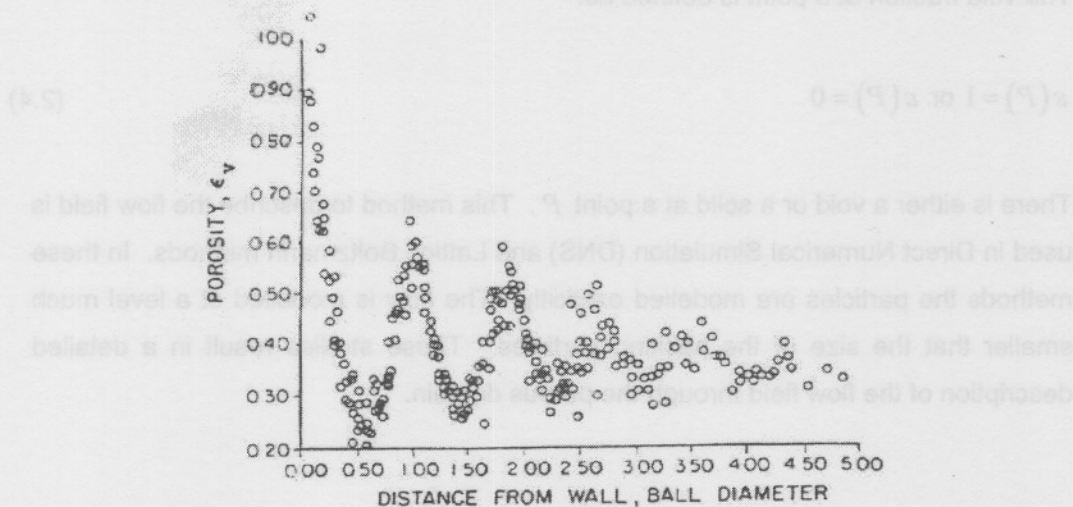


Figure 2-1 Radial void fraction distribution, results obtained by Goodling *et al.* (1980).

Figure 2-1 shows the results obtained by Goodling *et al.* (1980) for the radial void fraction distribution for cylindrical columns packed with spheres.

Roblee *et al.* (as quoted by Goodling *et al.*, 1980) used uniformly shaped particles, such as spheres, cylinders, Berl saddles and Raschig rings to determine the influence of the cylinder wall on the void fraction distribution. For spherical particles Roblee *et al.* obtained results that are in close agreement with the results reported by Goodling *et al.* (1980).

Sederman *et al.* (2001) conducted experiments with magnetic resonance imaging (MRI). The results that were obtained by Sederman *et al.* (2001) are in excellent agreement with the results of Goodling *et al.* (1980). Figure 2-2 is a graphical representation of the void fraction averaged over the height of the column, obtained by the MRI techniques. The dark regions represent higher void fraction.

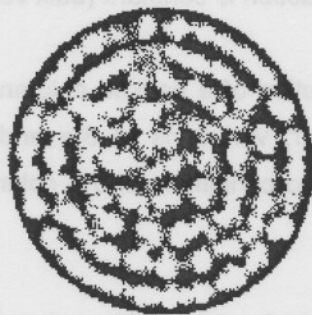


Figure 2-2. Average void fraction image obtained by Sederman *et al.* (2001) (dark regions have higher void fraction).

2.4.2 Particle shape and size

Goodling *et al.* (1980) also conducted experiments with multi-sized particles. Particles were mixed on an equal number basis, and on an equal volume basis. When equal numbers of two sizes of particles were used, the oscillations were still apparent up to three particle diameters from the cylinder wall. For three sizes of particles mixed on an equal number basis, the oscillations were observed up to two-particle diameters from the wall of the column. This is the same result obtained for two sizes of particles mixed on equal volume basis. When three sizes of particles were mixed on equal volume basis, the variations were damped out after about one particle diameter. In this case, the void fraction decreased regularly to the bulk value of the packed column, and did not display the characteristic damped oscillations.

For uniform particles of complex shape, such as Berl saddles, the void fraction decreases regularly from unity at the wall, to the bulk value of the column at about $\frac{1}{2}$ -particle diameter from the cylinder wall (Roblee *et al.* (as quoted by Goodling *et al.*, 1980)). This result is comparable to the results reported by Goodling *et al.* (1980) for a packing of three sizes of spheres mixed on an equal volume basis, discussed previously.

When Raschig rings are used, the void fraction exhibits a hump at about $\frac{1}{2}$ -half particle diameter from the wall, after which it decreases to the average value of the central part of the packed column.

2.4.3 Axial void fraction variation

The cylinder wall of a packed column exerts a definite influence on the void fraction of the column. As a result the packing in the wall region varies regularly, while in the core of the column, the void fraction is constant (bulk void fraction).

The axial void fraction distribution of a packed column should, theoretically, remain constant. There are however, variations at the ends of the column due to the constraints imposed by the end conditions of the column. This has been shown in the work of Bedenig (1966).

Bedenig (1966) defined the solid fraction (Füllfactor) as follows:

$$f_m = \frac{U_s}{U_T} \quad (2.5)$$

With U_s the volume occupied by the solids in the packing and U_T the total volume of the packing. This solid fraction is the mathematical complement of the void fraction for a packed column.

$$\varepsilon = 1 - f_m \quad (2.6)$$

Bedenig (1966) conducted experiments to determine the change in average void fraction of a packed column with height. For the purposes of this experiment, the cylinder was filled consecutively to higher axial levels to find the change in void

fraction for each axial level. The D/d_p -ratio used in this experiment was 15. It was found that the average void fraction of the packed column approached a constant value (bulk void fraction) for axial levels higher than 50 [mm] ($6\frac{1}{4}d_p$). This tendency can be seen in Figure 2-3.

Roblee *et al.* (as quoted by Goodling *et al.*, 1980) found significant differences in the void fraction of radial concentric rings. No significant differences were found at different axial levels within the column. This indicates that the axial void fraction distribution within a packed column can be considered constant.

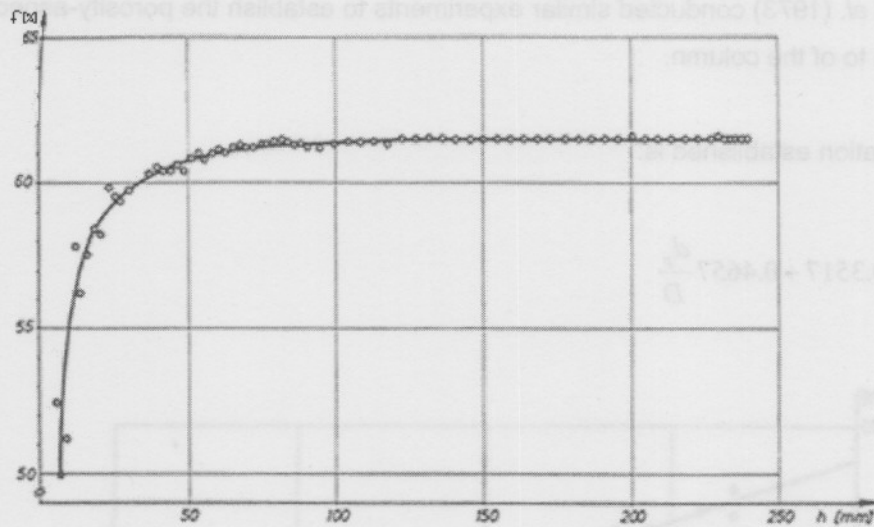


Figure 2-3. Solid fraction (in percentage) versus height above the column floor, (Bedenig (1966)).

2.4.4 Aspect ratio of column - equivalent for annulus

Bedenig (1966) conducted a further experiment to determine the bulk void fraction for various aspect ratios. For the purposes of this experiment the bulk void fraction was determined for the region above the $6\frac{1}{4}$ -particle diameter level (the floor of the column affects the void fraction distribution in this region, refer to Figure 2-3)). The range for which the experiment was conducted is $5 < D/d_p < 48$. The results are shown in Figure 2-4. A linear fit performed on the data gave:

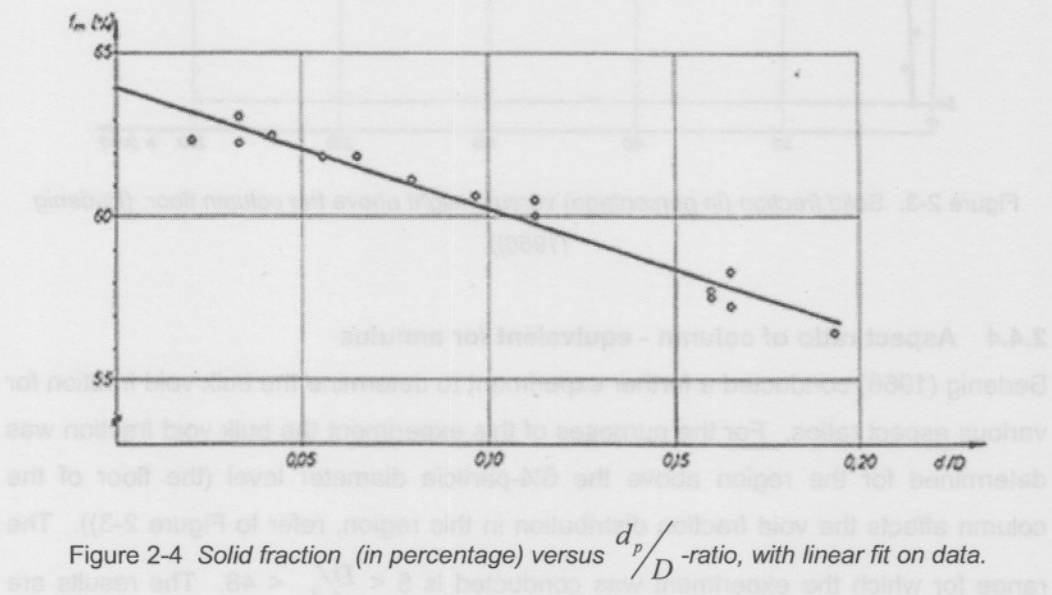
$$f_m = 0.64 - 0.352 \frac{d_p}{D} \quad (2.7)$$

Care was taken to load the columns to the maximum packing density possible. It is interesting to note that the y-intercept of this linear fit is the exact value of the maximum possible bulk solid fraction for an infinite sized randomly packed column (Bedenig (1966)). It is therefore reasonable to conclude that the data used in the prediction was obtained from maximum packing densities for the various aspect ratios.

Sato *et al.* (1973) conducted similar experiments to establish the porosity-aspect ratio relation to of the column.

The relation established is:

$$\varepsilon_{ave} = 0.3517 + 0.4657 \frac{d_p}{D} \quad (2.8)$$



This is similar to the work of Bedenig (1966). The coefficient associated with the aspect ratio differs by 32% from that obtained by Bedenig (1966). The difference can possibly be ascribed to a different experimental setup and packing procedure to that of Bedenig (1966).

Assuming that for annular columns, the average void fraction is also proportional to the aspect ratio Sodrè & Parise (1998) proposed the following relationship:

$$\varepsilon_{ave} = 0.3517 + B \frac{d_p}{D_h} \quad (2.9)$$

Here the hydraulic diameter is used to characterise the annular column, and B is the proportionality constant. The hydraulic diameter is given as:

$$D_h = 2(r_e - r_i) \quad (2.10)$$

The outer radius of the annular column is r_e , and the inner radius is r_i . They established the value for B from only one data point as:

$$B = 0.387 \quad (2.11)$$

This value for the coefficient associated with the aspect ratio is comparable to that obtained by Bedenig (1966) and Sato *et al.* (1973).

2.5 Methods to measure void fraction

There are various methods to measure the void fraction of a medium. In this section some of the experiments referred to in the literature are discussed. The results of these and other experiments have been discussed in section 2.4.

2.5.1 Average void fraction

To determine the average void fraction of a packed column the following experiment was conducted by Gordon (2001). A cylindrical vessel with known dimensions was filled with the maximum number of spherical particles, to ensure a consistent packing arrangement. The void fraction of the region above the 5-particle diameter level was determined by measuring the volume of water needed to fill the cylinder to a specific height h . The void fraction ε , was then calculated by means of eq. (2.12).

$$\varepsilon = \frac{U_v}{U_t} \quad (2.12)$$

Where U_v is the volume of the voids i.e. the volume of water needed to fill the cylinder to the prescribed height. U_t is the total volume of the cylinder between the prescribed axial planes.

It is important to note that the wall effects are included in this calculation of the void fraction. The effects of the wall on the void fraction extend to 5-particle diameters from the wall (Goodling *et al.*, 1980). To eliminate the wall effect due to the floor (bottom) of the column, this (5-particle) region is not included in the measurements.

Figure 2-5 is a schematic representation of the setup for this experiment.

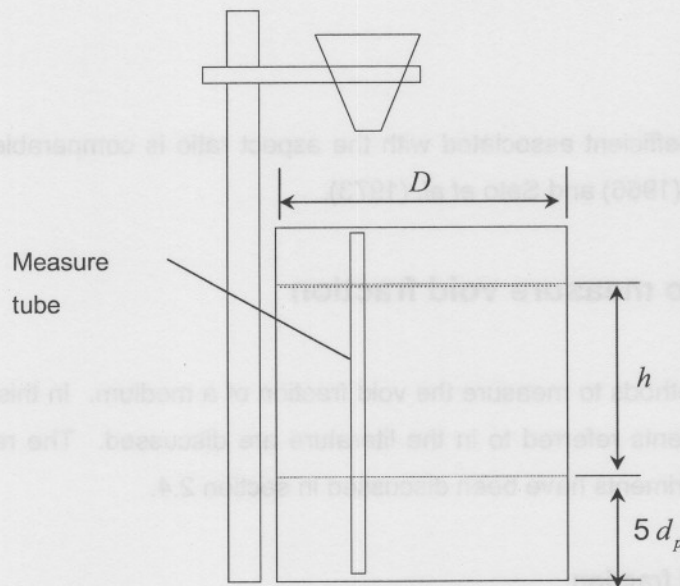


Figure 2-5. Schematic representation of the set-up to calculate the average void fraction.

2.5.2 Radial void fraction distribution

It is well documented that the void fraction varies with radial position in packed columns. There is no evidence to suggest that there exists any axial variation in packed columns (except in the regions close to constraining walls for example the floor of the column). Goodling *et al.* (1980), Roblee *et al.* (as quoted by Goodling *et*

al., 1980), Gordon (2001), Sederman *et al.* (1997) and others investigated the radial void fraction distribution of packed columns.

Goodling *et al.*

Goodling *et al.* (1980), Roblee *et al.* (as quoted by Goodling *et al.*, 1980) and Gordon (2001) conducted similar experiments to determine the radial void fraction distribution.

Goodling *et al.* (1980) constructed packed columns by pouring the maximum number of spheres into a cylinder. The spheres were set in this configuration by curing it in liquid epoxy.

From these samples thin annular rings were consecutively machined on a lathe. The void fraction $\varepsilon(r)$ of each annular ring was then determined by eq. (2.13).

$$\varepsilon(r) = \frac{\rho_T - \rho_S}{\rho_M - \rho_S} \quad (2.13)$$

Here ρ_T represents the total density of the annular ring (at radial position r), ρ_S the density of the spheres and ρ_M the density of the epoxy matrix. To determine the density of an annular cut the difference in mass $\Delta m(r)$, and volume $\Delta U(r)$, of the sample between consecutive cuts are used (eq. (2.14)).

$$\rho_T(r) = \frac{\Delta m(r)}{\Delta U(r)} \quad (2.14)$$

Figure 2-6 is a diagrammatic representation of the way in which the samples were shaped. It shows consecutive cuts made on the outside of the sample.

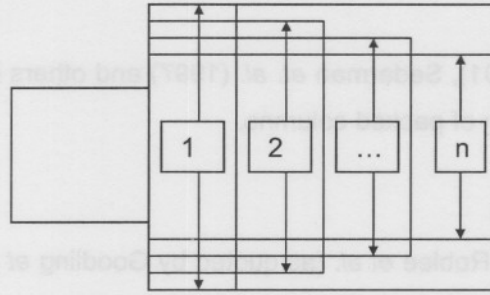


Figure 2-6. Annular rings were cut from the outside of the sample.

It is important to remember that the void fraction determined in this way is the average void fraction over the distance L (length of the machined annulus), and around (tangentially) the annulus with thickness Δr .

With the void fraction of an annular ring at radial position r , given by:

$$\varepsilon(r) = \frac{\Delta U_v(r)}{\Delta U_T(r)} \quad (2.15)$$

For a very thin annular ring, the volume of the ring can be obtained as:

$$\Delta U_T(r) = 2\pi r \Delta r L \quad (2.16)$$

where Δr is the thickness of the annular ring and L the length of the cylindrical packed bed. If $\Delta r \rightarrow 0$, then the volume $U_T(r)$ becomes an area, $A_T(r)$. This is the area-based void fraction.

$$\varepsilon(r) = \frac{A_v(r)}{A_T(r)} \quad (2.17)$$

The area-based void fraction and the volume-based void fraction obtained in this manner can be considered the same, for sufficiently small Δr .

Sederman et al.

Sederman *et al.* (2001) probed columns packed with spherical particles, using high resolution magnetic resonance imaging (MRI) volume-visualisation, to determine the

structure of the columns. For more information on MRI techniques consult Callaghan (1991).

2.6 Analytical radial porosity distribution approximations

Some authors have assumed simplified void fraction distributions in their calculations of the flow velocity and other dependent mechanisms. White and Tien (1987) and Vortmeyer and Schuster (1983) both used void fraction distributions, decreasing exponentially from unity at the cylinder wall, to the bulk value of the packed column at about $1\frac{1}{2}$ -particle diameters from the wall. This is typical of beds packed with irregularly shaped particles.

The relation of White and Tien (1987) is:

$$\varepsilon\left(\frac{r}{d_p}\right) = \left[1 + \left(1 - e^{-\frac{2r}{d_p}} \right)^{\frac{1}{2}} \left(\frac{1 - \varepsilon_{\infty}}{\varepsilon_{\infty}} \right) \right]^{-1} \quad (2.18)$$

The relation employed by Vortmeyer and Schuster (1983) is:

$$\varepsilon(r) = \varepsilon_{\infty} \left[1 + C e^{\left(\frac{D/2 - r}{d_p} \right)} \right] \quad (2.19)$$

Where C is a constant that has to be adjusted according to the value of ε_{∞} (the porosity at the wall must equal unity). These correlations are shown in Figure 2-7.

For annular packed columns, Sodrè & Parise (1998) and Cheng & Hsu (1986) assumed a void fraction distribution decreasing exponentially from unity at the wall to the bulk value in the centre of the column. The annular cross-section was divided into three regions, namely the internal wall region, transition region and the external wall region. The transition region includes the bulk region, if it exists. Both the wall regions extend one particle diameter radially into the column.

Sodré & Parise (1998) used the void fraction distribution of Cheng & Hsu (1986).

$$\varepsilon(r) = \varepsilon_{\infty} \left[1 + c_1 e^{\frac{-c_2(r-r_i)}{d_p}} \right] \quad r_i \leq r \leq \frac{r_e + r_i}{2} \quad (2.20)$$

$$\varepsilon(r) = \varepsilon_{\infty} \left[1 + c_1 e^{\frac{-c_2(r_e-r)}{d_p}} \right] \quad \frac{r_e + r_i}{2} \leq r \leq r_e \quad (2.21)$$

With c_1 calculated by setting the value of the void fraction at the wall to unity. This gives:

$$c_1 = \frac{1}{\varepsilon_{\infty}} - 1 \quad (2.22)$$

By taking the integral of eq. (2.20) and eq. (2.21) the average column void fraction is obtained.

$$\varepsilon = \varepsilon_{\infty} \left\{ 1 + \frac{2c_1 d_p \left[1 - e^{\frac{-c_2(r_e-r_i)}{2d_p}} \right]}{c_2(r_e - r_i)} \right\} \quad (2.23)$$

The coefficient c_2 can be solved for iteratively from eq. (2.23). The void fraction of an infinite column ε_{∞} was taken to be $\varepsilon_{\infty} = 0.3517$ (Sato *et al.* (1973), eq. (2.8)). The value of ε_{∞} was obtained from experiments with particles "gently dumped" into a cylindrical column.

Cohen and Metzner (1981) divided the packed column into three distinct regions. The first is the wall region, nearest to the wall and extends 1-particle diameter into the column. The second region is the transition region. For ease of mathematical modelling the transition region was assumed to extend 8-particle diameters into the

column. This part of the column includes the void fraction oscillations, and extends to where the local void fraction remains constant (does not change with radial position). The bulk region consists of the inner part of the column. In this region the void fraction is constant and equal to the bulk void fraction of the packed column.

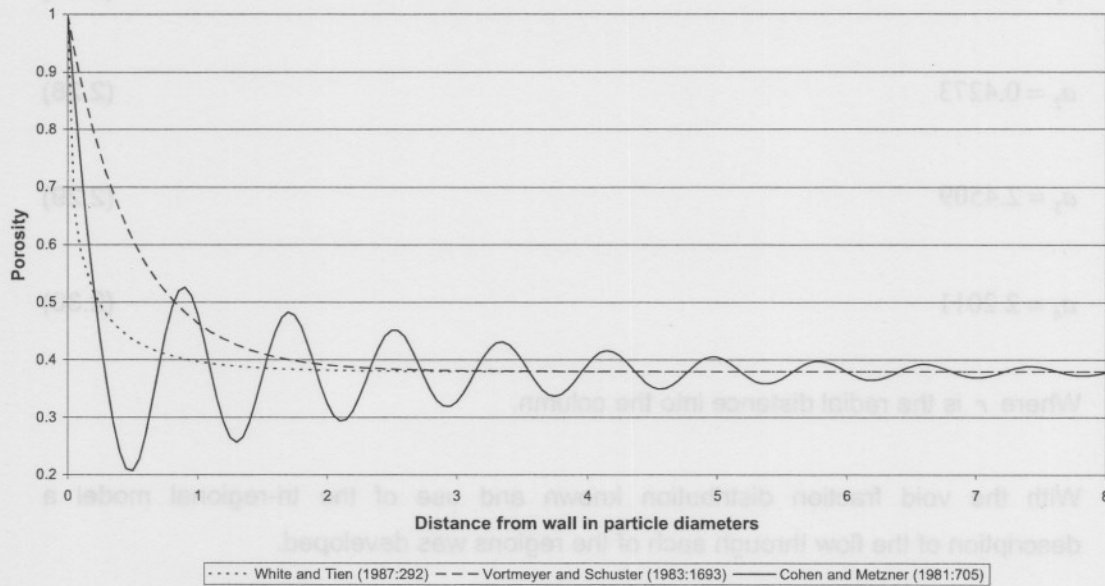


Figure 2-7. Void fraction distribution assumed by Cohen and Metzner (1981), also showing the approximations of White and Tien (1987) and Vortmeyer and Schuster (1983).

Cohen and Metzner (1981) used the experimental data obtained by other workers to fit a curve (Figure 2-7), which describes the radial variation of the void fraction with an average deviation of 0.5%.

The following are the relations used to fit the curve in Figure 2-7.

$$\frac{1-\varepsilon}{1-\varepsilon_b} = 4.5 \left(\frac{\left(\frac{D}{2}-r\right)}{d_p} - \frac{7\left(\frac{D}{2}-r\right)^2}{9d_p^2} \right) \quad \text{for } \frac{D}{2} - 0.25d_p \leq r \quad (2.24)$$

$$\frac{\varepsilon - \varepsilon_b}{1 - \varepsilon_b} = a_1 e^{-a_2 \left(\frac{D}{2}-r\right)/d_p} \cos \left(\left(\frac{\left(\frac{D}{2}-r\right)}{d_p} - a_4 \right) \pi \right) \quad \text{for } \frac{D}{2} - 8d_p < r < \frac{D}{2} - 0.25d_p \quad (2.25)$$

$$\varepsilon(x) = \varepsilon_b \quad \text{for } -\infty \leq r \leq \frac{D}{2} - 8d \quad (2.26)$$

$$a_1 = 0.3463 \quad (2.27)$$

$$a_2 = 0.4273 \quad (2.28)$$

$$a_3 = 2.4509 \quad (2.29)$$

$$a_4 = 2.2011 \quad (2.30)$$

Where r is the radial distance into the column.

With the void fraction distribution known and use of the tri-regional model a description of the flow through each of the regions was developed.

A study of Figure 2-7 suggests that the exponential relationship proposed by White and Tien (1987) may be a better representation of the radial variation of the "average" porosity than the relationship proposed by Vortmeyer and Schuster (1983).

2.7 Numerical procedures to calculate void fraction

Mueller (1992) performed a numerical investigation into the void fraction of packed columns. Mueller (1992) developed a model to calculate the radial void fraction distribution from the position data of packed columns. He (Mueller (1997)) applied this procedure to columns packed numerically using four different deterministic sequential packing models. He also conducted a physical experiment to obtain the positions of the spheres in a column.

He investigated the radial void fraction distribution for different aspect ratios, corresponding to that of experiments of other authors. He found that for smaller aspect ratios the deterministic models approximate real packings well.

Mueller (1992) calculated the porosity distribution numerical as follows; the porosity was calculated for a series of annular layers (similar to the experiments of Goodling *et al.* (1980), Roblee *et al.* (as quoted by Goodling *et al.*, 1980) and Gordon (2001)). This was achieved by calculating the solid volume contributions of the spheres being cut by the annular layer.

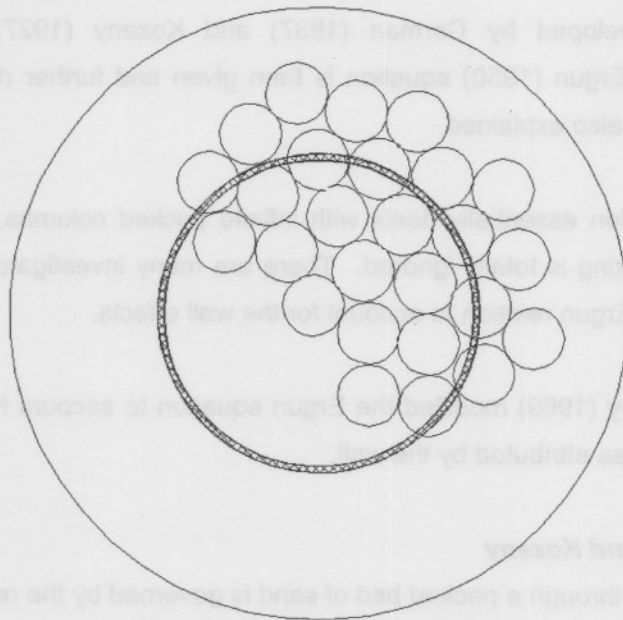


Figure 2-8. $X-Y$ plane of a radial annular layer in a column (Mueller (1992)).

2.8 Flow of fluids through packed columns

Closely related to the problem of the void fraction distribution in a packed column, is the problem of the flow distribution through the column.

There are essentially two effects on the flow through packed columns that are attributed to the presence of the wall. The discussions in the previous sections highlighted the effect of the wall on the packing arrangement of the particles in the column. The additional wetted surface area introduced by the wall also has a significant effect on the flow through the column.

There are various models and methods used by investigators to predict the flow, and pressure drop flow rate relation through packed columns. These methods are now overviewed briefly.

2.8.1 One-dimensional models

The relationships discussed in this section are one-dimensional solutions to the problem of flow through packed columns. In these models simplified void fraction distributions are assumed.

The models developed by Carman (1937) and Kozeny (1927) will firstly be discussed. The Ergun (1950) equation is then given and further developments by other authors are also explained.

The Ergun equation essentially deals with infinite packed columns, where the wall effect on the packing is totally ignored. There are many investigators that modified and adapted the Ergun relation to account for the wall effects.

Mehta and Hawley (1969) modified the Ergun equation to account for the additional wetted surface area attributed by the wall.

Carman and Kozeny

The flow of water through a packed bed of sand is governed by the relationship:

$$\frac{(\Delta p)}{L} \propto \bar{V} \quad (2.31)$$

Where Δp is the pressure drop over the column, L the (axial) length of the column, and $\bar{V}$ the superficial velocity of the fluid. The superficial velocity $\bar{V}$ of the fluid is defined as the volume flow rate Q , per cross-sectional area A , of the column.

$$\bar{V} = \frac{Q}{A} \quad (2.32)$$

Carman (1937) and Kozeny (1927) modelled the flow of fluids through packed columns as the flow through a parallel bundle of channels. They modified the Hagen-Poiseuille equation (eq. (2.33)) for laminar flow through a single tube, to model the flow through a bundle of tubes.

Equation (2.33) is the Hagen-Poiseuille relationship for a single tube.

$$\frac{(\Delta p)}{L} = \frac{32\mu\bar{V}}{D^2} \quad (2.33)$$

With D the tube diameter and μ the viscosity.

The modified Hagen-Poiseuille relationship of Carman (1937) and Kozeny (1927) is given by eq. (2.34).

$$\frac{(\Delta p)}{L_e} = K_1 \frac{\mu V_i}{D_h^2} \quad (2.34)$$

The equivalent diameter (hydraulic diameter) of the tubes is D_h , and the equivalent length L_e , is the length of the tortuous path that the fluid will follow. The interstitial velocity of the fluid through the bed is V_i . The constant of proportionality is K_1 .

The Dupuit-Forchheimer assumption states that the actual (interstitial) velocity of the fluid through the voids in the packing is:

$$V_i = \frac{\bar{V}}{\varepsilon} \quad (2.35)$$

The equivalent length of the bed can be assumed proportional to the actual length L .

$$L_e = K_2 L \quad (2.36)$$

And the tube equivalent diameter (hydraulic diameter) is defined as:

$$D_h = \frac{\text{flow area}}{\text{wetted perimeter}} \quad (2.37)$$

This can be shown to reduce to:

$$D_h = \frac{\varepsilon}{S_v(1-\varepsilon)} \quad (2.38)$$

Where S_v is the surface area per unit volume of the particles. Eq. (2.34) can now be written as:

$$\frac{(\Delta p)}{L} = K_3 \frac{(1-\varepsilon)^2}{\varepsilon^3} \mu \bar{V} S_v^2 \quad (2.39)$$

This relation is known as the Carman-Kozeny equation. From the literature there is general consensus on the value of $K_3 = 5$. It can be shown that for spherical particles the surface area per unit volume is:

$$\frac{S_{\text{sphere}}}{U_{\text{sphere}}} = \frac{6}{d_p} \quad (2.40)$$

S_{sphere} is the surface area of a particle and U_{sphere} is the volume of a particle.

Thus eq. (2.39) becomes:

$$\frac{(\Delta p)}{L} = 180 \frac{(1-\varepsilon)^2}{\varepsilon^3} \frac{\mu \bar{V}}{d_p^2} \quad (2.41)$$

Ergun

The Ergun equation was derived using columns with large D/d_p -ratios. In these columns the effect of the wall on the flow through the column is negligible. The Ergun equation is, accordingly, applicable to packed columns where the wall effects are negligible. This requirement is satisfied in columns with large aspect ratios (the ratio of the cross-sectional area influenced by the wall to the total cross-sectional area decreases with increasing aspect ratio). Some authors suggested that the effect of the wall on the Ergun equation might be important for aspect ratios smaller than 50.

Ergun (1952) established that the pressure drop-flow rate relation for the flow of a fluid through a column packed with spherical particles could be stated as:

$$\left(\frac{\Delta p g}{L}\right) = 150 \frac{(1-\varepsilon)^2}{\varepsilon^3} \frac{\mu \bar{V}}{d_p^2} + 1.75 \frac{1-\varepsilon}{\varepsilon^3} \frac{G \bar{V}}{d_p} \quad (2.42)$$

Where g is the gravitational acceleration, and G is the mass flux through the column.

Equation (2.42) (also referred to as the single region model by some authors) states that the energy loss in packed columns can be treated as the sum of the viscous (laminar flow region, Carman-Kozeny) and kinetic (turbulent flow region) energy losses. The viscous energy losses are proportional to $\frac{(1-\varepsilon)^2}{\varepsilon^3}$ and the kinetic energy losses are proportional to $\frac{1-\varepsilon}{\varepsilon^3}$. Therefore, the first term in equation (2.42) expresses the viscous energy loss per unit length of the column, and the kinetic energy losses are given by the second term.

KTA

The Nuclear committee (Kerntechnische Ausschuss (1980)) adapted the Ergun (1952) equation for a packing of uniform spheres, to the following form:

$$\left(\frac{\Delta p}{L}\right) = 160 \frac{(1-\varepsilon)^2}{\varepsilon^3} \frac{\mu \bar{V}}{d_p^2} + 3 \frac{(1-\varepsilon)^{1.1}}{\varepsilon^3} \frac{G \bar{V}}{d_p} \left[\frac{\mu}{\rho \bar{V} d_p} \right]^{0.1} \quad (2.43)$$

This, modified relationship is valid for:

$$10^0 < \frac{\text{Re}}{1-\varepsilon} = \left(\frac{\rho \bar{V} d_p}{\mu} \right) \frac{1}{1-\varepsilon} < 10^5 \quad (2.44)$$

$$0.36 \leq \varepsilon \leq 0.42 \quad (2.45)$$

$$L > 5d_p \quad (2.46)$$

Extension of the Ergun equation by Metha & Hawley

As explained previously the effect of the wall on the flow through a packed column can be attributed to the additional wetted surface area introduced by the wall, and the variations in porosity due to the presence of the wall.

To take account of these effects on the Ergun equation, modifications are made to this equation. If the aspect ratio is less than 50, the effect of the wall on the hydraulic radius (i.e. the effect of the wall on the wetted surface area) is assumed significant. The hydraulic radius is the characteristic length dimension in the Reynolds number.

Mehta and Hawley (1969) modified the hydraulic radius in order to account for the additional wetted surface introduced by the wall. They assumed a constant void fraction for the whole bed. Therefore, the total effect of the wall on the flow through the column was not taken into account.

For large aspect ratios, the Ergun correlation should remain unchanged. For smaller aspect ratios, the effect of the wall region on the flow through the bed becomes more important. For small aspect ratios, the characteristic length should reflect the effect of the wall on the flow.

The modified hydraulic radius is dependent on the cylinder diameter and the particle diameter, and is given by:

$$\frac{D_h}{2} = \frac{\frac{\text{volume of voids}}{\text{volume of bed}}}{\frac{\text{wetted surface of particles}}{\text{volume of bed}} + \frac{\text{wetted surface of wall}}{\text{volume of bed}}} \quad (2.47)$$

Therefore, the hydraulic radius for a cylindrical column packed with spheres is given by:

$$\frac{D_h}{2} = \frac{\varepsilon d_p}{6(1-\varepsilon)M} \quad (2.48)$$

Where:

$$M = 1 + \frac{4d_p}{6D(1-\varepsilon)} \quad (2.49)$$

With the above definition, the resulting form of the Ergun equation is:

$$\left(\frac{\Delta p g}{L} \right) = 150 \frac{(1-\varepsilon)^2}{\varepsilon^3} \frac{\mu \bar{V}}{d_p^2} M^2 + 1.75 \frac{1-\varepsilon}{\varepsilon^3} \frac{G \bar{V}^2}{d_p} M \quad (2.50)$$

From the definition of M it is easy to see that if $d_p/D \ll 1$, equation (2.50) reduces to equation (2.42).

The outcome of this work by Mehta and Hawley (1969) is an improved form of the Ergun equation that is valid for $7 \leq D/d_p \leq 91$. This adapted form was tested at low Reynolds numbers and it predicted the experimental results well.

2.8.2 Two (more)-dimensional models

In this section more advanced models to describe the flow through packed columns are discussed. These models introduce more detailed porosity distributions.

Parallel channel model (Capillary Model):

The packed bed is modelled as a bundle of parallel channels of appropriate geometry. The flow through each of these channels can be assumed to follow the same expression as for flow through a tube, but with an effective diameter representing the tube diameter. For Newtonian fluids (in the absence of inertial effects, that is, for low Reynolds numbers) the velocity-pressure drop relationship is (Cohen and Metzner (1981)):

$$V_i = \left[\frac{\Delta p}{2KL_e} \right] \frac{(D_e/2)^2}{2K_0} \quad (2.51)$$

Where V_i is the velocity through the channel (interstitial velocity), L_e is the length of the channel or the effective path length followed by the fluid, D_e is the effective channel diameter. In the case of a round tube D_e is the true tube diameter. K is a rheological power law parameter (consistency index). The factor K_0 essentially accounts for the inadequacy in the choice of a proper effective diameter. The effective diameter is usually based on the concept of hydraulic radius, where four times the hydraulic radius replaces the effective diameter. The hydraulic radius is defined as:

$$R_h = \frac{\text{volume for flow}}{\text{wetted surface area}} \quad (2.52)$$

For a column composed of spherical particles, this can be shown to be:

$$R_h = \frac{\varepsilon D}{6(1-\varepsilon)} \quad (2.53)$$

Now eq (2.51). becomes:

$$V_i = \left[\frac{\Delta p}{2KL_e} \right] \frac{(2R_h)^2}{2K_0} \quad (2.54)$$

The value of K_0 can in principle be calculated for a channel of known geometry, by comparing eq (2.54). with the exact solution. In the case of porous media the shape of the channels is too complex, hence the value of K_0 cannot be determined.

The interstitial velocity V_i can be replaced by $V_i = \frac{\bar{V}}{\varepsilon} \frac{L_e}{L}$ (Cohen and Metzner 1981).

Here $\bar{V}$ is the superficial velocity (refer to eq.(2.32)). Now eq.(2.54) becomes:

$$\bar{V} = \left[\frac{\Delta p}{2KL_e} \right] \frac{(2R_h)^2}{2K_0} \frac{\varepsilon}{(L_e/L)^2} \quad (2.55)$$

Alternatively, in terms of the mass flux G , through the column:

$$G = \rho \left[\frac{\Delta p}{2KL_e} \right] \frac{(2R_h)^2}{2K_0} \frac{\varepsilon}{(L_e/L)^2} \quad (2.56)$$

Since there are two unknown parameters $C^* = L_e/L$ and K_0 in eq (2.57), they cannot be uniquely determined and are, therefore, grouped together:

$$K_0 (C^*)^2 = B_c \quad (2.57)$$

The value of B_c for Newtonian fluids in columns packed with spheres range between 4.166 and 5. The resulting maximum scatter reported for most pressure drop flow rate relationships is about 20%. From the literature there is a general consensus on the value of $B_c = 5$, this is the value used by (Cohen and Metzner 1981).

Tri-regional model of Cohen and Metzner

Cohen and Metzner (1981) argue that for columns with $D/d_p > 30$ the single region model proposed by Ergun (1950), is adequate to estimate the mass flow through the column.

Cohen and Metzner (1981) divided the column into three regions. For each region they gave a description of the radial void fraction distribution, explained in section 2.5.2. They also included the modification by Mehta and Hawley (1969) in the Ergun equation. With this model they calculated the mass flux through each region.

This model accounts for both the primary effects of the wall on the flow through the column.

Sodré & Parise

Sodré & Parise (1998) analysed the pressure-drop-flow rate relation for annular columns packed with spherical particles over a wide range of particle Reynolds numbers ($0 < \frac{Re}{1 - \varepsilon_{ave}} \leq 2000$).

The void fraction distribution used by Sodré & Parise (1998) is discussed in section 2.5.2. Sodré & Parise (1998) divided the annulus into the outer wall region, the transition region and the inner wall region. For each of the regions the ratio of the average velocity for that region to the total average flow velocity (superficial velocity) was calculated. In the wall regions the effects of the walls are included similar to the treatment given by Cohen and Metzner (1981). For the transition region they used the Ergun equation to predict the flow, with no adjustments.

With this model they predicted the flow velocities in the various regions in relation to the superficial velocity. They also compared these results with results from physical experiments they conducted. The experimental results are in close agreement to that obtained from the model over a wide range of particle Reynolds numbers.

2.9 Velocity distribution

In a packed column reactor the void fraction varies sharply near the wall, since the geometry of the packing is interrupted there. As a result the velocity profile inside a packed column is severely distorted near the wall, reaching a maximum in the near-wall region.

In the design of packed column devices the mass flow rate, velocity distribution and temperature distribution are often important parameters. The theoretical aspects of the void fraction distribution and the implementation in investigations have been discussed in previous sections. It is now necessary to give a brief overview of the work that has been done to evaluate the extent of velocity variations in packed columns.

In this section, the radial velocity distribution in packed columns will consequently be investigated.

2.9.1 Vortmeyer & Schuster

Brinkman (as quoted by Vortmeyer and Schuster (1983)) formulated the differential equation that describes the flow profile within porous media bounded by a rigid wall. Vortmeyer and Schuster (1983) solved the Brinkman equation by an equivalent variational method and approximated the radial variation of the void fraction with a smooth exponential expression.

Figure 2-9 (a) shows the shape and position of the velocity peaks calculated by Vortmeyer and Schuster (1983), for different Reynolds numbers. The velocity has been normalized with the superficial velocity $\bar{V}$.

In Figure 2-9 (b) the calculated velocity profiles of Vortmeyer and Schuster (1983) in the packing are compared with experimental measurements and calculations of the flow profile 10 millimetres above the packing.

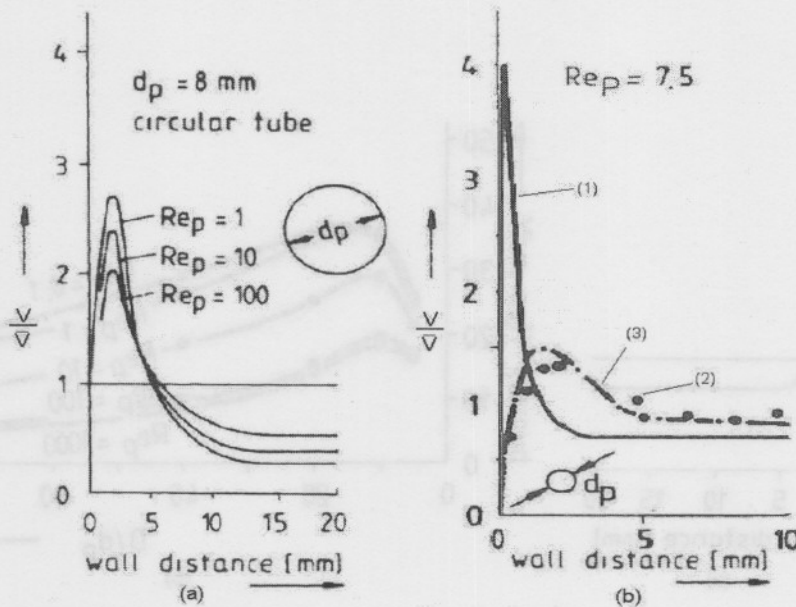


Figure 2-9. (a)- Calculated dimensionless flow profiles at various Re . (b)- Comparison of calculated flow profile in bed (1), vs. measured flow profile 10mm above bed (2); and calculated profile 10mm above bed (3). Adapted from Vortmeyer and Schuster (1983)

From Figure 2-9 it is clear that there can be notable velocity peaks near the wall of the column. Further, the (traditional) measurements of the velocity profile above the

packing cannot be considered an accurate description of the flow distribution in the column.

Figure 2-10 (a) is a diagrammatic representation of the definition of bypass flow as given by Vortmeyer and Schuster (1983). From Figure 2-9 it can be seen that much of the flow goes through the packing in the wall region in the form of bypass flow. The result is that the velocity in the central region of the column is lower than predicted by the superficial velocity.

Figure 2-10 (b) shows the percentage of flow going through the wall region in the form of bypass flow for different column aspect ratios. It is notable that this percentage has a definite maximum (for all Reynolds numbers). This maximum is close to an aspect ratio of 10. It is also interesting to note that the higher the Reynolds number is, the smaller the maximum velocity peak and the amount of bypass flow becomes.

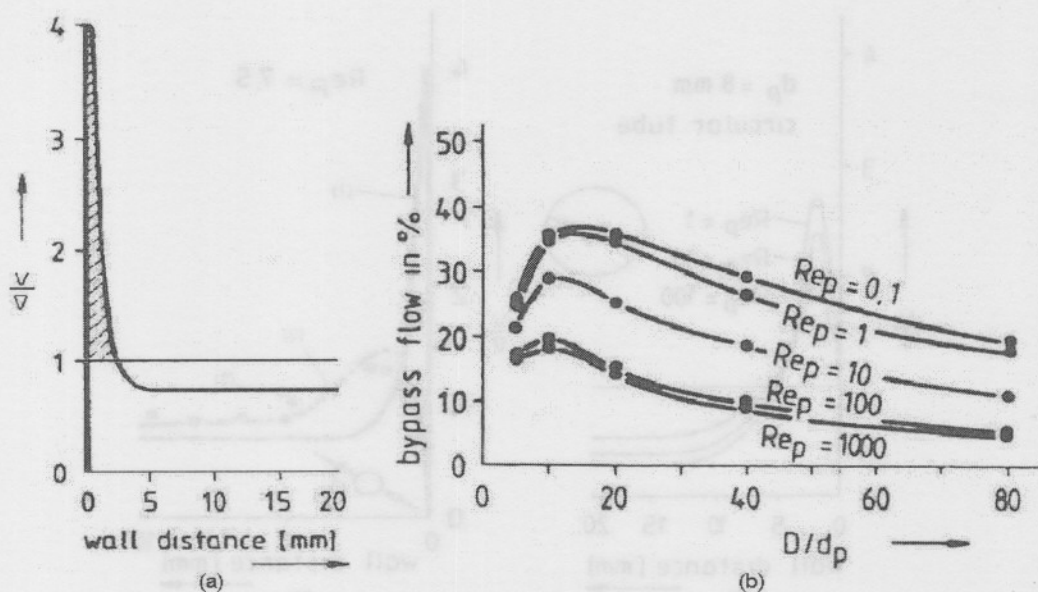


Figure 2-10. (a)-The definition of bypass flow. (b)- Percentage of flow in the bypass region vs. aspect ratio of the column, for different particle Reynolds numbers. Adapted from Vortmeyer and Schuster (1983)

White and Tien (1987) also did an analysis of the wall channelling in packed columns. In their model they used a radial porosity distribution similar to that of

Vortmeyer and Schuster (1983). The results they obtained, for the flow distribution are in good agreement with those of Vortmeyer and Schuster (1983).

2.9.2 Du Toit

Du Toit (2002) used the finite element approach to solve the one-dimensional momentum equation for the radial distribution of the axial velocity for the PBMR configuration. The void fraction distribution used is the same as that of Vortmeyer and Schuster (1983).

Du Toit (2002) obtained the dimensionless mass flux distribution as shown in Figure 2-11 (only the last 10% of the column radius is shown). The average dimensionless mass flux (plug flow) is also shown (dashed line). The mass flux in the central region of the column is only about 80% of the average mass flux. The maximum mass flux achieved is 19.5 times the average mass flux.

The bypass flow defined by Vortmeyer and Schuster (1983) in Figure 2-10-a, were determined to be 26.2% of the total mass flow. The percentage of bypass flow as a function of particle Reynolds number is plotted in Figure 2-12.

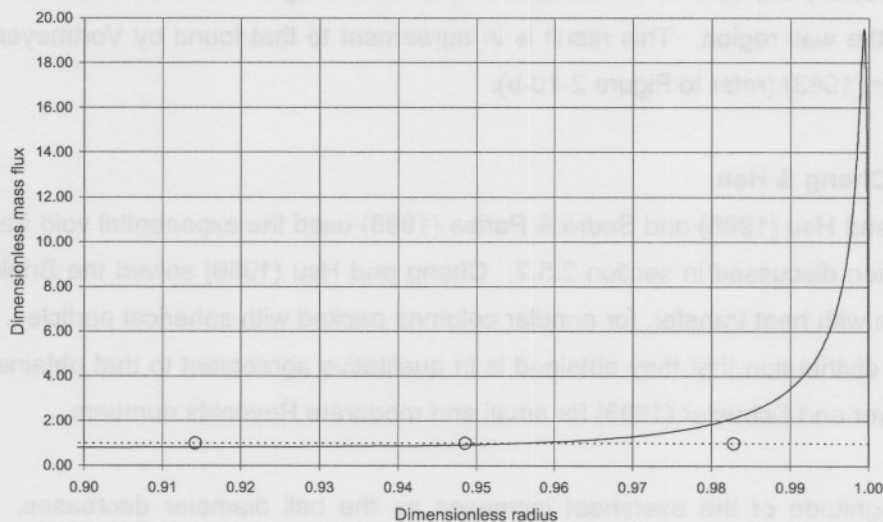


Figure 2-11. *Dimensionless mass flux as a function of dimensionless radius at design mass flow rate. Du Toit (2002).*

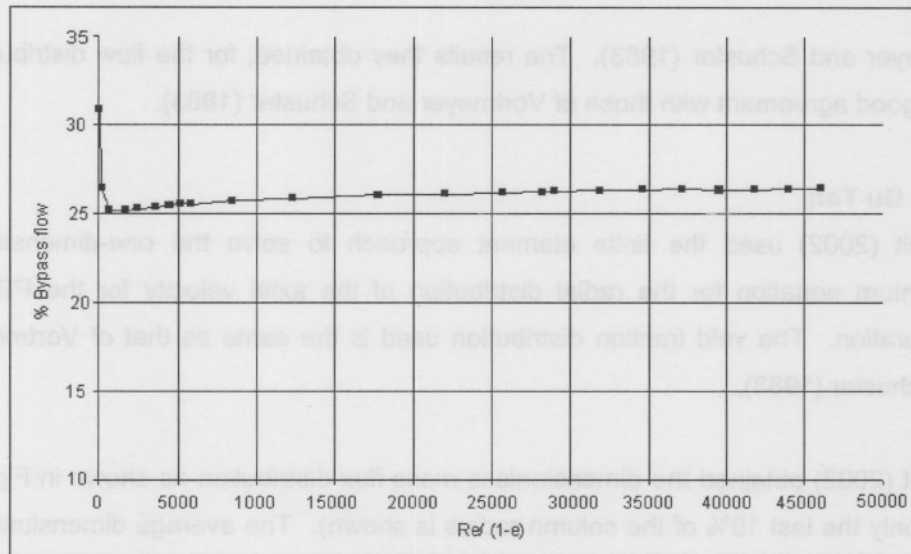


Figure 2-12. Percentage of bypass flow as a function of particle Reynolds number. Du Toit (2002).

As the Reynolds number decreases, the percentage of bypass flow gradually decreases. At very low Reynolds numbers, the amount of bypass flow drastically increases. This is probably due to the viscous effects that dominate the flow region and especially the core of the column where the average void fraction is much less than in the wall region. This result is in agreement to that found by Vortmeyer and Schuster (1983) (refer to Figure 2-10-b).

2.9.3 Cheng & Hsu

Cheng and Hsu (1986) and Sodrè & Parise (1998) used the exponential void fraction distribution discussed in section 2.5.2. Cheng and Hsu (1986) solved the Brinkman equation with heat transfer, for annular columns packed with spherical particles. The velocity distribution that they obtained is in qualitative agreement to that obtained by Vortmeyer and Schuster (1983) for small and moderate Reynolds numbers.

The magnitude of the overshoot increases as the ball diameter decreases. The velocity overshoot is slightly higher at the inner wall than at the outer wall. The velocity peaks are respectively a $\frac{1}{4}$ -particle diameter from the inner wall, and a $\frac{1}{3}$ -particle diameter from the outer wall.

Velocity distributions obtained by Cheng and Hsu (1986), for various particle diameters are given in Figure 2-13.

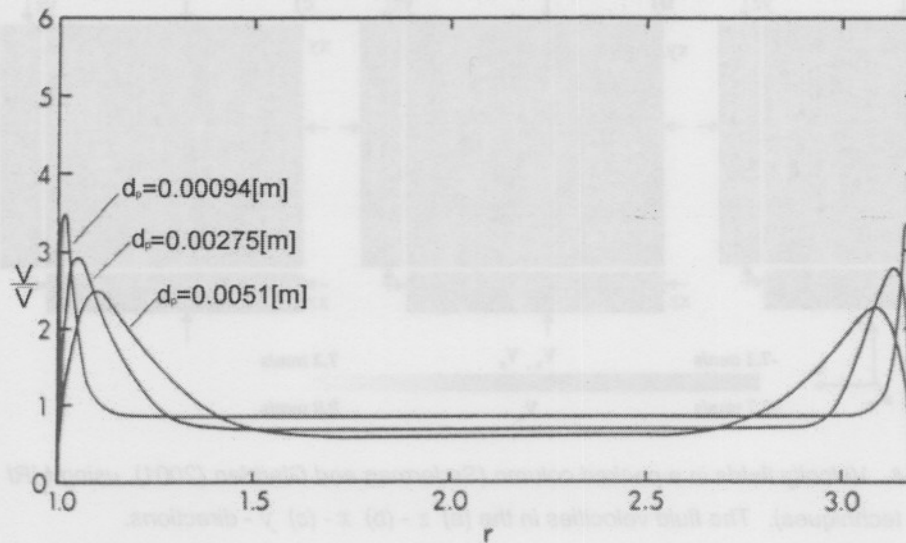


Figure 2-13. Wall channelling effect on axial velocity distribution, for annular columns.

Adapted from Cheng and Hsu (1986:1848).

2.9.4 Magnetic Resonance Imaging (MRI) techniques

Using high resolution MRI it is possible to probe packed columns for information into the spatial distribution of flow effects and its relation to the topology of the pore space. Experimental and theoretical studies into flow through porous media often treat the medium as a continuum. These approaches neglect the local inhomogeneities in the column, and concentrates only on bulk properties. Some of the most common of these models have been discussed in the previous section.

Sederman and Gladden (2001), Sederman, Johns *et. al.* (1998), Sederman, Johns *et. al.* (1997), and Sederman, Alexander *et. al.* (2001) experimentally studied the flow distribution through packed columns using MRI. The experimental setup and other aspects of the experiments are also discussed. MRI techniques are discussed by Callaghan (1991).

From the work of Sederman and Gladden (2001) it is clear that the flow in packed columns is non-homogeneous. There are significant variations in local flow rate through the column. In some regions the flow velocity is enhanced significantly (Figure 2-14).

From Figure 2-14 it is clear that the velocity over most of the column is nearly the same. This is close to the superficial velocity of the column. There are regions that have much higher velocities. There are also regions in which reverse flow is present.

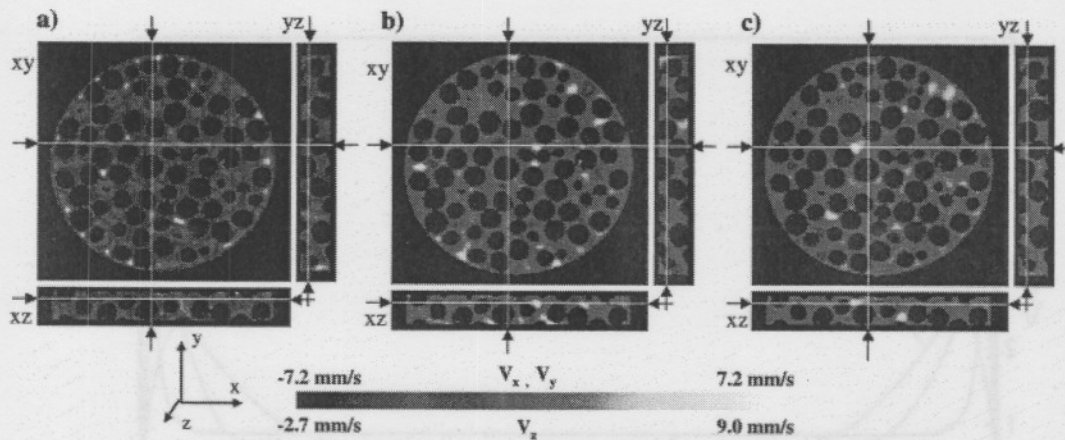


Figure 2-14. Velocity fields in a packed column (Sederman and Gladden (2001), using MRI techniques). The fluid velocities in the (a) z - (b) x - (c) y - directions.

Sederman, Johns *et. al.* (1998) found that a relatively small fraction of the inter-particle space carries a high percentage of the flow.

The results in Figure 2-15 represent a horizontal slice through the column, at a typical axial location.

Figure 2-15 is a plot of the volume flow fraction ($Q(A)/Q(0)$) through pores with cross-sectional areas greater than A , as a function of the area fraction ($a(A)/a(0)$), and as a function of the number fraction ($N(A)/N(0)$) of pores with cross-sectional area greater than A .

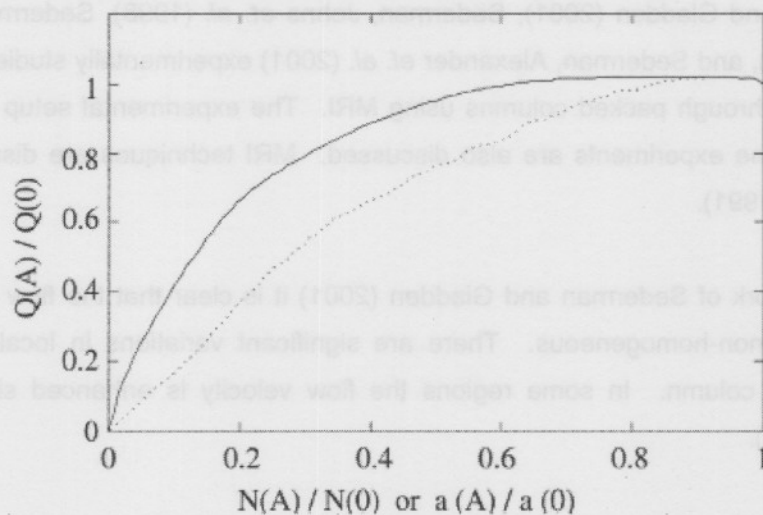


Figure 2-15. The fraction of the volume flow carried by pores with cross-sectional area greater than A , versus the number fraction (—), and the area fraction of these pores (···).

$Q(A)$ is the volume flow rate through the pores with cross-sectional area greater than A . $Q(0)$ is the total volume flow rate through the column. $a(A)$ is the total cross-sectional area of all pores with cross-sectional area greater than A . $a(0)$ is the total cross sectional area of all pores. $N(A)$ is the number of pores with cross-sectional area greater than A . $N(0)$ is the total number of pores at that slice.

Sederman, Johns *et al.* (1998) also found that the pores carrying high volume flows are characterised by larger volumes, and higher interfacial surface area adjoining neighbouring pores. These pores are also typically located in the wall region of the column. This is due to the ordering introduced by the walls. The result is consistent with predictions.

2.9.5 Other methods

Becker & Laurien (2001) applied CFD analysis techniques to describe the flow through the PBMR core. In their development of the problem they used a heterogeneous model, with an assumed void fraction distribution (similar to that used by Cheng & Hsu, 1986). The interaction of the gas and solid phases was modelled with the Ergun equation for the pressure drop, and a heat exchange term.

Hassan & Yesilyut (2002) investigated the flow distribution through packings of spheres using Large Eddy Simulation (LES). Specific attention was given to flow curvature. In this investigation the wall effects were not considered. In their study they constructed a detailed mesh of the flow domain through a cubic packing of 27 spheres. (To simulate one second took approximately 80 hours with a 4 processor (400MHz) Ultra Spark 2 Sun System.)

Inamuro *et al.* (1999) used the Lattice Boltzman Method (LBM) to simulate the flow through a packing of 9 spheres in a cubic domain. Again the flow field was explicitly defined, and no void fraction distribution needed to be assumed.

Brenner *et al.* (2001) applied LBM to a column randomly packed with spheres. In this investigation they show that LBM can predict flows through complex geometries. This includes turbulence, diffusion processes and more.

2.10 Conclusions made from the literature

In this chapter the porosity distribution in packed columns was investigated. There exist significant variations in porosity in the region the column wall and other packing discontinuities, for example the column wall.

These porosity variations in the wall region lead to velocity peaks, and consequently to irregular mass flux distribution through the porous medium. This can lead to poor predictions of the mass flow, or pressure drop over the column.

In the literature studied there are very few references to numerical studies of the packing structure of packed columns. There are codes and procedures that simulate the packing of particles. Mueller (1997) discuss several deterministic methods available to pack spherical particles in cylindrical columns. Other random procedures are also available to achieve these simulations. With the information supplied from these codes it is possible to study the packings in more detail with numerical methods. In this study numerical procedures will be developed to study packed columns. These procedures will form the basis for further development and investigations into packed column devices.

Chapter 3

Theoretical Background

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3.3	Axial Void Fraction Distribution	45
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3.1 Introduction

In the previous chapters the objectives of this study were stated, and the context of the problem was established. The importance of packed column devices was presented and the presence of the void fraction variations discussed. The work done by other investigators were reviewed. This introduction has given the reader an insight into the problem of the void fraction variation present in packed columns and the resultant flow through packed columns.

This chapter will now focus on the models that can be used to investigate packed columns numerically. For the purposes of this study the columns are assumed to be cylindrical or annular. The packing particles used are spherical and uniform in size, the position of each particle is given in Cartesian coordinates.

The numerical models that are developed are:

- A model to check for overlap between particles,
- a model to calculate the axial porosity distribution,
- a model to calculate the radial porosity distribution, and
- a model to determine the representative elementary volume (REV) about a point in the column.

Before the data for a packed column can be analysed, the quality of the data must first be established. To this end the overlap between particles is determined. Some software used to pack particles numerically allow for some overlap. If the overlap between the spheres is too much, further analysis will have little value.

The axial- and radial porosity distributions of the packing are also calculated. This can be compared with experimental data of other investigators. It is very difficult to determine the REV of a packed column experimentally. The REV can however be determined numerically. This can give some interesting insight into the definition of porosity.

Commercial software was used to generate the packing of spheres into cylindrical columns. This software supplies the positions of the centres of the spheres in the packing. There are several software packages employing different models that can be used to perform these packings. The details of these methods will not be discussed in this report.

3.2 Overlap Analysis of Packing

The data obtained for the positions of the spheres in a packed column must be analysed to determine the quality of the data. This study will not attempt to prove the reality of the packing as compared to a real packing. The method used to test the quality of the data is to determine the overlap between spheres. Many numerical procedures that simulate the packing arrangement of particles in a vessel allow some overlap between particles.

If the overlap between particles is too large, then the calculated porosity will have little value. The packing will not be a useful approximation of a real packed column, and thus any information extracted will be of little use. The packed columns used in this study are therefore first tested for the overlap between adjacent spheres.

3.2.1 Development of model

A simple check to determine the overlap between spheres was implemented. The distance between the centres of two spheres was determined. If this distance is smaller than a sphere diameter, then some overlap exists. In this procedure, the overlap is defined as a percentage of the sphere diameter (eq.(3.1)).

$$overlap = \frac{\left(d_p - \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \right)}{d_p} \times 100 \quad (3.1)$$

Here the subscripts i , and j denotes the specific spheres being tested. The position of the overlap is also determined and recorded. The position of the overlap is located halfway between the overlapping spheres.

3.2.2 Implementation of model

To implement the model an exhaustive search is done to locate all possible combinations of sphere pairs to test for overlap. The algorithm employed is shown in the pseudocode in Figure 3-1.

```
for (iSphere = 1; iSphere <= Number_Of_Spheres; iSphere++)
{
    for (jSphere = iSphere + 1; jSphere <= Number_Of_Spheres; jSphere++)
    {
        Calculate distance between the i'th sphere and the
        j'th sphere (Spheres_Distance)

        if ( Spheres_Distance < Sphere_Diameter)
        {
            Calculate overlap between spheres (eq.(3.1)).

        } // End overlap test
    } // End for loop over jSphere
} // End for loop over iSphere
```

Figure 3-1. Pseudocode to explain the algorithm employed to search for overlapping spheres.

This algorithm in Figure 3-1 can be explained as follows; for each sphere calculate the distance between this sphere and all other spheres with sphere identity numbers greater than this one, if the distance is smaller than a sphere diameter, calculate the overlap.

3.3 Axial Void Fraction Distribution

The void fraction distribution of a packed column does not change significantly with axial position. This is true except in regions where there is a wall (or other form of discontinuity, for example at the top of the cylinder). Therefore, in the floor region of a packed column there will be void fraction variations present. There are references in the literature to studies investigating the void fraction change present in the floor region of packed columns (these studies are discussed in Chapter 2).

The procedure that is explained here is used to determine the void fraction distribution along the axis of a cylindrical packed column. The experimental data from other investigators can be used to verify and validate the procedure.

3.3.1 Development of model

To calculate the axial porosity distribution in a packed column, the area porosity can be calculated on consecutive axial planes, situated a small axial distance Δz from each other. Figure 3-2 is a schematic representation of an axial plane cutting the column.

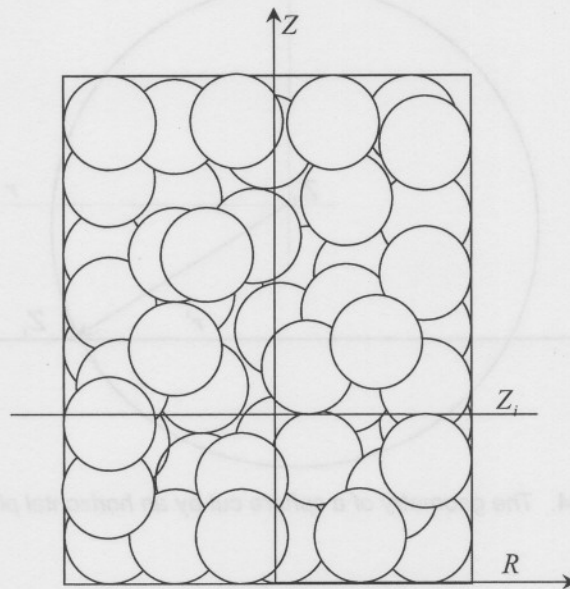


Figure 3-2. Schematic representation of the numerical packed column used in the calculation of the axial void fraction distribution.

The area porosity can be determined for any horizontal plane Z_i , cutting the column. To calculate the area porosity on a plane cutting the column, the individual spheres being cut by the plane needs to be located. Then the cut area A of each sphere must be determined. Figure 3-3 is an illustration of the area A , of an individual sphere to be determined in order to calculate the porosity at an axial level.

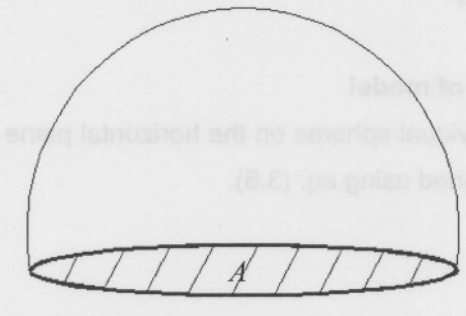


Figure 3-3. Illustration of the area A , to be determined for each sphere cut by the horizontal plane.

Figure 3-4 shows the relevant geometric relationships for an arbitrary sphere with centre height Z_0 , cut by a horizontal plane at height Z_i .

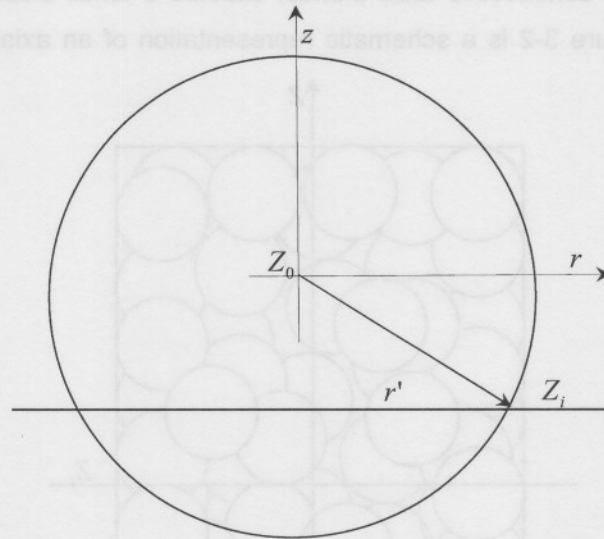


Figure 3-4. The geometry of a sphere cut by an horizontal plane Z_i .

The area A is calculated as follows:

$$r' = \sqrt{\left(\frac{d_p}{2}\right)^2 - |Z_0 - Z_i|^2} \quad (3.2)$$

$$A = \pi r'^2 \quad (3.3)$$

Where A is the cut area as indicated in Figure 3-3, and r' is the radius of the area as calculated by eq. (3.2).

3.3.2 Implementation of model

With the areas from individual spheres on the horizontal plane known, the porosity at that axial level is determined using eq. (3.5).

$$\varepsilon = \frac{A_v}{A_t} \quad (3.4)$$

$$\varepsilon = 1 - \frac{\sum A}{A_T} \quad (3.5)$$

Here A_v is the area on the plane occupied by voids. The term $\sum A$ is the sum of all the cut areas A , of the spheres, and is therefore the area, occupied by spheres on the cutting plane. A_T is the total area of the plane, and D the column diameter:

$$A_T = \frac{\pi D^2}{4} \quad (3.6)$$

```

while (Zi < Column_Height)
{
    for (iSphere = 1; iSphere <= Number_Of_Spheres; iSphere++)
    {
        Test to determine if the particular sphere is
        cut by the cutting plane.

        if (absolute_Value(Z0 - Zi) < (dp/2))
        {
            Calculate the cut area A of the sphere.
        }

        Sum all areas A, contributed by spheres cut by
        horizontal plane Zi.

    } // End loop over iSphere

    Calculate total area of column on cutting plane.
    Calculate porosity.
    Increment axial position of cutting plane.
} // End loop over axial levels

```

Figure 3-5. Pseudocode to explain the algorithm used to calculate the axial porosity distribution in a packed column.

The implementation of the model developed for calculating the porosity, on a horizontal plane, cutting the column, is shown in Figure 3-5.

The algorithm in Figure 3-5 can be explained as follows; for each axial cutting plane, and all spheres in the column, check if the plane cuts the sphere, calculate the cut

area A of that sphere, sum all cut areas contributed by spheres (on a plane), use eq. (3.5) to calculate area porosity, on the axial plane.

3.4 Radial Void Fraction Distribution

As explained in the literature survey, many studies have been conducted to determine the radial void fraction distribution in packed columns. Void fraction is a measure of the area available for flow.

3.4.1 Development of model

In this model, the area void fraction at a radial position in the column is determined. To determine the area porosity at a radial position, it is necessary to determine the total area occupied by spheres, at that radial position. From this information, it is then possible to determine the void fraction. Figure 3-6 is a schematic representation of a radial cut trough a column packed with spheres.

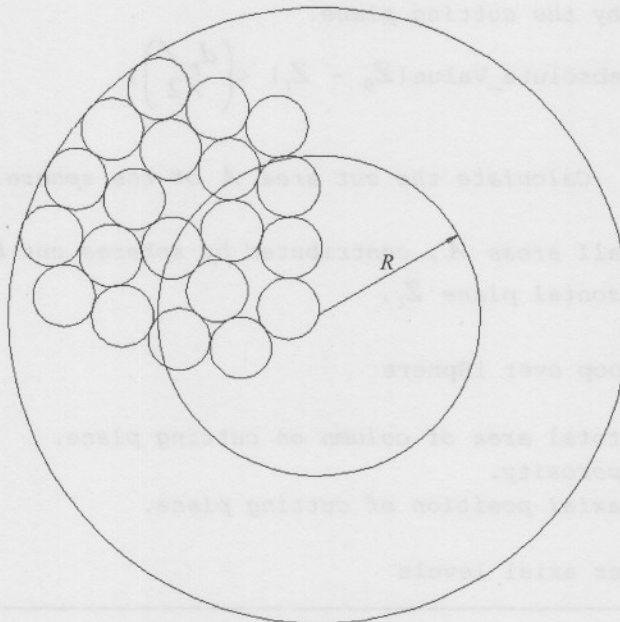


Figure 3-6. Schematic representation of radial cut through packed column.

To calculate the porosity, first determine the cut areas of the individual spheres cut by the radial plane. Figure 3-7 is a schematic representation of the area of a sphere cut by the radial plane R .

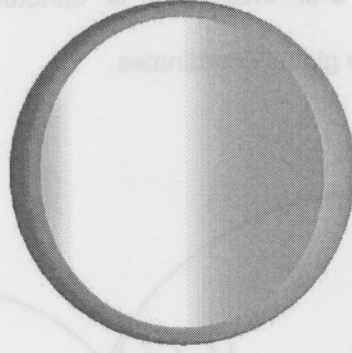


Figure 3-7. Illustration of the area A of a sphere cut by the radial plane.

Any point (X, Y, Z) in the global coordinate system can be converted to (x, y, z) in the local coordinate system, situated on an individual sphere as follows (Figure 3-8):

$$x = X - R_0, \quad y = Y, \quad z = Z - Z_0 \quad (3.7)$$

Where R_0 is the radial position of the sphere and the X -direction is taken as the horizontal line connecting the centre line (axis) and the centre of the particle. For all points on the intersection of the radial cutting plane (with radius R) and the surface of the sphere, constituting the cutting line, the following holds:

$$X_s^2 + Y_s^2 = R^2 \quad (3.8)$$

Where X_s and Y_s are any point on the intersection, in global coordinates. In local coordinates:

$$x_s^2 + y_s^2 + z_s^2 = \left(\frac{d_p}{2} \right)^2 \quad (3.9)$$

Where x_s , y_s and z_s is the coordinates on the cutting line. The plane $z_s = 0$, is the horizontal centre plane through the sphere. The point $z_s = 0$ in eq.(3.9), is the intersection point of the radial cutting plane and the edge of the sphere, as viewed

from above, as in Figure 3-8. This point is denoted as (x_a, y_a, z_a) in local coordinates, or (X_a, Y_a, Z_a) in global coordinates.

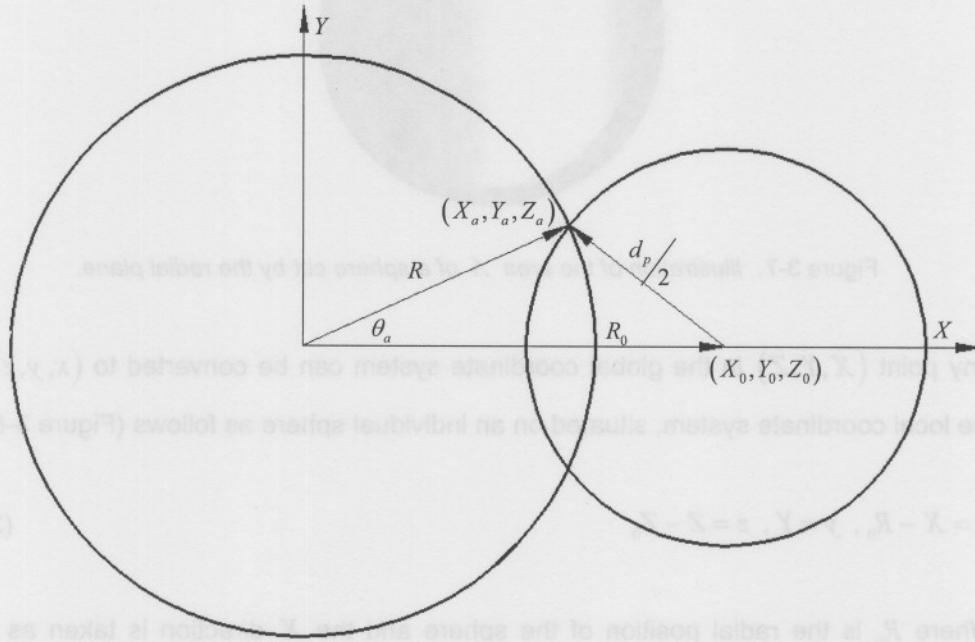


Figure 3-8. Radial plane cutting through a sphere with position (X_0, Y_0, Z_0) , at a distance R_0 from the origin.

From eq.(3.7) and eq.(3.9), follows (with R_0 the radial position of the sphere in the column):

$$(X_a - R_0)^2 + Y_a^2 = \left(\frac{d_p}{2}\right)^2 \quad (3.10)$$

$$X_a^2 - 2X_a R_0 + R_0^2 + Y_a^2 = \left(\frac{d_p}{2}\right)^2 \quad (3.11)$$

Now subtracting eq.(3.11) from eq.(3.8):

$$2R_0 X_a - R_0^2 = R^2 - \left(\frac{d_p}{2}\right)^2 \quad (3.12)$$

This can be solved for X_a :

$$X_a = \frac{R^2 - \left(\frac{d_p}{2}\right)^2 + R_0^2}{2R_0} \quad (3.13)$$

And then Y_a and θ_a follows:

$$Y_a = \sqrt{R^2 - X_a^2} \quad (3.14)$$

$$\theta_a = \arccos\left(\frac{Y_a}{X_a}\right) \quad (3.15)$$

For all points lying on the surface of the sphere:

$$x^2 + y^2 + z^2 = \left(\frac{d_p}{2}\right)^2 \quad (3.16)$$

And in global coordinates:

$$(X - R_0)^2 + Y^2 + (Z - Z_0)^2 = \left(\frac{d_p}{2}\right)^2 \quad (3.17)$$

And thus for all points on the cutting line follows:

$$Z_s - Z_0 = \sqrt{\left(\frac{d_p}{2}\right)^2 - X_s^2 + 2R_0X_s - R_0^2 - Y_s^2} \quad (3.18)$$

And in local coordinates:

$$z_s = \sqrt{\left(\frac{d_p}{2}\right)^2 - X_s^2 + 2R_0X_s - R_0^2 - Y_s^2} \quad (3.19)$$

Substituting eq. (3.8) into eq. (3.19) leaves:

$$z_s = \sqrt{\left(\frac{d_p}{2}\right)^2 - R^2 - R_0^2 + 2R_0 X_s} \quad (3.20)$$

And remembering that:

$$X = R \cos \theta \quad (3.21)$$

Eq. (3.20) becomes:

$$z_s = \sqrt{\left(\frac{d_p}{2}\right)^2 - R^2 - R_0^2 + 2R_0 R \cos \theta_s} \quad (3.22)$$

In this model two axial (horizontal) planes are specified (Z_{low} and Z_{high}) between which the porosity is calculated (shown in Figure 3-9). With this functionality, it is possible to choose to omit regions of the column where there are effects due to the floor, or any other discontinuity in the column.

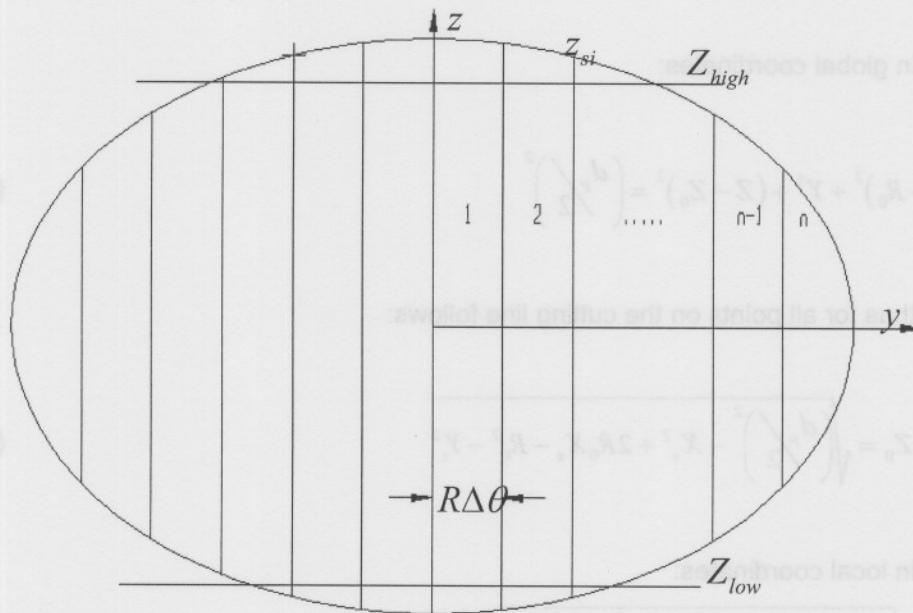


Figure 3-9. Schematic representation of the area to be calculated, showing the integration intervals.

The area of the cutting plane on the sphere is (Figure 3-9):

$$A = 2 \int_0^{\theta_a} (z_t + z_b) R d\theta \quad (3.23)$$

With:

if $z_s \leq Z_0 - Z_{low}$ then

$$z_b = z_s \quad (3.24)$$

else if $z_s > Z_0 - Z_{low}$ then

$$z_b = Z_0 - Z_{low}$$

and

if $z_s \leq Z_{high} - Z_0$ then

$$z_t = z_s \quad (3.25)$$

else if $z_s > Z_{high} - Z_0$ then

$$z_t = Z_{high} - Z_0$$

With θ ranging from $0 \leq \theta \leq \theta_a$. To calculate the cutting area, integrate eq.(3.23) numerically using the trapezium rule. Integrating from $\theta = 0$, in the positive θ -direction, the last z -value will be zero. Thus, the trapezium rule reduces to:

$$A = 2 \left[\frac{1}{2} (z_{t1} + z_{b1}) + \sum_{i=2}^n (z_{ti} + z_{bi}) \right] R d\theta \quad (3.26)$$

Here z_{ti} and z_{bi} is defined as the height of the cutting line in local coordinates, at an angle of θ_i with $0 \leq \theta_i \leq \theta_a$, and θ_a defined in the local coordinate system as shown in Figure 3-8. To integrate the cut area on a sphere numerically; θ_a is divided into a finite number of increments of size $\Delta\theta$.

Using equations, (3.13), (3.14), (3.15), (3.22) and eq.(3.26) it is now possible to calculate the area of each individual sphere cut by the radial cutting line.

3.4.2 Implementation of model

In order to calculate the area porosity on a radial plane (Figure 3-6), the areas from all the individual spheres cut by that plane must be determined. Figure 3-10 is the algorithm for calculating the cut area of an individual sphere.

```

Test to check if a sphere lies partially, or totally between the
two horizontal planes,  $Z_{low}$ , and  $Z_{high}$ .

if  $((Z_0 + \left(\frac{d_p}{2}\right)) > Z_{low})$  OR  $(Z_0 - \left(\frac{d_p}{2}\right)) < Z_{high}$ 
{
    Test to check if the radial plane  $R$  cuts the sphere,
    with centre position  $R_0$ .

    if  $(\text{absolute\_value}(R_0 - R) < \left(\frac{d_p}{2}\right))$ 
    {
        Determine the coordinates of  $(x_a, y_a, z_a, \theta_a)$  (equations (3.13),
        (3.14), (3.15), and (3.22)).
        Calculate the size of an integration interval,  $\Delta\theta$ .

        for  $(\theta_i = 0; \theta_i \leq \theta_a; \theta_i + \Delta\theta)$ 
        {
            Calculate the height  $z_{si}$  in local coordinates, of the
            cutting line at the specified angle,  $\theta_i$ .

            Use eq. (3.24) (3.25) to determine the appropriate
            height of the cutting line in local coordinates.
        }
        Calculate the area by means of the trapezium rule (3.26).
    } //End loop over  $\theta_i$ 
} // End test radially
} // End test axially

```

Figure 3-10. Algorithm for determining the cut area of an individual sphere.

The area porosity on the radial plane can be calculated as follows:

$$\varepsilon(R) = \frac{A_v(R)}{A_T(R)} \quad (3.27)$$

The area on the plane occupied by voids is A_v , and the total area of the plane is A_T .

Thus:

$$\varepsilon(R) = 1 - \frac{\sum A(R)}{A_T(R)} \quad (3.28)$$

Where A is the cut area contributed by a sphere.

The algorithm in Figure 3-10 can be explained as follows; if a sphere lies partially or totally between z_{low} , and z_{high} , and if the sphere is cut by the radial plane R , determine the intersection coordinates $(x_a, y_a, z_a, \theta_a)$ (equations (3.13), (3.14), (3.15) and (3.22)), calculate the size of an integration interval $\Delta\theta$, calculate the height of the cutting plane at each angular interval, use trapezium rule to calculate the cut area of the sphere.

3.5 Determining the REV

The representative elementary volume (REV) is discussed in detail in the literature survey. The aim of this procedure is to establish the REV about a point in a packed column. It is important to realise that the REV will change with position in a packed column, due to the random nature of the packing, and wall effects.

3.5.1 Development of model

The REV about a certain point P in a packed column can be determined by taking consecutively larger volumes about that point, and calculating the porosity for each volume. This is equivalent to the procedure discussed in section Chapter 2 explaining the REV.

In this procedure, a spherical volume U_i is constructed about point P in the column. The porosity of this volume is determined, and the size of the volume is incremented.

$$0 \leq U_i \leq U_n \text{ with } i = 1, 2, 3 \dots n \quad (3.29)$$

The volume of U_i is varied from $U_1 = 0$ to U_n , where U_n is the predetermined maximum size of U_i about point P .

To determine the porosity of U_i analytically is extremely difficult. This involves finding the intersections of the spheres with the boundary of the spherical volume, which is very complex. Consequently, an approximation to the porosity is calculated in this procedure.

Thus to determine the porosity of the volume U_i , an equally spaced grid is first generated about point P . For each differential (control) volume in the grid, a point in the centre of this volume is taken to represent the average of all properties of the volume. Each of the points lying in the volume U_i , is checked whether it lies inside a particle or outside. The point is assigned a value of one if the point is situated within a sphere, and zero is assigned, if the point is not situated in a sphere. To calculate the porosity of the volume U_i the total volume of the points lying in particles in this volume $((U_s)_i)$, is calculated. The porosity of volume U_i then follows:

$$\varepsilon(U_i) = 1 - \frac{(U_s)_i}{U_i} \quad (3.30)$$

The REV is reached when the porosity of the elementary volume U_i , does not change significantly when making small changes to the volume U_i . The data generated from this procedure are analysed in a spreadsheet application to determine the REV.

The implementation of this model will be considered in Chapter 4, where the structure of the code is discussed.

3.6 Conclusion

In this chapter numerical models were developed to analyse packed columns. These models will form the basis of the codes that are developed in the next chapter.

The axial- and radial void fraction distribution models determine the area porosity on a series of consecutive cutting planes through the column. In the experiments that was conducted by Goodling *et al.* (1980), Roblee *et al.* (as quoted by Goodling *et al.*, 1980) and Gordon (2001), the porosity of a thin annular ring is determined. This is

the average volume porosity at that position in the column. This will again be discussed in Chapter 5.

Chapter 4

Experimental Method and Analysis

Chapter outline:

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Chapter 4

Experimental Method and Analysis

Chapter outline:

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4.1 Introduction

In the previous chapter, models were developed to:

- analyse the quality of the numerical data,
- calculate the axial- and radial porosity distributions in a packed column, and
- determine the size of the REV about a point in the packed column.

In this chapter specific issues that were encountered in the development of the codes, are discussed. The aim of this chapter is to provide the reader with a deeper understanding of the codes.

The nature of the problems investigated in this study are very similar, and it is necessary to search for particles with specific attributes from a, potentially, very large collection. Therefore, in most of the codes that were developed, the particles are sorted into bins. These bins are collections of particles with similar position attributes. This makes it much faster to locate the particles with desired characteristics.

In this chapter, the following issues are addressed.

- The basic structure of the codes is discussed. The codes with similar structures are grouped together and the functions and sub-functions that constitute the codes are discussed together.
- Each of the sub-functions is discussed in detail. The emphasis is put on the implementation of the code.

In order to validate the codes, test cases are discussed and the solutions are checked against the analytical solutions, or the results of other methods.

4.2 Basic structure of codes

In this section the basic structure of the codes are discussed. To take advantage of the similarities of the problems, the codes are structured similarly. The functions and sub-functions employed share the same function and general form. Thus, it is useful to discuss these sub-functions together here. In each of the codes, the calculation of the desired solution (i.e. axial porosity distribution, or radial porosity distribution) is located in a separate sub-function. These sub-functions are discussed individually in section 4.3.

The following codes share the same structure:

- Code to calculate overlap between spheres (calcoverlap.cpp).
- Code to calculate axial porosity distribution (axialporos.cpp).
- Code to calculate radial porosity distribution (radialporos.cpp).

The code used to calculate the representative elementary volume (REV.cpp) about a point in a column has a similar structure, with particular differences. This code is discussed separately in section 4.4.

4.2.1 General structure and function of codes

Figure 4-1 is an illustration of the basic structure of the codes. The sub-functions that share the same function are discussed, and detailed explanations of the algorithms employed are given in this section.

This schematic diagram clearly shows the similarities that exist between the codes. The only sub-function that differs between the codes is the calculate functions. Here the relevant solution for the specific problem is calculated.

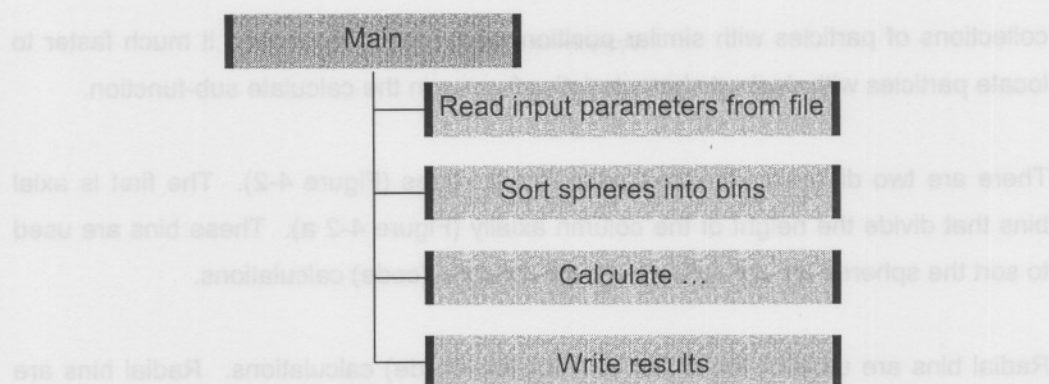


Figure 4-1. *The basic structure of the codes calculating, the overlap between spheres, the axial porosity distribution and the radial porosity distribution.*

4.2.2 Main

The main function is the controlling function in all the codes. In the main function, the filename of the input file is obtained from the user. The main function also controls all the sub-functions (as shown in Figure 4-1).

4.2.3 Read input parameters from file

The main function calls the ReadInput sub-function. In this sub-function, the input file (extension .inp) is opened, and all the input parameters are read from the file. Refer to Appendix A for an example and an explanation of the contents of the input files.

The input file contains information concerning the geometry, and other properties of the specific case being studied. The data of the sphere positions is contained in another file (extension .dat). The filename of the data file is also contained in the input file. The data file is opened. A unique identification number and the Cartesian coordinates of each sphere are read from the data file.

The data from these files are used to generate a sphere-list that stores the identification number and coordinates of each of the spheres. Both the input and the data files are now closed. Control is returned to the main function.

4.2.4 Sort spheres into bins

The nature of the problems investigated in this study are very similar, in that it is necessary to search for particles with specific position attributes from a, potentially, very large collection. Therefore, the particles are sorted into bins. These bins are

collections of particles with similar position attributes. This makes it much faster to locate particles with desired characteristics for use in the calculate sub-function.

There are two different bin types used in the codes (Figure 4-2). The first is axial bins that divide the height of the column axially (Figure 4-2 a). These bins are used to sort the spheres for use in the axial void fraction (code) calculations.

Radial bins are used in the radial void fraction (code) calculations. Radial bins are situated concentrically about the Z-axis of the column (Figure 4-2 b). These bins are used to sort the spheres for use in the radial void fraction (code) calculations.

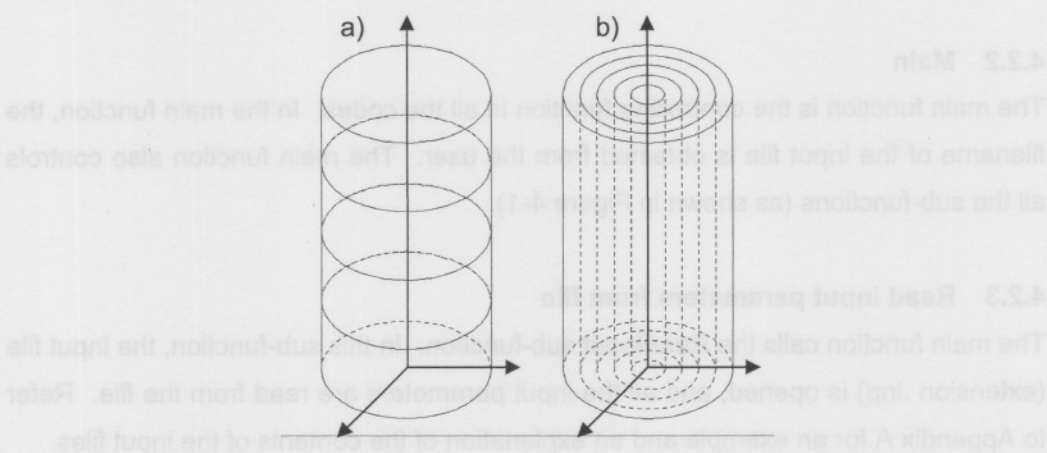


Figure 4-2. Illustration of: a) axial- and b) radial bins used in the codes.

Axial bins

In the axial void fraction distribution procedure, the spheres are sorted into bins according to their axial position. Two horizontal planes define an axial bin.

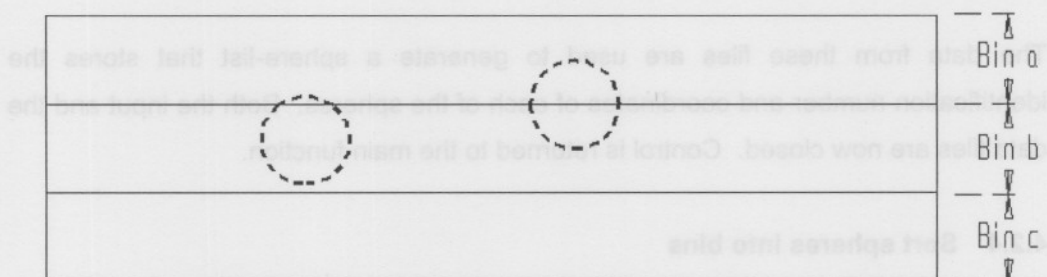


Figure 4-3. Illustration of some axial bins, showing that a sphere can be associated with more than one bin.

In this sub-function, the cylindrical packed column is divided into bins. The size of the bins are defined by the "binratio". The *binratio* is the ratio of the bin height to the diameter of a particle d_p , eq. (4.1):

$$h_b = \text{binratio} * d_p \text{ with } h_b > \frac{1}{2} d_p \quad (4.1)$$

Here h_b is the height of a bin.

```

for (Sphere = 1; Sphere <= Number_Of_Spheres; Sphere++)
{
    bin1 = ceiling((Z0 - (dp/2)) / hb);

    bin2 = ceiling(Z0 / hb);

    bin3 = ceiling((Z0 + (dp/2)) / hb);

    If (bin1 = bin2 = bin3)
    {
        This sphere is associated only with one bin, the bin
        number is bin1.
    }
    If (bin1 > bin2 = bin3)
    {
        This sphere lies in the bins numbered bin1 and bin2.
    }
    If (bin1 = bin2 > bin3)
    {
        This sphere lies in the bins numbered bin2 and bin3.
    }
    If (bin1 > bin2 > bin3)
    {
        This sphere lies in the bins numbered bin1, bin2, and bin3.
    }
    Save the sphere identification number in a list containing
    all the sphere identification numbers for the relevant bin.
} //End for loop over spheres

```

Figure 4-4. Algorithm to sort the spheres into axial bins.

If the whole sphere or a part thereof is contained in the bin, then the sphere is arranged into that bin. This means that a sphere can be associated with more than one bin (Figure 4-3).

Figure 4-4 is the pseudocode for the algorithm to sort spheres into axial bins. Here Z_0 is the axial coordinate position of the sphere. The algorithm can be explained as follows; for each sphere in the column, calculate the bin number(s) associated with it. The identification numbers of the spheres located in a specific bin are then associated with that bin.

Radial bins

The algorithm employed to sort the spheres into radial bins is very similar to the one shown above.

For the codes calculating the radial porosity distribution, and the representative elementary volume (REV) in a packed column, it is advantageous to sort the spheres into bins according to their radial position. Two radial planes construct a radial bin. Again, the *binratio* is defined as the thickness of the bin relative to the particle diameter, eq. (4.2):

$$r_i = \text{binratio} * d_p \text{ with } r_i > \frac{1}{2} d_p \quad (4.2)$$

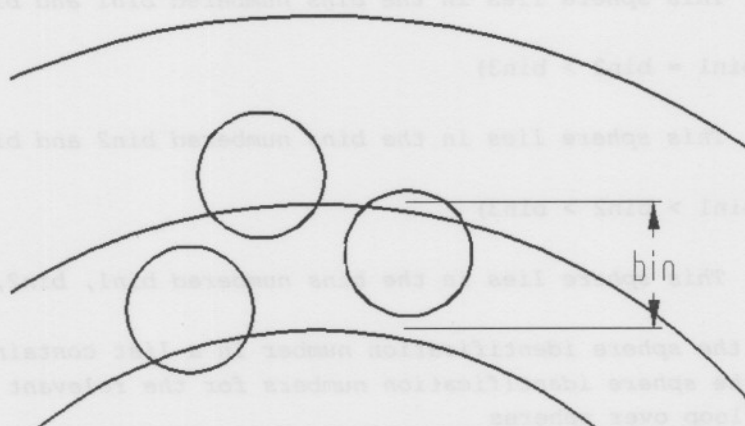


Figure 4-5. Illustration of a radial bin. A sphere can be associated with more than one bin.

Here r_i is the bin-thickness. If the whole sphere or a part thereof is contained in the bin, then the sphere is arranged into that bin. This means that a sphere can be associated with more than one bin (Figure 4-5).

Each sphere is tested to determine in which bins it is situated. The algorithm used to sort the spheres is similar to that given in the previous section for axial bins (Figure 4-4).

Here R_0 is the radial coordinate position of the centre of the sphere. The algorithm shown in Figure 4-6 can be explained as follows; for each sphere in the column, calculate the bin number(s) associated with it. The identification numbers of the spheres located in a specific bin are then associated with that bin.

```

for (Sphere = 1; Sphere <= Number_Of_Spheres; Sphere++)
{
    bin1 = ceiling(( $R_0 - \left(\frac{d_p}{2}\right)$ ) /  $r_i$ );
    bin2 = ceiling( $R_0$  /  $r_i$ );
    bin3 = ceiling(( $R_0 + \left(\frac{d_p}{2}\right)$ ) /  $r_i$ );

    If (bin1 = bin2 = bin3)
    {
        This sphere is associated only with one bin, the bin
        number is bin1.
    }
    If (bin1 > bin2 = bin3)
    {
        This sphere lies in the bins numbered bin1 and bin2.
    }
    If (bin1 = bin2 > bin3)
    {
        This sphere lies in the bins numbered bin2 and bin3.
    }
    If (bin1 > bin2 > bin3)
    {
        This sphere lies in the bins numbered bin1, bin2, and bin3.
    }
    Save the sphere identification number in a list containing
    all the sphere identification numbers for the relevant bin.
} //End for loop over spheres

```

Figure 4-6. Algorithm to sort spheres into radial bins.

4.2.5 Write results to file

The WriteResults sub-function is called by the main function. The results generated in the calculate sub-function are written to a result file (extension .res) with the same name as the input file. Some relevant information is also printed to the screen.

4.3 Calculate sub-functions

In this section the sub-functions that calculate the overlap, axial porosity distribution, and the radial porosity distribution in the respective codes, are discussed.

4.3.1 Calculate the overlap between spheres

The CalcOverlap sub-function calculates the overlap between spheres. The overlap is calculated from the model developed in Chapter 3. After calculating the overlap between two spheres, the axial position of the overlap is determined. The position of the overlap is assumed to be situated half way between the relevant spheres. The positions of overlap are sorted into axial bins. The algorithm to sort the positions of overlap into axial bins is the same algorithm used to sort the spheres into axial bins, in the axial porosity distribution procedure.

After executing the algorithm, control is returned to the main function.

Analysis of code

To determine the validity of the code, test cases were investigated, where only two spherical particles were positioned in a packed column (with $d_p = 1$). The results for three cases are shown in Table 4-1.

It is easy to verify that these results are correct. The positions (in Cartesian coordinates) of the two particles are given in Table 4-1 for each case. The maximum and average overlaps, for these test cases, are equal since there is only one (possible) overlap in the column.

From these tests it is clear that the code calculates the overlaps occurring in the column correctly.

Coordinates	X	Y	Z	Number of overlaps	Maximum overlap	Average overlap
Case 1	0	0	1	1	100%	100%
	0	0	1			
Case 2	0	0	0.5	1	50%	50%
	0	0	1			
Case 3	0	0	0.5	0	0%	0%
	0	0	1.5			

Table 4-1. The results for three test cases, to validate the calculations of the code calculating the overlap between two particles in the column with $d_p = 1$.

4.3.2 Calculate the axial void fraction distribution

In this code the CalcPoros sub-function is used to calculate the axial porosity distribution. The main function calls the CalcPoros sub-function, and control is returned to the main function after CalcPoros has executed.

In this sub-function, the model developed in Chapter 3 for calculating the porosity, on a horizontal plane, cutting the column, is used. Figure 3-5 is the pseudocode for the algorithm employed to calculate area of the horizontal cut through a sphere.

The cut areas A , of all the individual spheres cut by the axial plane is determined and summed. The cross sectional area A_T , of the column on that axial plane is calculated, and the area porosity ε , on the plane, then follows:

$$\varepsilon(Z) = 1 - \frac{\sum A(Z)}{A_T(Z)} \quad (4.3)$$

The sub function first calculates the porosity of an axial plane situated at the bottom of the column. Then, the axial position of the plane is incremented a small distance Δz , and the porosity is again calculated. Doing this over the full height of the column will give an approximation for the variation of the porosity in the axial direction.

Analysis of code

The axial porosity distribution is calculated with the axialporos.cpp (axialporos.exe) code. To validate the axial porosity distribution code, a few test cases were investigated. These were:

- Validate that the cut area A (on an arbitrary plane through a single particle) is calculated correctly. As explained in the sections detailing the algorithm and implementation of this code, these cut areas A are used to calculate the porosity on an axial plane.
- Calculate the volume of a sphere ($d_p = 1$), by numerically integrating the areas (A) over the height of the sphere.

For the purposes of these validation tests a particle with diameter $d_p = 1$ was used.

For the first test, two axial planes were constructed cutting the particle, and the cut areas (A) were calculated using the axialporos.cpp, and a CAD package. The results are summarised in Table 4-2. The results indicate that both the CAD package and the code developed for this study, returns the same solutions for these simple cases.

	$\frac{ Z_0 - Z_i }{d_p}$	A , Axial porosity code	A , CAD package
case 1	0.4	0.282743	0.282743
case 2	0	0.785398	0.785398

Table 4-2. Validation test results calculating A for a particle, at different axial plane positions.

In the numerical integration to find the volume of the particle, the integration intervals are an important parameter. The slice ratio (the ratio of the distance between two slices to a particle diameter) is an indication of the number of axial planes cutting the particle. This parameter was varied to determine what influence it has on the calculated volume of the particle.

To calculate the volume of the particle the trapezium rule was used. This reduces to:

$$\text{Volume}_{\text{sphere}} = \text{slice ratio} \times d_p \left(\frac{1}{2} A_1 + \sum_{i=2}^{n-1} A_i + \frac{1}{2} A_n \right) \quad (4.4)$$

Where n is the number of cutting planes through the sphere, and A_i is area cut by the i 'th plane through the particle.

	Slice ratio	Volume of sphere	Error (%)
Analytical value	-	0.523598775	-
case 1	0.125	0.515417545	1.5625
case 2	0.0625	0.521553468	0.3906
case 3	0.03125	0.523087449	0.0977
case 4	0.015625	0.523470944	0.0244

Table 4-3. Volumes calculated with the axial porosity code, with the analytical solution, and error.

Table 4-3 shows the results, versus the analytical value. The percentage error with a slice ratio of 0.125 is less than 1.6%. This is an indication of the quality of the solution (for the axial porosity distribution) generated by this code. In this study the slice ratio will consequently be set to 0.03125. This will lead to an average error of less than 0.1 %.

4.3.3 Radial void fraction distribution

In this code the CalcPoros sub-function is used to calculate the radial porosity distribution. The main function calls the CalcPoros sub-function, and control is returned to the main function after CalcPoros has been executed.

In the CalcPoros sub-function the cut area A , contributed by a single sphere cut by the radial plane, is calculated as shown in Chapter 3. The total area of the radial plane occupied by cut spheres is obtained by summing all the contributions from the individual spheres. The total area of the radial cutting plane is calculated, and the area porosity at that radial plane (r) follows:

$$\varepsilon(r) = 1 - \frac{\sum A(r)}{A_T(r)} \quad (4.5)$$

Here A_r is the total area of the radial plane, and ε is the porosity.

To find the radial porosity distribution, the area porosity is calculated on a series of radial planes. The first radial plane is constructed at the wall of the column. The area porosity is calculated on this plane. The radial position of the plane is then incremented a small distance Δr into the column. Again the area porosity is calculated. Doing this over the radial span will give an approximation for the variation of the porosity in the radial direction.

Analysis of code

The radial porosity distribution is determined using the `radialporos.cpp` code. To validate this code the following steps were taken:

- Validate that the cut area A (on an arbitrary plane through a particle) is calculated correctly. As explained in the sections detailing the algorithm and implementation of this code, these cut areas A are used to calculate the porosity on a radial plane. Firstly a sphere ($d_p = 1$) was situated 1-particle diameter radially into the column. The radial cutting plane is then used to cut the sphere at four arbitrary positions. The cut area is calculated each time, for different number of integration intervals, and compared with a CAD model calculation.
- Determine the effect of radial position of the particle in the column on the calculation of cut area A .
- Calculate the volume of a spherical particle.

No analytical solution for the cut area A , constructed by a radial plane cutting a spherical particle, could be found. To test the results generated by the radial porosity code, a CAD package was used to determine the area. The estimated error in the CAD solution is 0.5%.

Table 4-4 is a summary of the results. In all the cases investigated the difference between the results for the CAD package and the code is less than 0.6%. For 64 integration intervals the average difference is 0.072%.

	16 Integration intervals	32 Integration intervals	64 Integration intervals	128 Integration intervals
Average difference %	0.580	0.205	0.072	0.039

Table 4-4. The average error (%) between the methods used to calculate A .

For the next test the spherical particle was positioned at different radial positions in the column. In the radial void fraction code the porosity distribution is only calculated to a distance of one sphere radius from the axis of the column. The minimum radial position of a sphere for this test was therefore taken to be $r_0 = 1d_p$. The maximum centre position of a sphere in the proposed PBMR core will be $r_0 = 30d_p$, hence this was used in this test for the maximum radial position.

Table 4-5 shows the results for this test. In all cases investigated the average difference between the CAD package and the radial porosity code is less than 0.1%.

These results suggest that the radial position of the particle has only a small effect on the calculation of the cut area of the sphere.

	$r_0 = 1d_p$	$r_0 = 9\frac{1}{2}d_p$	$r_0 = 30d_p$
Average difference %	0.060	0.095	0.090

Table 4-5. The average difference between results for the methods used to calculate A , for different radial particle positions.

The volume of the sphere was also determined, using numerical integration. For this test the number of angular integration intervals (to calculate cut area A) was varied, and the number of radial integration intervals (over the particle) was also varied. The trapezium rule was employed to do the integration.

Figure 4-7 is a graphical summary of the results for this validation test. There is an average difference of 0.048 % between the solutions for 64- and 128 angular integration intervals (all other parameters remaining constant). There is no real improvement in the solution for 128 radial integration intervals over 64 radial

integration intervals. In this study the angular integration intervals will be set to 64 for all further cases analysed.

These tests suggest that the calculation of the area of the radial cut through a particle has been implemented correctly.

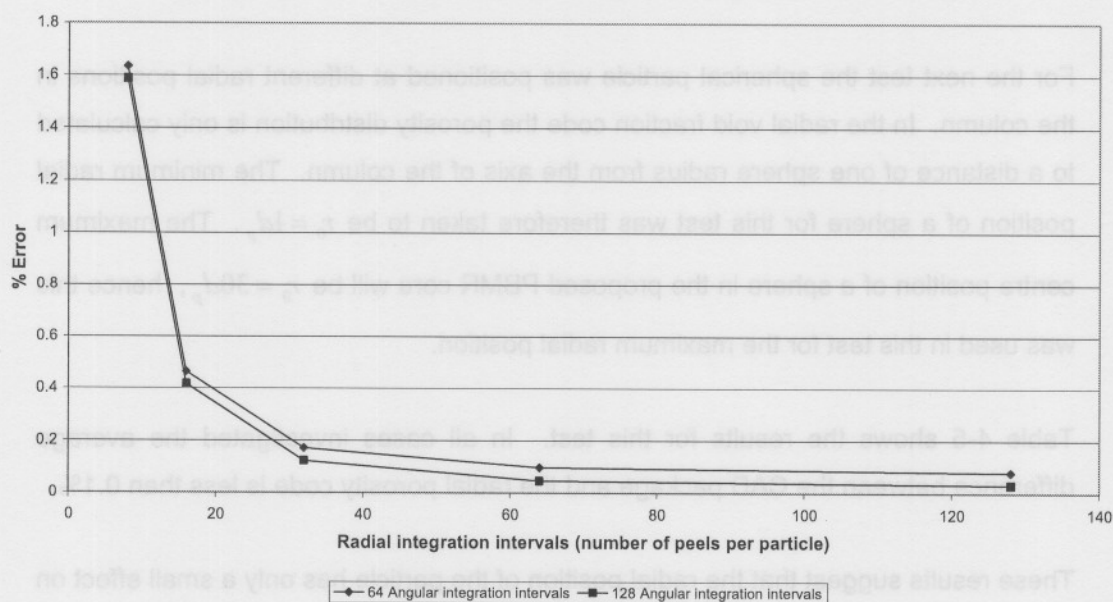


Figure 4-7. Validation test results calculating the volume of a sphere, accounting for angular and radial integration intervals.

4.4 Representative elementary volume (REV)

The basic structure of the code to calculate the REV, is similar to that of the other codes discussed. The input parameters are read from an input file and the results are written to an output file, and the spheres are sorted into concentric radial bins (refer to section 4.2.1 for a more complete discussion on these sub-functions).

In Chapter 3, the model developed to calculate the porosity associated with a spherical volume U_i , situated in a packed column, has been explained. In order to implement this model the sub-functions: generate grid, and sort grid points into bins are used. In the next sections, these sub-functions are explained. First, the algorithm used in this code is overviewed briefly.

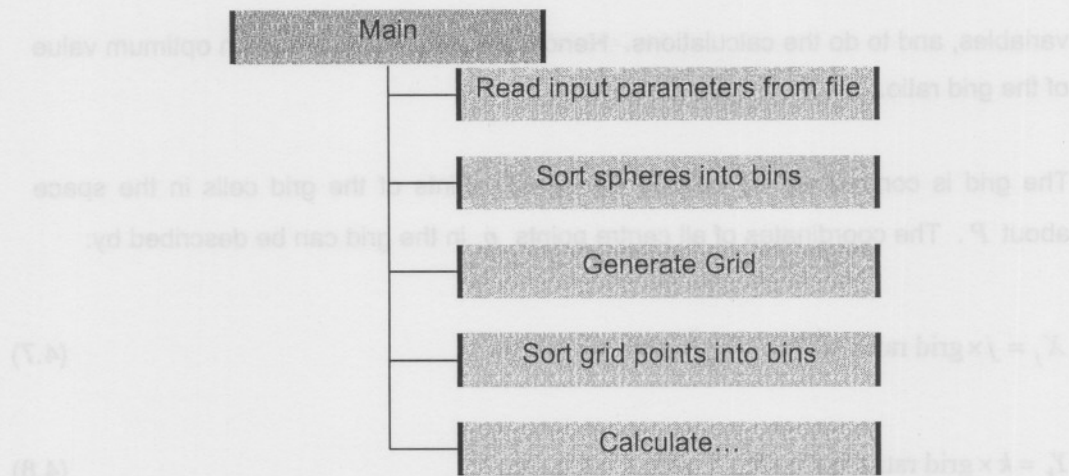


Figure 4-8. The basic structure of the REV code developed in this study.

The spheres are sorted into cylindrical bins (explained in Figure 4-6, these bins will now be called particle bins), and the grid points are sorted into spherical bins (explained and illustrated in Figure 4-13 and Figure 4-14, these bins will be called grid bins). The grid bins are gradually grown out to the maximum volume (with radius R_{max} , defined in Figure 4-10) from a small volume. For each of the grid bins the grid points lying in that bin is identified. The grid points (associated with a grid bin) lying in particles are counted, and the porosity of the grid bin is determined. From this the REV can be determined in a spreadsheet application.

4.4.1 Generate grid

The user supplies the coordinates of the point P (in the input file), about which the REV is to be determined. As explained in Chapter 3, consecutive spherical volumes U_i (with $i = 1, 2, 3 \dots n$) is constructed about point P . The porosity of these volumes is determined. From this the REV can be determined.

A cubic grid is generated about point P . The length of the side of a grid cell dl is dependent on the size of the particles in the porous domain. This length is specified by the user in the input file, with:

$$\text{grid ratio} = \frac{dl}{d_p} = \text{Constant} \quad (4.6)$$

The smaller the grid ratio, the more grid cells are generated per unit volume. This will lead to a more accurate approximation of the porosity in that volume. The drawback associated with a fine grid is that it takes more time to set up the needed

Chapter 4: Experimental Method and Analysis

variables, and to do the calculations. Hence, it is necessary to find an optimum value of the grid ratio.

The grid is constructed by placing the centre points of the grid cells in the space about P . The coordinates of all centre points p_i in the grid can be described by:

$$X_j = j \times \text{grid ratio} + (X_p - R_{\max}) \text{ with } j = 1, 2, \dots, n \quad (4.7)$$

$$Y_k = k \times \text{grid ratio} + (Y_p - R_{\max}) \text{ with } k = 1, 2, \dots, n \quad (4.8)$$

$$Z_l = l \times \text{grid ratio} + (Z_p - R_{\max}) \text{ with } l = 1, 2, \dots, n \quad (4.9)$$

Where n is the total number of cells in a Cartesian coordinate direction. X_p , Y_p and Z_p is the coordinates of the point P . There are a total of n^3 points p_i in the grid (i.e. $i = 1, 2, \dots, n^3$). The pseudocode for the algorithm is given in Figure 4-9. Note how equations (4.7), (4.8), and (4.9) is used to generate the grid points.

```

i = 0
for (l = 0; l <= 2 * Rmax / grid ratio * dp; l++) //z-direction
{
    for (k = 0; k <= 2 * Rmax / grid ratio * dp; k++) //y-direction
    {
        for (j = 0; j <= 2 * Rmax / grid ratio * dp; j++) //x-direction
        {
            i++
            Use eq.(4.7), eq.(4.8) and eq.(4.9) to calculate the
            coordinates of the grid points.
            pi = f(Xj, Yk, Zl)

        } //End for loop in x-direction
    } //End for loop in y-direction
} //End for loop in z-direction

```

Figure 4-9. Algorithm to calculate the position coordinates of the grid points.

It is important that each grid bin is situated entirely inside the boundaries of the column (porous domain). Figure 4-10 shows the top view of the cylindrical column,

with origin O . The maximum size (U_n) of the volume U_i (to fit into the column), and the cubic grid constructed about U_n is illustrated. The radius of U_n is R_{max} .

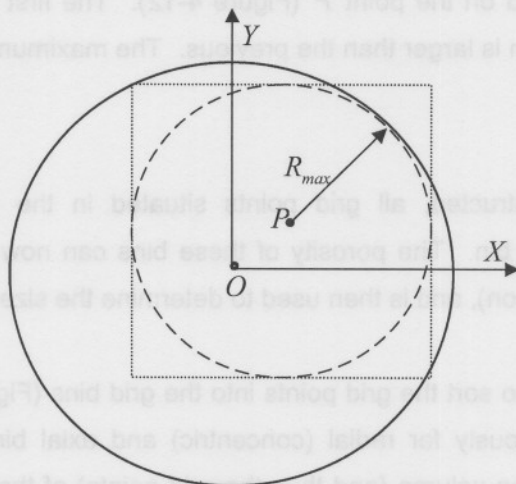


Figure 4-10. Illustration of the cubic grid about point P , and the largest grid bin fitting into the column (top view).

Figure 4-11 is an illustration of the grid points generated by this sub-function.

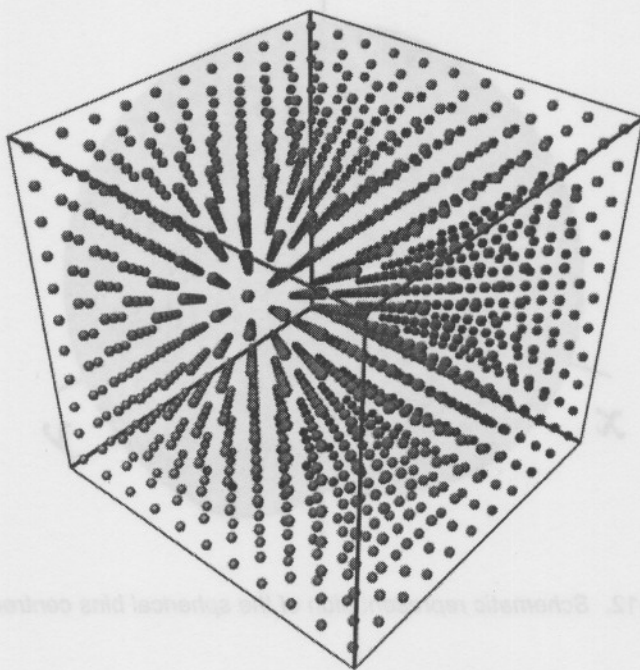


Figure 4-11. Illustration of a grid generated to show grid points.

4.4.2 Sort grid points into grid bins

The centre points of the cubic grid constructed in the previous section is now sorted into grid bins centred on the point P (Figure 4-12). The first grid bin is small, and every subsequent bin is larger than the previous. The maximum radius for these bins is R_{max} .

For every bin constructed, all grid points situated in the bin is identified and associated with that bin. The porosity of these bins can now be calculated (in the CalcPoros sub-function), and is then used to determine the size of the REV.

The algorithm used to sort the grid points into the grid bins (Figure 4-13) is similar to that explained previously for radial (concentric) and axial bins. Each grid bin is defined to exclude the volume (and thus the grid points) of the previous bins. Each grid point has an associated flag that is set to zero at initialisation. If a point is situated in a specific grid bin, then the value of the flag is set to 1. Each grid point is tested to determine the value of the flag, if the flag value is 1 it is not again included in any other bins.

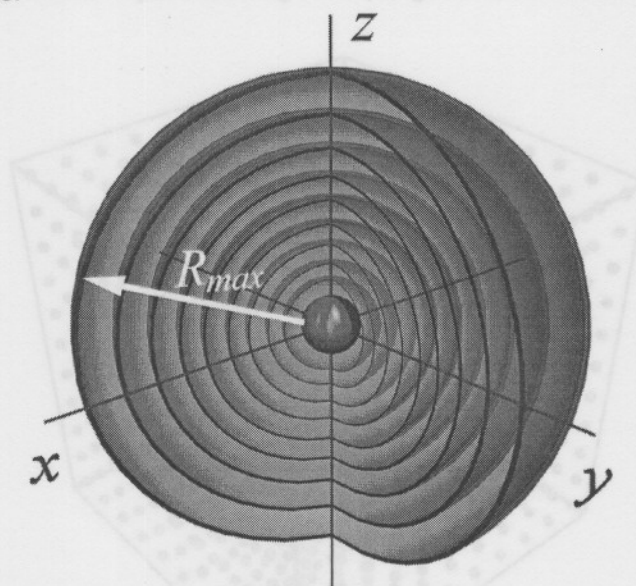


Figure 4-12. Schematic representation of the spherical bins centred on P .

The algorithm can be explained as follows; for each grid bin check all grid points to determine if it lies within the spherical bin or outside, and check the value of the flag associated with that point. If a grid point lies inside the grid bin, and the flag value is 0 then associate that grid point with that bin. Now set the flag value to 1.

```

for (Grid_bin = 1; Grid_bin <= Number_of_Bins; Grid_bin++)
{
    for (grid_point = 1; grid_point <= Number_of_Points; grid_point++)
    {
        Determine the distance between point  $P$  and the grid point.

        if (distance <= Grid_bin_radius, and point_flag == 0)
        {
            Associate this grid point with this spherical bin.
            Set point_flag to 1.
        }
    }
} //End FOR over grid points
} //End FOR over grid bins

```

Figure 4-13. Algorithm to sort grid points into grid bins.

Figure 4-14 is an illustration of the points collected in a grid bin, constructed in the manner explained above.

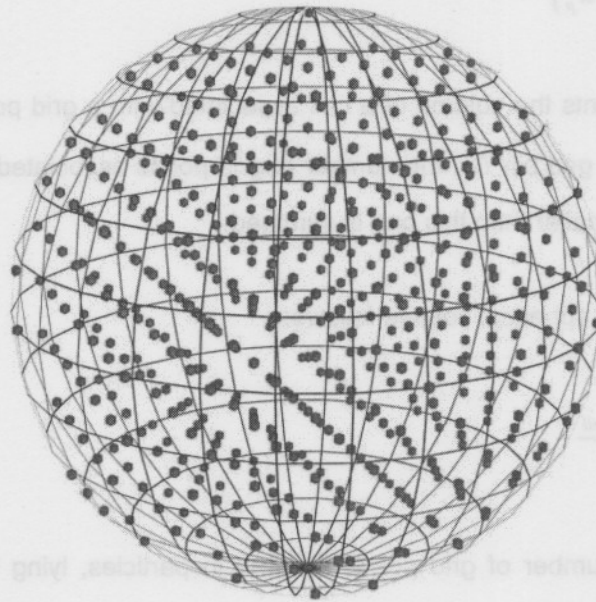


Figure 4-14. Illustration of the points collected in a spherical bin.

4.4.3 Calculate porosity of grid bins

In this code, the CalcPoros sub-function is used to calculate the porosity of the grid bins. This information are written to a file (extension *.res) and can be used to determine the REV for the point P .

To calculate the porosity of a grid bin, all the grid points in that bin is tested to determine if it is situated inside a particle (sphere) or outside. To determine if a grid point is situated in a particle, the *distance* between the centre of the sphere and the grid point is calculated.

$$distance = \sqrt{(X_i - x_j)^2 + (Y_i - y_j)^2 + (Z_i - z_j)^2} \quad (4.10)$$

Here (X_i, Y_i, Z_i) is the coordinates of the i^{th} grid point, and (x_j, y_j, z_j) is the in the position coordinates the j^{th} spherical particle. If this *distance* is smaller than a particle radius, then the grid point lies within that sphere.

The volume of each cell is:

$$U_{cell} = (\text{grid ratio} \times d_p)^3 \quad (4.11)$$

Here U_{cell} represents the volume of a cell associated with a grid point. To calculate the porosity of the grid bin U_i , the number of grid points associated with this grid bin and all grid bins smaller than this one is summed.

The porosity of the spherical volume follows:

$$\varepsilon(U_i) = 1 - \frac{N_{U_i} \times U_{cell}}{U_i} \quad (4.12)$$

Here N_{U_i} is the number of grid points situated in particles, lying in the i^{th} , and smaller, grid bins.

Figure 4-15 shows the pseudocode for the algorithm, used to determine the porosity of each grid bin. The algorithm can be explained as follows; count the number of grid points, in a grid bin, that lies inside spherical particles. Do this only for spheres lying in cylindrical bins being cut by the grid bin. Do this for all grid bins.


```

for (Grid_bin = 1; Grid_bin <= Number_of_Grid_Bins; Grid_bin++)
{
    For loop over all grid bins.

    for (Grid_Point = 1; Grid_Point <= Number_of_Points; Grid_Point++)
    {
        For loop over all the grid points in the grid bin.

        for (Particle_bin = bin1; Particle_bin <= bin3; Particle_bin++)
        {
            For loop over particle bins.

            for (Sphere = 1; Sphere <= Number_of_Spheres; Sphere++)
            {
                For loop over all spheres in particle bin.

                if (distance <  $d_p/2$ )
                {
                    Count the number of grid points that
                    lies in particles.
                }
                else if (distance ==  $d_p/2$ )
                {
                    Count the number of grid points that
                    lies on the surface of a sphere, and
                    assume that half the volume associated
                    with these points lies in the sphere.
                }
            }
        }
    }
}
//End for over particles
//End for over particle bins
//End for over grid points
//End for over grid bins

```

Figure 4-15. Algorithm to determine if a grid point is situated in a sphere.

Analysis of code

To validate this code the following steps have been followed:

- The point P about which the REV is calculated will be situated at the centre of a particle. For this configuration the porosity should be 0 until the grid bin diameter is greater than the particle diameter.

- The volume of the particle will be determined by summing the volume of all the cells situated in the particle, and checked against the analytical value for the particle.

Figure 4-16 shows the expected tendency for the porosity distribution about point P situated in the centre of a particle.

For the purposes of this validation test, the effect of delta ratio was also investigated. The delta ratio is the ratio of the length of the side of a grid cell to a particle diameter. This is an indication of the coarseness of the grid. A larger delta ratio implies a larger cell volume.

It is clear that a spherical volume will be very poorly approximated by a single (or even 2, or 3) cubic cells. The more grid cells are used in the approximation of an arbitrary volume, the more accurate the approximation will be. From Figure 4-16 it is clear that the approximation to the volume of the grid bin is very poor for small grid bin volumes. Negative values for the porosity of the grid bin are obtained when the cubic cells underestimate the volume of the grid bin.

The REV analysis of a packed column is dependent on the size of the grid cell volumes constructing the grid bins. It is clear that when the cell volume and the grid bin volume is on the same scale, the error accompanying the approximation of the spherical bin with cubic cells will be very large.

Kaviany (1991) states that for the REV $\ell \gg d_p$, where ℓ is the characteristic length scale for the REV and d_p is a particle diameter. Thus, this error in the approximation for small volumes (for grid bin diameters smaller than $\frac{1}{2}$ -particle diameter) is not important, and can be ignored.

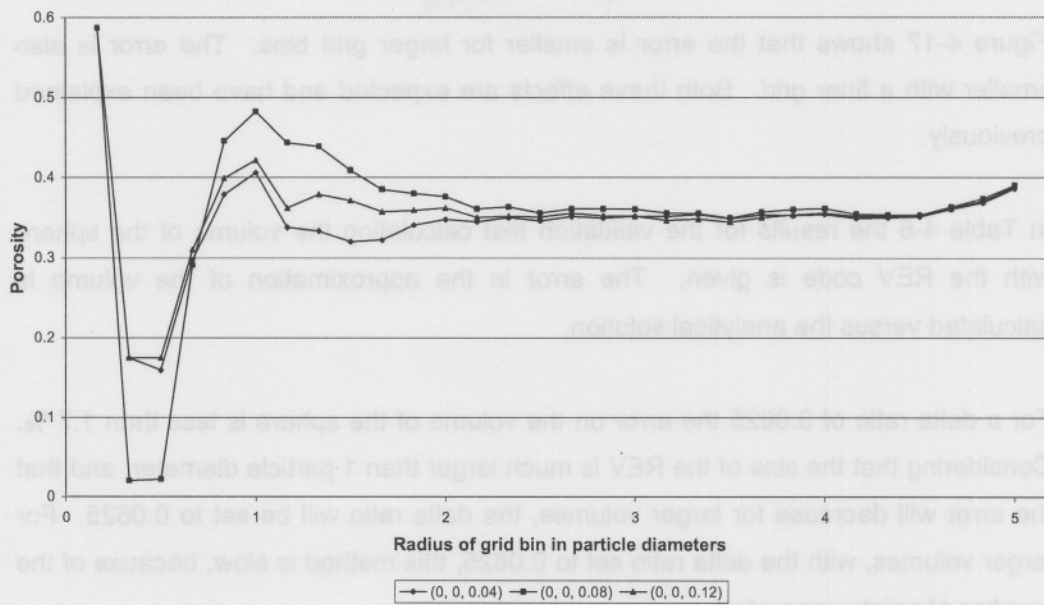


Figure 4-16. The porosity distribution about point P , for P situated in the centre of a particle. Showing the effect of delta ratio on the solution.

Figure 4-16 shows the trends that were expected for the test case. The error in the approximation for different grid bin sizes, and different delta ratios is shown in Figure 4-17.

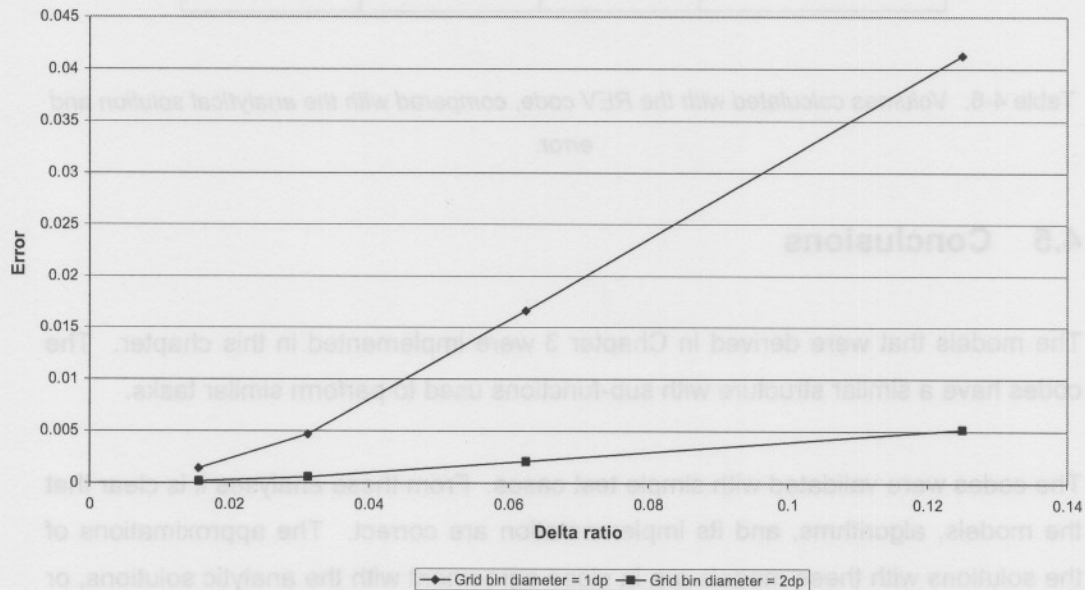


Figure 4-17. Analysis of error for different grid bin volumes.

Figure 4-17 shows that the error is smaller for larger grid bins. The error is also smaller with a finer grid. Both these effects are expected and have been explained previously.

In Table 4-6 the results for the validation test calculating the volume of the sphere with the REV code is given. The error in the approximation of the volume is calculated versus the analytical solution.

For a delta ratio of 0.0625 the error on the volume of the sphere is less than 1.7 %. Considering that the size of the REV is much larger than 1 particle diameter, and that the error will decrease for larger volumes, the delta ratio will be set to 0.0625. For larger volumes, with the delta ratio set to 0.0625, this method is slow, because of the number of points generated.

	Delta ratio	Volume of sphere	Error (%)
Analytical value	-	0.523598775	-
case 1	0.125	0.501953125	4.134
case 2	0.0625	0.514892572	1.663
case 3	0.03125	0.521148682	0.468
case 4	0.015625	0.522861481	0.141

Table 4-6. Volumes calculated with the REV code, compared with the analytical solution and error.

4.5 Conclusions

The models that were derived in Chapter 3 were implemented in this chapter. The codes have a similar structure with sub-functions used to perform similar tasks.

The codes were validated with simple test cases. From these analyses it is clear that the models, algorithms, and its implementation are correct. The approximations of the solutions with these models are in close agreement with the analytic solutions, or the solutions obtained by other methods.

5.1 Introduction

The purpose of this study is to develop procedures to analyse packed columns. In this chapter, the results that were generated are discussed. This is only a qualitative study of the results that are generated by the procedures. More data must be analysed in order to quantify the effects present in packed columns.

Chapter 5

Results

The procedure to calculate the overlap between particles was developed to test the quality of the data. This procedure cannot evaluate the quality of the packing (in terms of representation of reality). Thus, all the results must be evaluated, while considering the influence of the packing method.

In this chapter, four packed columns are analysed. First, the positions of the spheres are shown graphically. Then the data are analysed by the codes developed.

5.2 Data

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5.1 Introduction

The purpose of this study is to develop procedures to analyse packed columns. In this chapter, the results that were generated are discussed. This is only a qualitative study of the results that are generated by the procedures. More data must be analysed in order to quantify the effects present in packed columns.

The numerical packings, which were analysed in this study, were generated using PFC3D, a commercial discrete element method (DEM) code. There are other methods to (numerically) generate such structures. These methods are not discussed in this report. It is important to realise that the method employed may not give a good representation of a real packing.

The procedure to calculate the overlap between particles was developed to test the quality of the data. This procedure cannot evaluate the quality of the packing (in terms of representation of reality). Thus, all the results must be evaluated, while considering the influence of the packing method.

In this chapter, four packed columns are analysed. First, the positions of the spheres are shown graphically. Then the data are analysed by the codes developed.

5.2 Data

Table 5-1 summarises the data of the packed beds that are investigated in this study:

Case	Sphere diameter d_p m	Cylinder diameter D m	Cylinder height H m
1	0.008	0.088	0.160
2	0.008	0.104	0.160
3	0.00476	0.0714	0.0952
4	0.00476	0.0952	0.0952

Table 5-1. Data for the cases analysed in this study.

In the simulation of the packing of the particles into the column with PFC3D, the required average porosity of the column is specified. For these columns, the specified average porosity was 0.39.

5.3 Analysis

The packed columns were probed with the software developed in this study to extract all possible information. As a first step in the analysis of the packing, the positions of the particles are plotted. The overlap between the particles in the column will then be analysed, and the axial and radial porosity distributions are determined. The REV will then be calculated for a few points in the column.

Figure 5-1 shows the positions of the particles in the X - Y coordinate plane, for case 1. From this plot, it is clear that the packing in the wall region of the column is considerably more ordered than the packing of particles in the central part of the column.

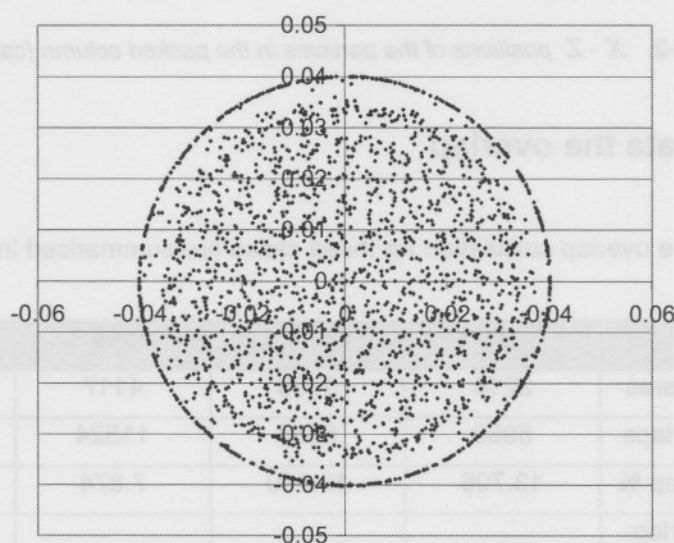


Figure 5-1. X - Y positions of the particles in the packed column (case 1).

Figure 5-2 is a plot of the positions of the particles (case 1) in the X - Z coordinate plane. Here the characteristic ordering of the particles can be seen at the bottom, and the top of the column.

The particles are not expected to be ordered at the top in the way that it seems to be in this plot. This will be further discussed when the axial porosity distribution is investigated.

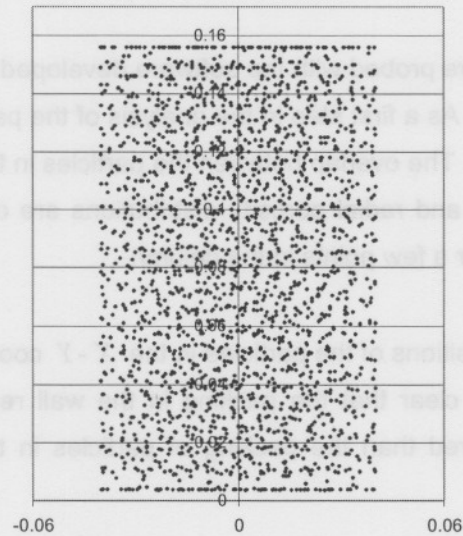


Figure 5-2. $X - Z$ positions of the particles in the packed column (case 1).

5.4 Calculate the overlap

The results of the overlap calculation for these cases are summarised in Table 5-2.

Item	Case 1	Case 2	Case 3	Case 4
Number of spheres	2214	3093	4117	7320
Number of overlaps	5988	8256	11524	20283
Maximum overlap %	13.706	13.410	7.874	6.755
Degree of overlap (average overlap) %	2.639	2.533	2.065	1.920

Table 5-2. Summary of the results for the overlap analysis.

There are significant individual overlaps. However, the average overlap for the cases analysed are smaller than 2.7%. There are on average 1.41 overlaps per particle in all the columns.

The quality of the data are (for the purposes of this study) good enough to continue with further analyses. The overlap that occurs will have some influence on the results. With the average overlap, less than 2.7% it is reasonable to assume that the effect on the results will be negligible.

5.5 Axial porosity distribution

Figure 5-3 is a plot of the axial porosity distribution in the column for all the cases investigated. The characteristic damped oscillation that exists in the wall region of a column packed with spherical particles is present at the bottom of the column, as expected. This tendency is also present at the top of the column. This effect is unexpected. It is probable that, in the simulation of the packing of the column, a "lid" was put on the column. This might have been done to press the particles into the column to obtain the prescribed bulk porosity of 0.39.

In the range from 4- to 16-particle diameters (from the bottom of the column), the porosity show small variations around the mean value. The maximum deviation from the average (for the central region of the column) for each column is shown in Table 5-3.

Item	Case 1	Case 2	Case 3	Case 4
Maximum deviation from average porosity in central region of column (%)	10.57	8.49	6.36	5.59

Table 5-3. Maximum deviation from the average porosity in the central region of the column.

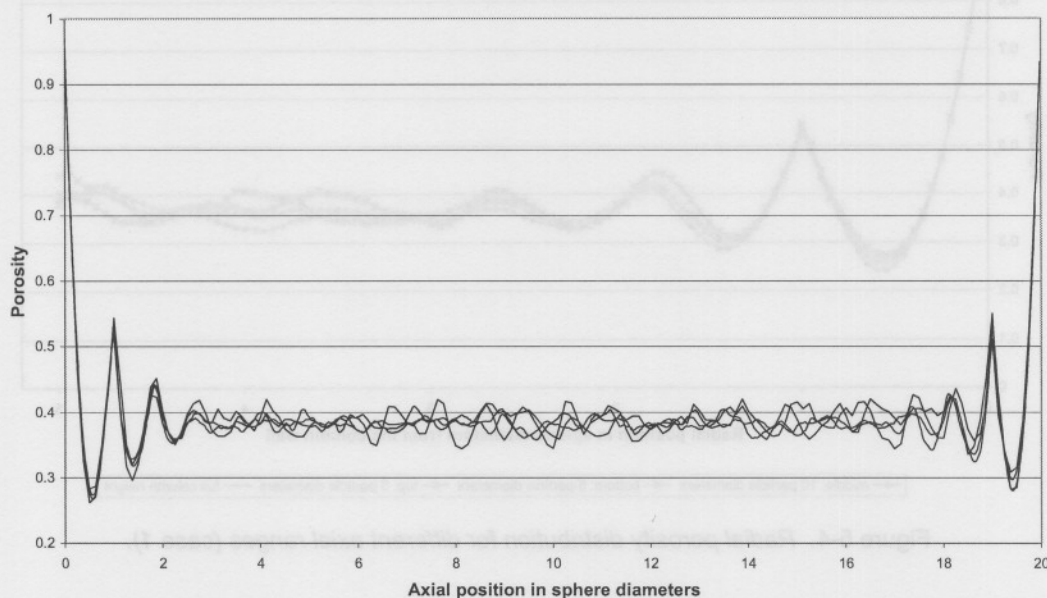


Figure 5-3. Axial porosity distribution.

The deviations from the average (can clearly be seen in Table 5-3) are more pronounced for the columns with lower aspect ratios. This effect is expected if the size of the REV, which is discussed later in this chapter, is taken into account.

The REV of the columns with lower aspect ratios, is larger than (or in the range of) the column diameter. In this case, the porosity of consecutive REV's will vary significantly, since local effects (such as wall effects, and other) will have a significant influence on the porosity.

5.6 Radial porosity distribution

The radial porosity distribution of the column is studied in this section. Two axial planes z_{low} and z_{high} are specified in the input file (Appendix A), between which the porosity is calculated. This enables the user to exclude certain regions of the column from the calculations. The 5-particle diameter regions at the bottom and the top of the column, display the expected variations in porosity (Figure 5-3). These regions can be excluded from the radial porosity calculations to get a clear picture of the radial porosity distribution.

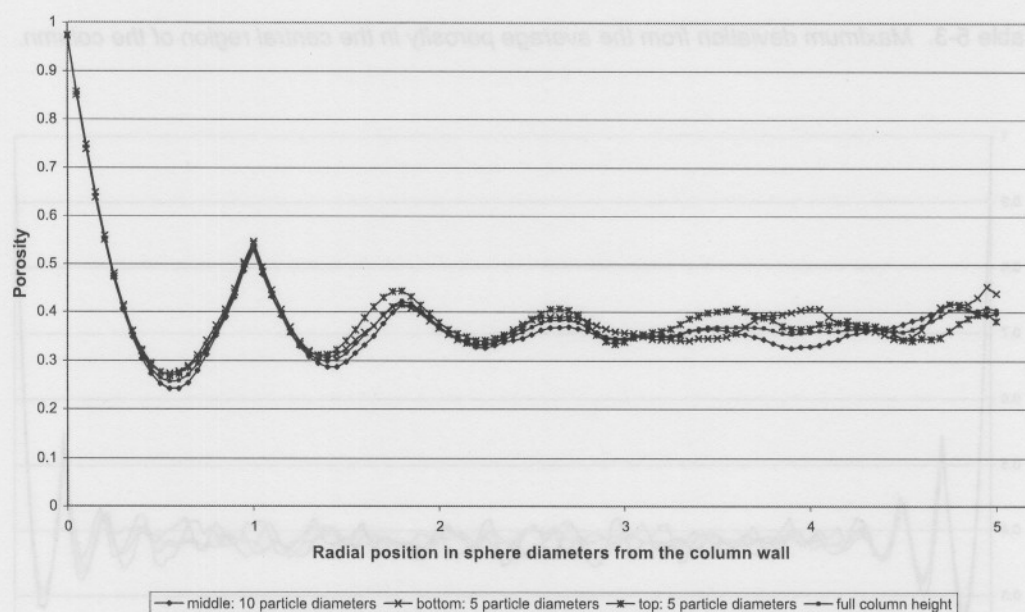


Figure 5-4. Radial porosity distribution for different axial ranges (case 1).

The parameters z_{low} and z_{high} are respectively defined in terms of particle diameters from the bottom and the top of the column. The porosity distribution is calculated

over the full height of the column, the middle 10-particle diameter region (thus excluding the top and bottom 5-particle diameter regions), the bottom 5-particle diameter region, and the top 5-particle diameters region. Figure 5-4 is a plot of the porosity distribution for different axial ranges for case 1.

In Figure 5-4, the characteristic porosity variations associated with the wall region is present for all axial ranges tested. There are notable differences in the porosity at a radial position, for the different axial ranges. The maximum difference in porosity at a radial position, for the different axial ranges (for the case shown below), is 21.43 %.

Importantly, for axial ranges of only five particle diameters there are significant variations in the radial porosity distribution in the "bulk porosity region". This is ascribed to the fact that the local (pore scale) variations in porosity have a significant effect on the average porosity, since the height of the sample is in the range of the pore scale of the column.

Figure 5-5 is a graph of the radial porosity distribution over axial ranges on the scale of the pore size, for case 1. Here it is evident that the variations in porosity are more dramatic for the cases where the height over which the sample was taken, is smaller.

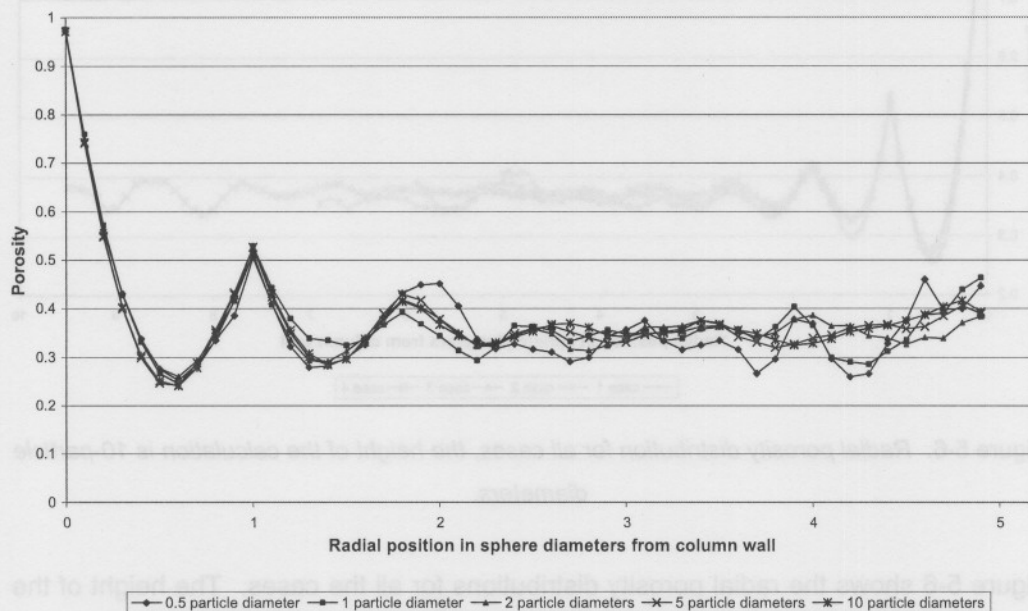


Figure 5-5. Radial porosity distribution for axial ranges on the pore scale (case 1).

The results obtained for the porosity distribution is very dependant on the height range over which the sample is calculated. This is in agreement with intuition, and with the discussion on the REV in Chapter 2.

It is important to realise that the radial porosity distribution obtained in this manner is an average value for the porosity at a radial position, and is averaged over the height for the specific calculation. Therefore, it follows that the smaller the height of the sample the more closely the porosity at a radial position will follow the local trend in the column at that position.

As explained in the first chapter, the porosity of a point can only be one or zero. The definition of porosity is really only applicable to an area or a volume of a certain minimum size. In the cases above, where the porosity changes dramatically in the "bulk porosity region" the criteria of the REV is not satisfied and the porosity is not well defined.

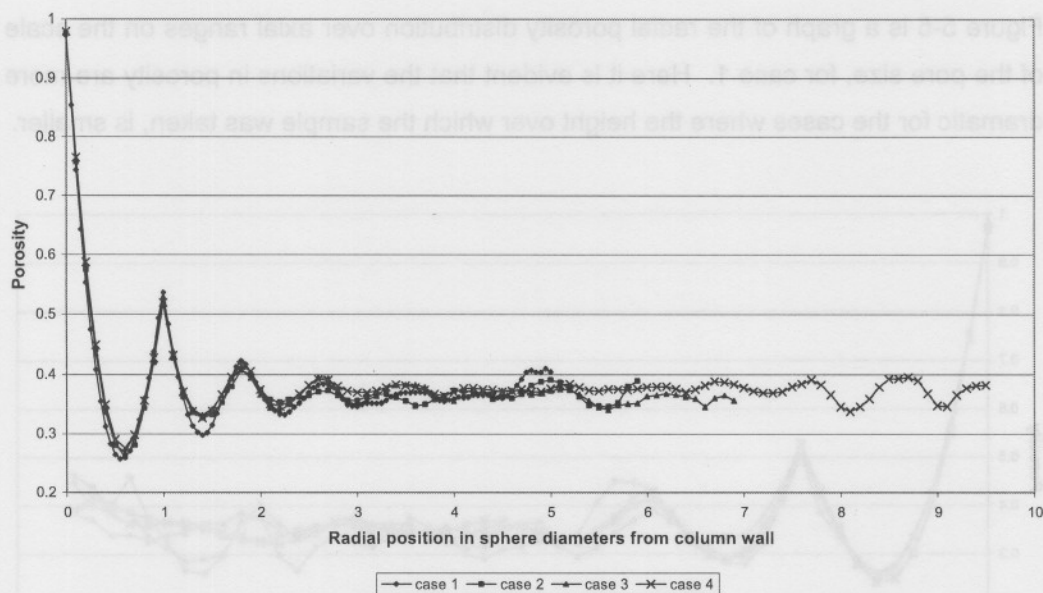


Figure 5-6. Radial porosity distribution for all cases, the height of the calculation is 10-particle diameters.

Figure 5-6 shows the radial porosity distributions for all the cases. The height of the samples is 10-particle diameters. The damped oscillations are clearly defined and are in close agreement with physical experimental results (in the literature). Interestingly there is a sharp peak in the porosity distribution graph at 1-particle diameter from the column wall. The results obtained from physical experiments

(Figure 5-7 and Figure 5-8) do not display the same sharp peak. This peak is an indication of the regularity of the packing of the first layer of particles against the wall.

The physical experiments conducted by Gordon (2001) and Goodling *et al.* (1980), are discussed in Chapter 2. In these experiments, thin annular rings are cut from the perimeter of the cured sample. The porosity of these annular rings is calculated, and is plotted in Figure 5-7 and Figure 5-8. These values are the average volume porosity at that average radial position, over the height of the sample. The averaging effect in the physical experiments will have the effect to smoothen the porosity distribution curve.

Figure 5-1 shows the positions of the particles in the $X-Y$ coordinate plane for case 1. Here the particles against the wall of the column are much more densely packed than in any other part of the column. This will give rise to the sharp peak present in the porosity distribution curve at 1-particle diameter from the column wall.

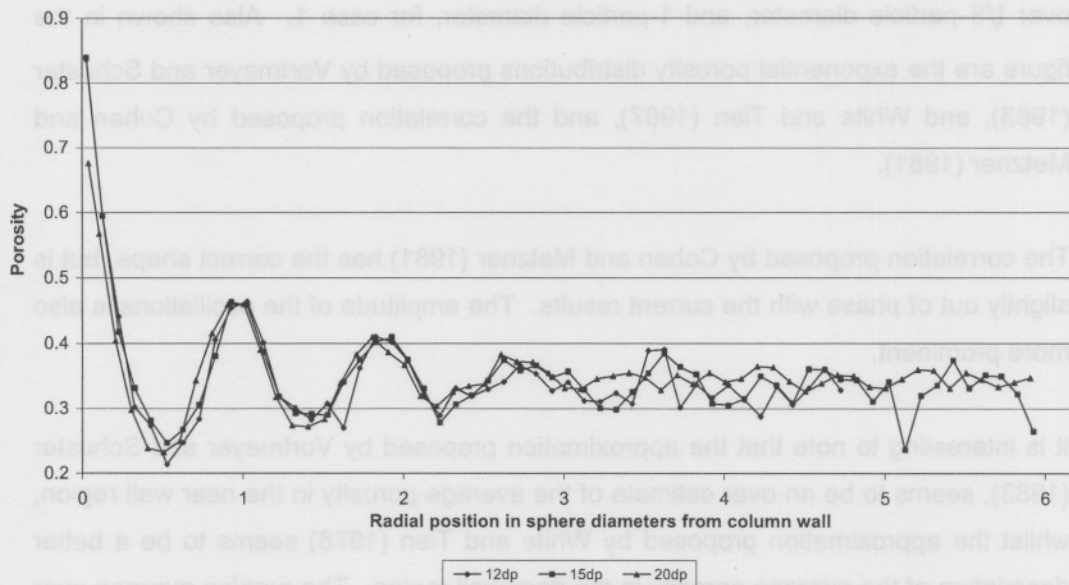


Figure 5-7. Experimental results of Gordon (2001).

Figure 5-7 and Figure 5-8 shows the experimental results of both Gordon (2001) and Goodling *et al.* (1980). The general trend is in good agreement to that obtained from the numerical experiments (Figure 5-6). The experimental results show more deviation about the mean porosity, in the region further away from the column wall.

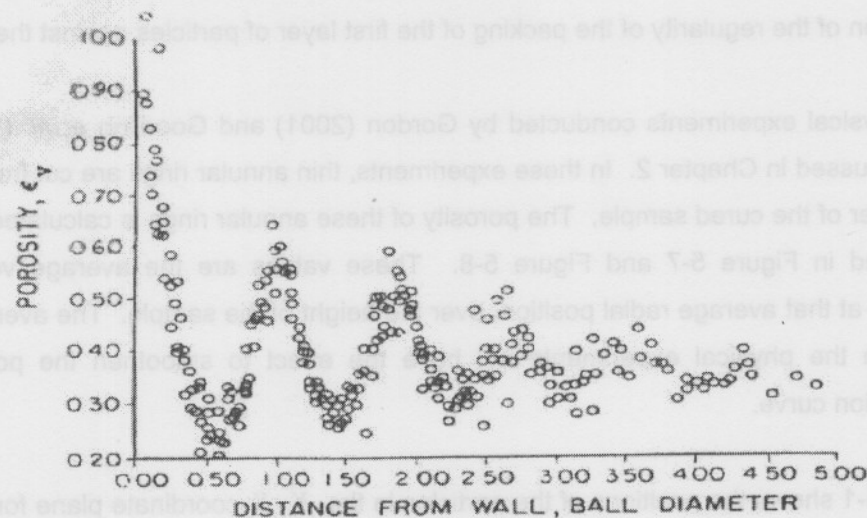


Figure 5-8. Experimental results of Goodling et al. (1980).

Figure 5-9 shows the radial porosity distribution, with the running averages calculated over $1/8$ -particle diameter, and 1-particle diameter, for case 1. Also shown in the figure are the exponential porosity distributions proposed by Vortmeyer and Schuster (1983), and White and Tien (1987), and the correlation proposed by Cohen and Metzner (1981).

The correlation proposed by Cohen and Metzner (1981) has the correct shape, but is slightly out of phase with the current results. The amplitude of the oscillations is also more prominent.

It is interesting to note that the approximation proposed by Vortmeyer and Schuster (1983), seems to be an over estimate of the average porosity in the near wall region, whilst the approximation proposed by White and Tien (1978) seems to be a better description of the average porosity in the near wall region. The running average over an $1/8$ -particle diameter is a good approximation to the experimental results of both Gordon (2001) and Goodling et al. (1980).

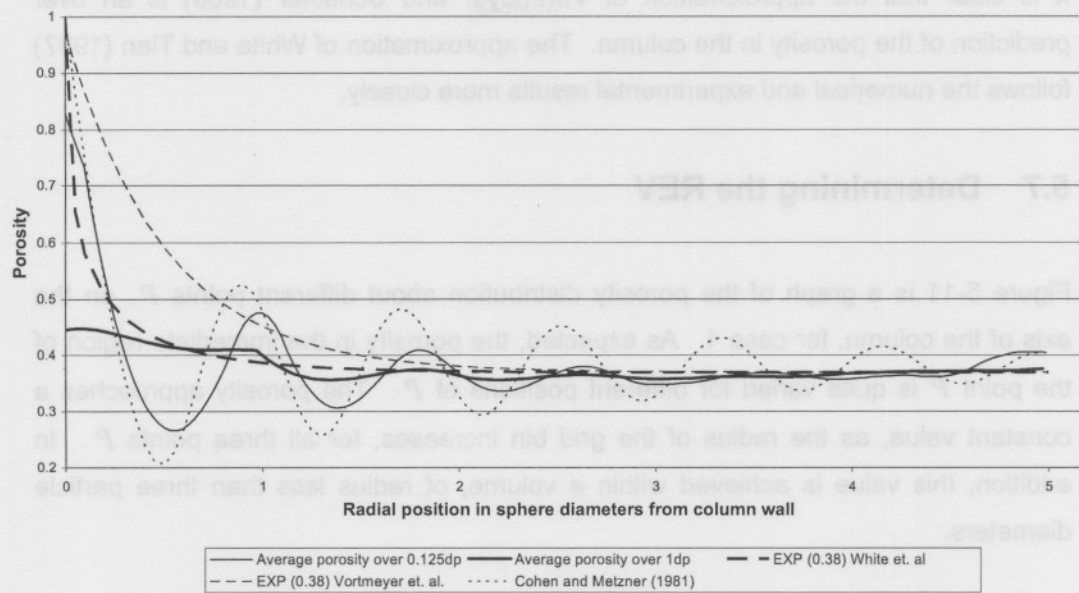


Figure 5-9. Radial porosity distribution, with running averages, and porosity distribution approximations used in the literature.

To get an indication of the quality of the approximations used by Vortmeyer and Schuster (1983), and White and Tien (1987), the cumulative void volume, as a function of the distance from the wall, was calculated by integration. This is shown in Figure 5-10. The void volume is an indication of the volume available for flow.

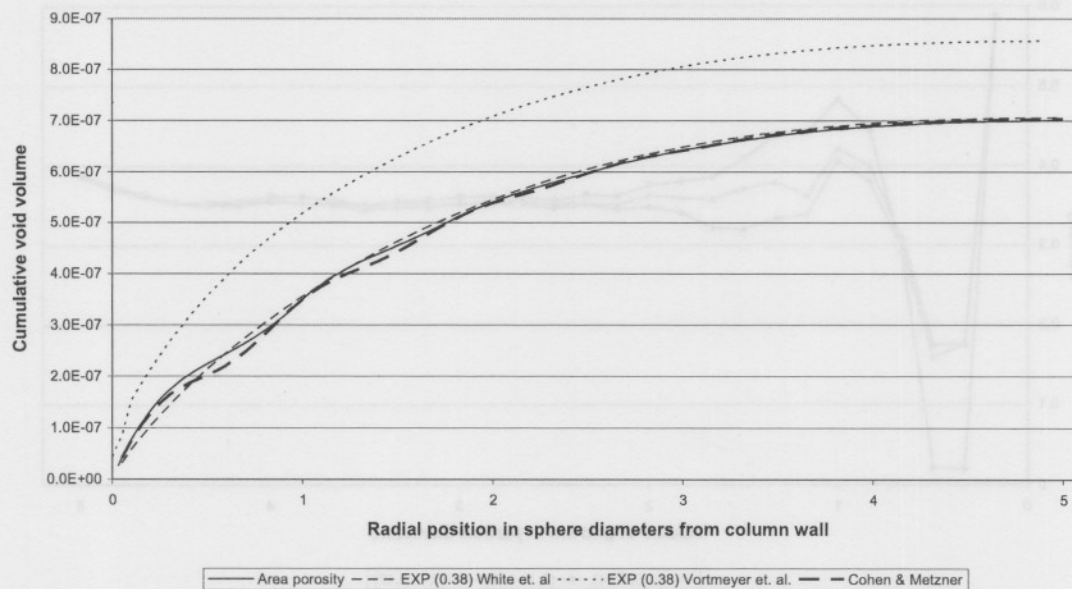


Figure 5-10. The cumulative void volume for different approximations to the radial porosity distribution (case 1)

It is clear that the approximation of Vortmeyer and Schuster (1983) is an over prediction of the porosity in the column. The approximation of White and Tien (1987) follows the numerical and experimental results more closely.

5.7 Determining the REV

Figure 5-11 is a graph of the porosity distribution about different points P , on the axis of the column, for case 1. As expected, the porosity in the immediate region of the point P is quite varied for different positions of P . The porosity approaches a constant value, as the radius of the grid bin increases, for all three points P . In addition, this value is achieved within a volume, of radius less than three particle diameters.

Note that for a grid bin radius in the region of five particle diameters (for this case), the porosity of consecutive volumes increases steadily. This can be explained by realising that the column radius is only 5.5 particle diameters. This means that for large grid bins the region close to the wall is included in the calculation of the porosity of the bin. The porosity of the wall region is higher than the bulk porosity of the column, and thus the porosity of the grid bin that includes this region will tend to be higher than the bulk porosity of the column.

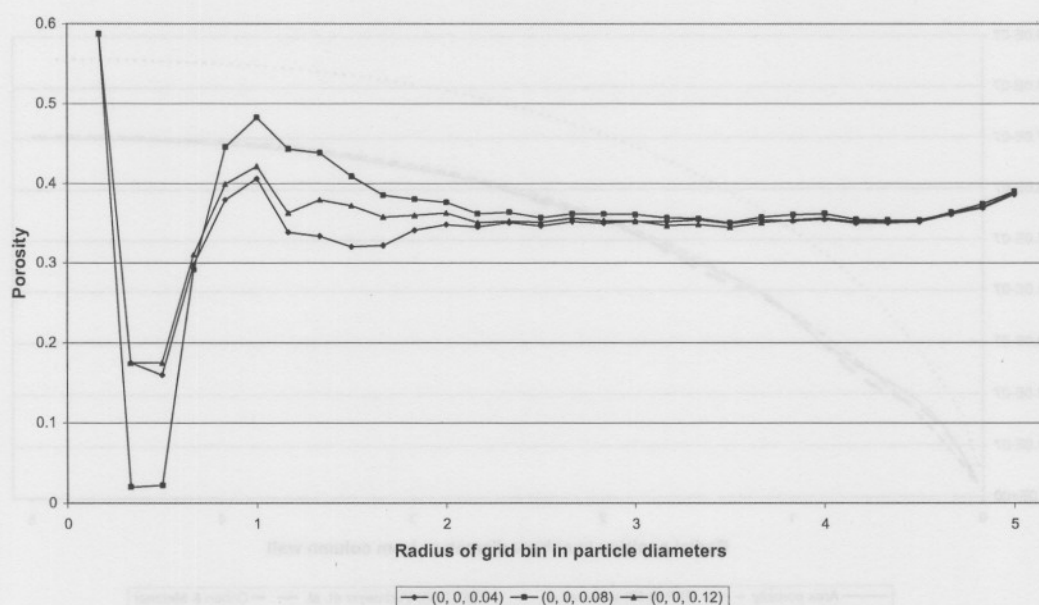


Figure 5-11. Porosity distribution about point P , for different points on the axis of the column.

Figure 5-12 shows the porosity distribution about points P , not lying on the axis of the column. A large part of the spherical bins about these points is situated inside the wall region (5-particle diameters from the column wall). The general tendency here is the same as that shown above in Figure 5-11. The porosity approaches a constant value for a grid bin radius in the region of two particle diameters.

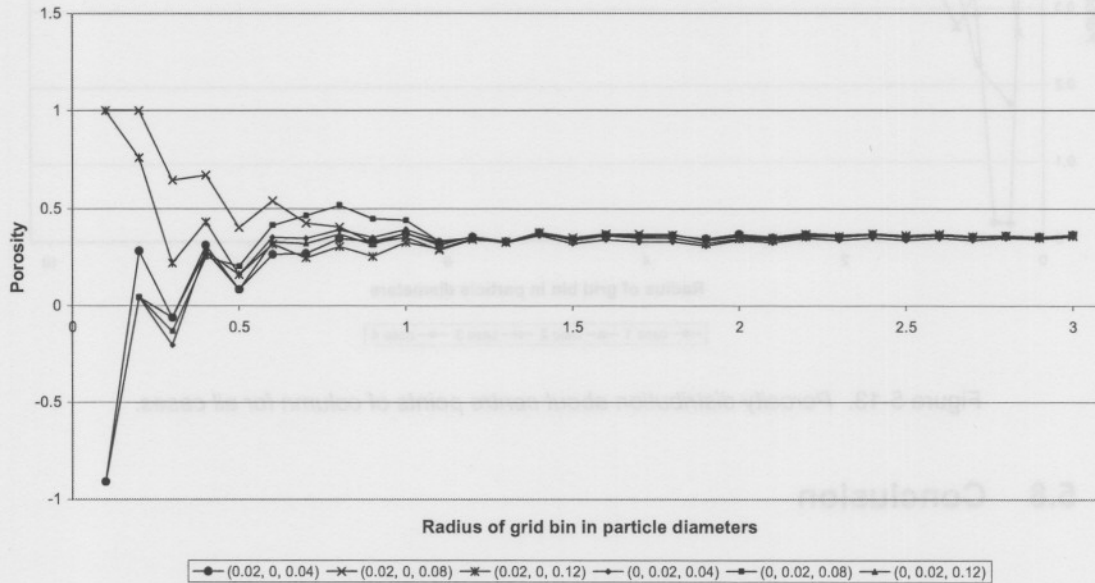


Figure 5-12. Porosity distribution about point P for points not lying on the axis of the column.

Figure 5-13 is a plot of the porosity distribution about the centre point of the column for all the cases investigated in this section.

The porosity distributions about the points P in Figure 5-13 approach a constant value (for all points P in this calculation) for a grid bin radius of two particle diameters. Kaviany (1991) predicted (in section 2.2.2) that for the REV $\ell \gg d_p$, where ℓ is a characteristic length scale for the REV and d_p is a particle diameter. Thus from this (preliminary) result it seems that the size of the REV is smaller than expected.

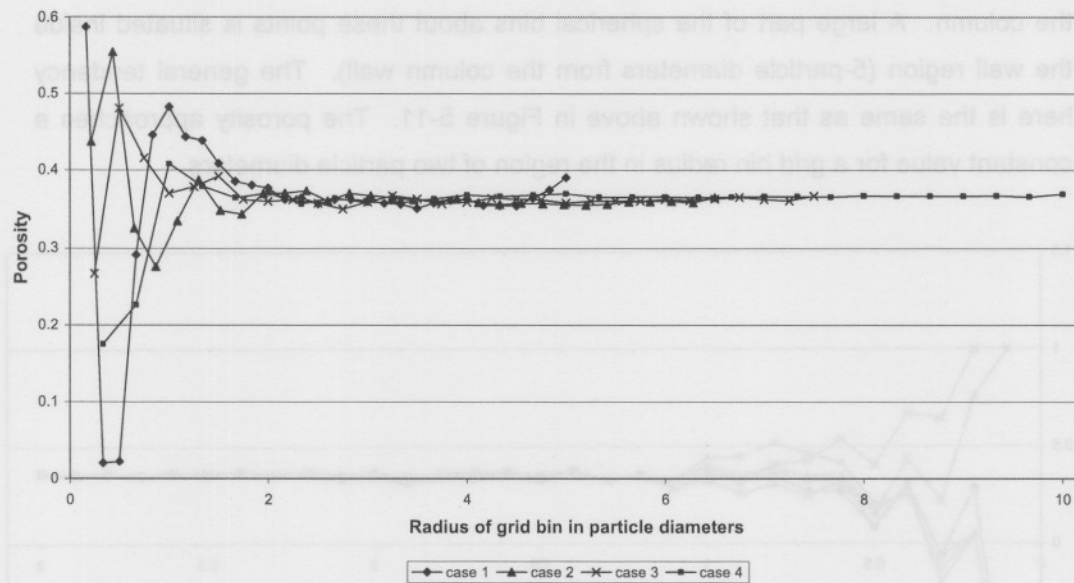


Figure 5-13. Porosity distribution about centre points of column for all cases.

5.8 Conclusion

The results that were obtained from the numerical procedures developed in this study are in good agreement to the experimental results of other authors. The expected tendencies were observed for the axial- and radial void fraction distributions. From the results for the REV calculations, it appears that the size of the REV is smaller than predicted in the literature.

The results generated in this study are only preliminary. More data is needed to do a thorough investigation of the effects present in packed columns.

Chapter 6

Conclusions and Recommendations

Chapter outline:

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6.4	Recommendations for further research	100

6.1 Introduction

In this chapter a brief summary of this report is provided, and the most important conclusions that can be reached are discussed. Recommendations for further research are also suggested.

6.2 Summary

The background to this study was given in Chapter one. It was shown that porosity variations exist in packed columns. Many physical experiments have been conducted to determine the structure and packing characteristics of packed column devices. There is little information in the literature on numerical investigations into packed columns. The objective of this study was consequently, to develop numerical tools to analyse the packing structure of packed columns.

In Chapter 2, a thorough literature survey was conducted. The porosity was rigorously defined in terms of the representative elementary volume (REV). Experimental results of other authors show that the porosity varies sharply, and in a definitive way near the column wall. These variations extend about 5-particle diameters into the column. In the central region of the column, where no significant variations exist, the porosity approaches a constant (bulk) value.

The models that are used in the literature to simulate the flow through packed columns are also discussed in the literature survey. Many of these flow models aim to account for the effect of the porosity variations on the flow in the wall region. From these studies it is clear that wall channelling occurs, and can have a significant influence on the mass flow and pressure drop over the column.

In Chapter 3 the derivation and implementation of the models to analyse the porosity of packed columns were discussed. For the purposes of this study four models were developed; a model to calculate the overlap between the particles in the column, a model to calculate the axial porosity distribution, a model to calculate the radial void fraction distribution, and a model to calculate the porosity distribution about a point in the column (this model can be used to determine the size of the REV).

The implementation and validation of the models were explained in Chapter 4. This chapter provides the reader with a thorough insight into the functioning of the codes.

In Chapter 5, a complete analysis of four data sets was discussed. The aim of this study was to develop the functionality to analyse the position data of packed columns. This chapter shows that the developed codes deliver the desired (expected) results, and that the codes function properly and correctly.

6.3 Conclusions

As stated in the summary, and in the introductory chapter, the objective of this study was to develop procedures to analyse the porosity of packed columns numerically. The validation tests that were conducted in Chapter 4, confirmed that the implementation of the models are correct. Furthermore, the results generated with the codes are in qualitative agreement to the experimental results of other authors.

The conclusion that can be reached, is that the codes are correct and therefore that the main study objectives has been achieved. Further, the results also indicate that the position data for the packed columns are a (relatively) good approximation to real packings.

6.4 Recommendations for further research

The output of this study is the implementation of numerical methods to analyse the porosity of packed columns. The results that were generated for this study, is only preliminary, and not sufficient to draw any (definite) conclusions about the porosity characteristics of packed columns in general.

For the purposes of further research the following studies can be conducted:

- The trends and properties (characteristics) of the porosity in packed columns can be investigated thoroughly with the use of these codes.
- With these codes as basis, other tools can be developed, for example to study the pore structure, the heat conduction properties, and the view factors (shape factors) for radiation heat transfer problems.

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APPENDIX A: Input files

All the input files for the codes described in this report have the same form. All the information in the input file is not used by all codes. All coordinates are given in meters [m]. The typical input file has the following form:

```

** Case 1
case11d2.dat
2214 0.008 0.0 0.088 0.160
1.0 0.1 0.0 15.0 50
6 0.2 30 0.0 0.0 0.052

```

Figure A-1. The information contained in a typical input file.

Line 1: ** Descriptive title for the problem

The descriptive title in the input file is there to help the user keep track of progress. The title can be less or equal to 81 characters. The title must start with an asterisk ("**") in the first column.

Line 2: Name of data file containing the coordinates of the centres of the spheres.

The data file that is opened contains the sphere data. This includes the sphere identification number, and the coordinates of the spheres, in Cartesian coordinates. The sphere identification numbers can agree with the number of spheres in the packing, however this is not always necessarily the case.

Line 3: Number of spheres, d_p , D_{inside} , D , L .

This is information directly relating to the packing. On this line the total number of particles in the column, the particle diameter, the inside diameter of the annular column, the column outside diameter, and the column height is given. If the column is not an annular column, the inside diameter set to zero.

Appendix A: Input files

Line 4: *binratio*, peel/slice-ratio, z_{low} , z_{high} , *ndteta*.

This is the information relating to the solution of the problem. The *binratio* is defined as the ratio of the bin height, or bin thickness, to the diameter of a sphere d_p . The peel/slice-ratio is defined as the ratio of the distance between consecutive peels (radial porosity code), or slices (axial porosity code) to sphere diameter. z_{low} is the lower cut-off plane for the radial porosity distribution procedure, and z_{high} is the upper cut-off plane for the radial porosity distribution procedure. The parameter *ndteta*, is the number of integration intervals that is used in the integration of the area A , in the radial void fraction procedure.

Line 5: Grid *binratio*, delta ratio, number of grid bins, (X_p, Y_p, Z_p) .

The grid *binratio* is defined as the ratio of the maximum spherical bin radius to sphere diameter. The delta ratio is defined as the ratio of the distance between grid points to the sphere diameter. (The smaller the delta ratio, the more grid points will be generated, thus the solution will be more accurate, and the code will take more time to execute.) The number of grid bins to be used is also specified. (X_p, Y_p, Z_p) is the Cartesian coordinates of the point P , about which the REV is calculated.

All this information need not be included for use in all the codes. The following figures show what information is needed by the various codes.

A.1 Calculate overlap

** Descriptive title
Name of data file to access.
Total number of spheres, d_p [m], column inside diameter, D [m], L [m]
<i>binratio</i>

Figure A-2. The information needed for the *calcoverlap* code.

A.2 Axial porosity distribution

** Descriptive title
Name of data file to access.
Total number of spheres, d_p [m], column inside diameter, D [m], L [m],
 $binratio$, sliceratio.

Figure A-3. The information needed for the axialporos code.

A.3 Radial porosity distribution

** Descriptive title
Name of data file to access.
Total number of spheres, d_p [m], column inside diameter, D [m], L [m],
 $binratio$, peelratio, z_{low} , z_{high} , number of angular integration intervals.

Figure A-4. The information needed for the radialporos code.

A.4 Representative elementary volume

** Descriptive title
Name of data file to access.
Total number of spheres, d_p [m], annular inside diameter, D [m], L [m],
 $binratio$, peel/slice-ratio, z_{low} , z_{high} , number of angular integration intervals,
Grid binratio, delta ratio, number of grid bins, (X_p, Y_p, Z_p)

Figure A-5. The information needed for the REV code.

