Large Scale Lattice-Boltzmann Simulations: Computational Methods and Applications

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Chapter 7

Hydraulic Permeability of Fibrous Media

7.1 Introduction

In the previous chapter we have demonstrated that the Lattice-Boltzmann method is a versatile tool for simulating fluid flow in realistic 3D geometries. In the remainder of the thesis we use LBM to study hydrodynamic properties of disordered porous media. We focus on porous media made of fibers. Fluid flow in porous media plays an important role in a wide variety of technical and environmental processes, such as oil recovery, paper manufacturing and spread of hazardous wastes in soils. The single-phase creeping flow through a porous substance is well described by Darcy's law [94, 95] which can be written in the form

\[ q = -\frac{k}{\nu} \nabla p, \]  

(7.1)

where \( q \) is the fluid flux through the medium, \( \nu \) and \( p \) are the kinematic viscosity and the pressure of the fluid, respectively, and \( k \) is the permeability coefficient that is a measure of the fluid conductivity through the porous medium. It depends on the geometrical properties of the medium.

Determination of the permeability, \( k \), for each particular substance is a long standing problem. The experimental methods that are currently used are based on sophisticated approaches, which utilize e.g. mercury porosimetry, electrical conductivity, nuclear magnetic resonance or acoustic properties of the medium [96, 97, 98]. Theoretical methods typically rely on analytical models based on simplified pore geometries, which allow solution of the microscopic flow patterns [94], or on more advanced methods that statistically take into account the structural complexity of the medium [94, 95].

Numerical simulations are often used to connect theory with experiments. Realistic three-dimensional flow simulations in complex geometries are however very demanding in terms of computing power. Until recently this approach has been hampered by the necessity of major simplifications in the pore structure or flow dynamics. New techniques based on massively parallel computers and increased single processor capabilities have now made 3D simulations of realistic
flow problems feasible. This development is further augmented by the intro-
duction of the lattice-gas-automaton (LGA) \cite{99,12} and lattice-Boltzmann (LB)
method \cite{21,28,46}, which have already been applied to a wide class of fluid-
flow problems and are particularly useful in complex and irregular geometries
\cite{100,40,41,49,101,6}.

In this chapter we report on the results of lattice-Boltzmann simulations of
creeping flow through various fibrous media and compare them with previous
experimental, analytical and numerical results. The aim of this study is three-
fold:

- First, we validate the Lattice-Boltzmann results rigorously by direct com-
  parison with analytical, numerical and experimental data for various mod-
  els of fibrous media with a large variation in geometrical properties (see
  section 8.2);

- Next, we study the effect of disorder on the hydraulic permeability and
  make a connection between the permeability and the geometry of the me-
  dia (see sections 8.2 and 8.3);

- Finally, we study the permeability of bounded fibrous media, cf. media
  placed between two parallel plates, as a function of the distance between
  the parallel plates (see section 8.4). These studies are particularly rele-
  vant as many fibrous media in practice are bounded systems.

### 7.2 Permeability of (dis)ordered fibrous media

#### 7.2.1 Background

For a specific fiber arrangement, the permeability depends on the size and con-
centration of fibers \cite{102}. It is assumed here that the fibers are uniform in di-
ameter and are long enough such that the logical metric for size is the fiber ra-
dius, \( r \). The fiber concentration is characterized by the fiber volume fraction, \( \phi \).
The main objective is then to study the functional behavior of the dimensionless
hydraulic permeability, \( \frac{k}{r^2} \) as a function of the volume fraction,

\[
\frac{k}{r^2} = f(\phi).
\]

*This chapter is based on the following publications:

- A. Koponen, D. Kandhai, E. Hellen, M. Alava, A. Hoekstra, M. Kataja, K. Niskanen, P.

- D.S. Clague, D. Kandhai, R. Zhang, P.M.A. Sloot, 'Hydraulic Permeability of
  Accepted for publication.
In the past years several studies have been conducted to explore $f(\phi)$ for various fiber arrangements. These studies were based on analytical, numerical and experimental methods. In this section we present a brief overview of the results. The theoretical approach has been to solve Stokes equation in a unit cell via mathematical methods. Due to several approximations in the analytical models, these results are usually only valid for small fiber volume fractions. For simplicity, the unit cell is often restricted to a circular rod placed at the center of a polygon with periodic boundaries. One of the first analytical expressions has been published by Langmuir in 1942 \[103\]. His work was based on flow parallel to an array of cylinders (one-dimensional flow) in a circular unit cell. This unit cell greatly simplifies the mathematics. Later, several other studies have been reported in which a square unit cell was used instead of circular unit cells. Alternatively, the cylinders were placed in a square, triangular or hexagonal array arrangement. A general equation for the dimensionless hydraulic permeability, $k$, in the case of flow parallel to an array of rods was published by Drummond and Tahir in 1984 \[104\],

$$
\frac{k}{r^2} = \frac{1}{4\phi} (-ln(\phi) + K + 2\phi - \frac{\phi^2}{2})
$$

(7.2)

where $K$ is a constant depending on the fiber arrangement. From this equation, we clearly see a dominant $ln(\phi)$ functionality for very small volume fractions. For higher volume fractions polynomial correction terms are included.

A more complicated case which has been studied rigorously, is flow perpendicular to an array of cylinders. Here the flow field is truly two-dimensional. Different analytical expressions have been proposed by several authors during the last years. The most notable is the result of Sangani and Acrivos (1982) for a square array of cylinders \[105\],

$$
\frac{k}{r^2} = \frac{1}{8\phi} (-ln(\phi) - 1.476 + 2\phi - 1.774\phi^2 + 4.076\phi^3).
$$

(7.3)

In addition to this expression, which is only valid in the dilute limit, Sangani and Acrivos reported a semi-analytical study of the hydraulic permeability of a 2D periodic array of cylinders for the full range of fiber volume fractions \[105\]. We clearly see that the hydraulic permeability for flow perpendicular to an array of cylinders (higher resistance as expected) is approximately half of the hydraulic permeability of flow parallel to an array of cylinders.

So far we discussed one- and two-dimensional flow in fibrous media. Jackson and James studied the hydraulic permeability of a three-dimensional cubic lattice model. They used the expressions of the permeability of flow parallel to an array of cylinders and perpendicular to an array of cylinders to derive the following results for the cubic lattice model \[102, 106\],

$$
\frac{k}{r^2} = \frac{3}{20\phi} (-ln(\phi) - 0.931 + O(ln(\phi))^{-1}).
$$

(7.4)

In Ref. \[102\] it is shown that this equation agrees reasonably well with experimental data for $\phi$ smaller than 0.25. Another very useful method to predict the
permeability is via the Kozeny-Carman equation, where the permeability is related to the fiber volume fraction and the specific surface area of the media. In the next section we will discuss the Kozeny-Carman equation in more detail. Besides these theoretical studies, Higdon and Ford recently reported, numerical simulations of the hydraulic permeability of different models of 3D fibrous media using spectral boundary element methods [107] for the full range of fiber volume fractions. Their results will be used and discussed in more detail in the next sections. Other numerical studies include those on fluid flow through random arrays of parallel cylinders and suspension of prolate spheroids [108, 109]. All these efforts neglect the disorder typical of real 3D fibrous media. The work of Clague and Philips [110] on permeability of disordered fibrous media is an exception. They used numerical slender body theory methods to calculate the permeability of 3D disordered fibrous media. However, their study was restricted to dilute systems due to inherent limitations of their numerical approach. Finally, we stress that a large body of experimental data has been published (see e.g. [102] for a comprehensive review). However, despite these numerous experimental, numerical and theoretical studies, permeability characteristics of three-dimensional disordered fibrous porous media are still poorly understood. Here we use the lattice-Boltzmann method to calculate the hydraulic permeability for different fibrous media and for a large range of fiber volume fractions.

### 7.2.2 Description of the fibrous media

The first model of fibrous media that is studied is a 2D periodic array of cylinders (see Fig. 7.1). As stated in the previous section, the hydraulic permeability of this simple configuration has been studied theoretically in detail by Sangani and Acrivos [105]. This problem is a well known and accepted benchmark for fluid flow in fibrous media. Additionally, we simulated fluid flow through a 3D BCC lattice configuration with periodic boundaries. In the BCC lattice configuration the fibers are placed such that their intersection points coincide with the BCC positions (see Fig 7.2). This simulation cell has been studied numerically by Higdon and Ford [107] for a wide range of solid fractions using spectral boundary element methods. The main motivation for performing simulations of the periodic array of cylinders and the BCC configuration, is to validate the LBM simulations for a wide range of solid fractions and to determine the minimum number of lattice points that are required for discretising the cylinders such that accurate results are guaranteed. Moreover, these simulation cells will be used in the next section to study in more detail the connection between the hydraulic permeability and the geometry of the medium. In that section we focus on the behavior of the hydraulic permeability as a function of $\phi$. Details of the geometry are not explicitly taken into account. Besides the simulations of flow through ordered fibrous media we studied media where the fibers are placed randomly. We considered two configurations, namely random fiber mats and fibrous media consisting of randomly placed overlapping cylinders.
Figure 7.1: A 2D array of periodic cylinders. \( r \) is the radius of the cylinder and \( \delta_{sqr} \) is the half-distance between the cylinders. \( \delta_{sqr} \) will be used in the next chapter.

Figure 7.2: A fibrous medium based on the BCC lattice.
The random fiber mats are constructed in discretized space using a recently introduced growth algorithm [57]. Within this algorithm, fiber webs are grown by sequential random deposition of flexible fibers of rectangular cross-section on top of a flat substrate (the xy plane). Each fiber is randomly oriented either in the x or y direction, and is then let to fall in the negative z direction until it makes its first contact with the underlying structure. After this it is bent downwards without destructing the structure, and subject to the constraint

$$|z_i - z_j| \leq F.$$  \hspace{1cm} (7.5)

Here $z_i$ and $z_j$ are the elevations of the fiber surface above two nearest-neighbor cells $i$ and $j$, and $F$ is an effective fiber flexibility. Notice that for long fibers the resulting web structure solid fraction, and contact area of fibers, are determined by $F$ [111]. A large $F$ produces a dense web while small $F$ leads to a more porous structure.

Figure 7.3: A fiber-web sample constructed with the deposition model. The fiber volume fraction of the web is 0.17.

In order to construct structures that are homogeneous in the z direction, the samples used in the simulations were extracted from inner parts of thicker webs. Based on preliminary simulations (data not shown), ten grid layers of void space were then added on the top of samples, and the system was made periodic in all directions. In Fig. 7.3 we show a sample created by this algorithm.
It has been shown that these structures closely resemble that of materials like paper (see e.g. Ref. [112]) and non-woven fabrics (restriction to the x and y directions can be relaxed and does not play an important role here).

Besides the random fiber mat we also studied fluid flow through fully disordered fibrous networks. These networks are built of overlapping cylinders that are placed randomly in a cubic volume and thus their orientation in the z-direction is not constrained by a flexibility parameter [113]. In Fig. 7.4 we show a sample created by this method. In Ref. [113] it has been shown that the generated structures are indeed statistically random. A few years ago, Clague and Philips have studied the permeability of similar disordered media using numerical slender body theory [110]. The main differences between our simulations and that of Clague and Philips is that in their approach the cylinders were not allowed to overlap due to limitations of their numerical method. Therefore their study was restricted to dilute systems, e.g. in the limit of low fiber volume fractions, $0 < \phi < 0.25$.

![Figure 7.4: Part of a disordered fiber-network sample constructed with the random fiber generator described in Ref. [113]. The fiber volume fraction of the network is 0.1.](image)

**7.2.3 Hydraulic Permeability as a function of the fiber volume fraction**

In the LBM simulations a uniform velocity field is first initialized. Next, flow is induced by applying a body force on the fluid [49]. This is accomplished simply by adding at each time step a fixed amount of momentum in the direction
of the force to all 'particles' within the void space. Unless stated otherwise the relaxation parameter in the simulations is equal to 1. The permeability of the medium is simply found by computing the total flux \( q \) through the sample from the stationary hydrodynamic state for a given pressure gradient and fluid viscosity and using Eq. 7.1.

It is well known that the permeability of a porous medium determined by the present method depends on grid resolution. Resolution sensitivity is caused by the bounce-back boundary condition applied to the solid-fluid interface, and by Knudsen effects in small pores (see [12, 46, 49] and chapter 3). These effects are viscosity dependent, and they determine the minimum size of obstacles and pores that can be used in simulations. We will therefore perform a few preliminary simulations to address the resolution effects.

### Periodic Array of Cylinders

The hydraulic permeability for a periodic array of cylinders is shown in Fig. 7.5. In this plot we have included the semi-analytical solution of Sangani and Acrivos [105]. The cylinders have been discretized using radii of 5.5 to 23.5 lat-
tice points for the full range of fiber volume fractions. It is clear that there is a very good agreement between our simulations and the semi-analytical curve of Sangani and Acrivos [105] for the complete range of fiber volume fractions, as the cylinder radius is increased.

**BCC Lattice Configuration**

The results for the BCC lattice configurations are shown in Fig. 7.6.

![Graph showing calculated dimensionless permeability](image)

Figure 7.6: The calculated dimensionless permeability $k/r^2$ as a function of fiber volume fraction for the full range of solid fractions. For $\phi < 0.4$, $R = 6$ lattice points, for $0.4 < \phi < 0.6$ $R = 12$ and $R = 18$ lattice points otherwise. To guide the eye a dashed curve through the numerical results of Higdon and Ford is included [107].

From preliminary studies we found that accurate results are guaranteed when the cylinder radius is varied from 6 to 30 lattice points for increasing fiber volume fractions (data not shown). In Fig. 7.6 we have included the hydraulic permeabilities computed by Higdon and Ford using Spectral Boundary Element Methods. We clearly see that the Lattice-Boltzmann results are in excellent agreement with Higdon and Ford’s calculations. A further increase of the cylinder radii does not have a significant effect on the accuracy of the results.
As noted in Ref. [114] the agreement between the LBM results for the ordered fibrous media and that described in Refs [105, 107] is important because it shows that the LBM is accurate over a larger range of fiber volume fractions compared to the results obtained by the approach based on numerical slender body theory. Moreover, its accuracy is comparable to Spectral Boundary Element methods used by Higdon and Ford for the full range of fiber volume fractions.

Disordered media I: Random Fiber Mats

Before performing flow simulations in the random fiber webs we have first conducted a convergence study in order to gain insight in the minimum grid resolutions that guarantee acceptable accuracy for different fiber volume fractions. For this we made a series of test runs using fibers of aspect ratio 10, i.e. of size \( w_F \times w_F \times 10 w_F \), with \( w_F = 5, 10 \) and 20 grid units. In these tests the size of the simulation lattice was \( L_x \times L_y \times L_z = 20 w_F \times 20 w_F \times 10 w_F \). Moreover, the relaxation parameter \( \tau \) of the LBGK collision operator was varied from 0.668 to 2 corresponding to the dynamic viscosity \( \nu = (2 \tau - 1)/6 \) [21] ranging from 0.056 to 0.5 (in grid units). The main reason for varying the relaxation parameter is to compare the results obtained on different grid resolutions for varying \( \tau \). It is expected that as \( \tau \) approaches to 0.668 (\( \nu = 0.056 \), the numerical errors due to the bounce-back boundary condition will decrease [49].

In Fig. 7.7 we show the computed permeability as a function of viscosity \( \nu \) for two test systems of different fiber volume fractions. The nearly linear dependence of \( \nu \) on permeability [49] is clearly seen in this figure. For \( \phi = 0.33 \) (Fig. 7.7a), the result is already almost independent of the grid resolution for the smallest value of the viscosity. For low fiber volume fractions (with \( \nu = 0.056 \)), resolution \( w_F = 5 \) can be used. For a higher fiber volume fraction finite-size effects become more pronounced. Comparing the simulated permeabilities for \( \phi = 0.61 \) (Fig. 7.7b) at \( \nu = 0.056 \), we can conclude that \( w_F = 10 \) is satisfactory for high fiber volume fractions.

In the actual permeability simulations fibers of aspect ratio 20, i.e. of size \( w_F \times w_F \times 20 w_F \), and a lattice of dimensions \( 80 w_F \times 80 w_F \times 10 w_F \) were used. The flexibility parameter \( F \) was varied from 0 to 3 which corresponds to fiber volume fractions \( \phi \) ranging from 0.05 to 0.58. In the simulations \( \tau = 0.668 (\nu = 0.056) \) and two different values for \( w_F \) were used. For \( \phi < 0.4 \), \( w_F = 5 \) was used, and the size of the simulation lattice was \( 400 \times 400 \times 60 \) grid points. For \( \phi > 0.4 \), \( w_F = 10 \) and a lattice of \( 800 \times 800 \times 110 \) grid points were used. For these discretizations, the estimated finite-size errors of the simulated permeabilities were less than 15%. This is estimated from the calculated permeabilities for the different values for the \( w_F \) parameter and \( \nu = 0.056 \) (see Fig. 7.7).

When 32-bit floating point numbers were used, the larger simulation lattice required 5.4 GByte of core memory. The simulations were therefore carried out using 64 nodes (300 MHz CPUs with 128 MByte of memory) on a Cray T3E system. For parallelization of the method we refer to chapter 5. The required CPU time was typically between 1 and 4 hours. Notice that we have used the IMR method described in chapter 3 to reduce the saturation times of the simulations.
7.2 Permeability of (dis)ordered fibrous media

Figure 7.7: Calculated dimensionless permeability $k/r^2$ as a function of viscosity $v$ for two test samples with fiber volume fraction $\phi = 0.33$ (on the left) and $\phi = 0.61$ (on the right). Here $r = w_f/2$ is the hydraulic radius of the fibers. The fiber widths (grid resolutions) are $w_f = 5, 10$ and $20$.

In Fig. 7.8 we show a simulated stationary velocity field for a flow in the z direction through the highly inhomogeneous sample shown in Fig. 7.3. It is evident that there are large fluctuations in the velocity field reflecting the variations in the local fiber volume fraction of the sample. These fluctuations, which are inherent in random porous structures, will affect the permeability, except at very low fiber volume fractions, such that it is expected to become higher than that for regular arrays of pores [102]. This effect will be seen in the results given below.

In Fig. 7.9 we show the simulated permeability of the random fiber web as a function of the fiber volume fraction. In this figure solid triangles denote the simulated values. It is evident that there are two distinct features in the simulated permeability curve. Firstly, it seems to diverge as expected when $\phi \rightarrow 0$, and, secondly, $k$ seems to be an exponential function of the fiber volume fraction for a rather wide range of: $0.15 < \phi < 0.58$.

A fit through the last five points with lowest fiber volume fractions of the form $k/r^2 = constant \cdot \phi^{-\mu}$ gives $\mu = 1.92$. The simple capillary-tube model by Kozeny and Carman [94] gives $k/r^2 \propto (1 - \phi)^3 \phi^{-2}$ in this limit so that, as expected, the
Figure 7.8: The velocity field of fluid flow through the fiber web shown in Fig. 7.3. Bright colors indicate high fluid velocity.

Simulated behavior of the permeability is in rather good agreement with this model.

A fit of the form $\ln(k/r^2) = A + B\phi$ to the rest of the simulated points gives $A = -9.5, B = -10.4$, with a very high correlation between the simulated points and the fitted curve. So far there have been no analytical results which would have produced this kind of exponential behavior at intermediate fiber volume fractions. It will not hold near the percolation threshold at which permeability vanishes. This critical region is however beyond the present computational capabilities.

Experimental results [115, 102], shown in Fig. 7.9 as open circles and squares, conform well with the simulated points. Notice that there is no free parameter in the present model as permeability is scaled by the square of the hydraulic radius of the fibers, and the relaxation parameter $\tau$ is only used to fix the necessary grid resolution. The level of agreement is therefore astonishingly high. It also shows that the model web used here captures the essential features of the fibrous filters and compressed fiber mats used in the experiments.

Also shown in Fig. 7.9 are three curves which are results of previous analytical [102] (curve (1)), numerical [107] (curve (2)) and semi-empirical [94, 115, 116] (curve (3)) considerations. Curve (1) is given by $k/r^2 = \frac{3}{20}(-\ln(\phi) - 0.931 + O(1/\ln(\phi)))$, an expression obtained in Ref. [102] for a cubic lattice model (see section 2), and curve (2) results from a numerical solution [107] for the Stokes flow in a face-centered-cubic (fcc) array of fibers. Both these curves are below the simulated points, especially for decreasing fiber volume fraction. Notice
7.2 Permeability of (dis)ordered fibrous media

Figure 7.9: The calculated dimensionless permeability \( k/r^2 \) as a function of fiber volume fraction, \( \phi \) (black triangles). Open squares and circles show the experimental results for fibrous filters [102] and compressed fiber mats [115, 102], respectively. Curve (1) is the analytical result for cubic lattice given in Ref. [102], curve (2) is the numerical result (crosses) for a FCC lattice from Ref. [107], and curve (3) shows the result of a fit with the Kozeny-Carman relation, Eq. (7.6).

that the fcc result also follows an exponential law at intermediate fiber volume fractions. It is 30-40% below the random fiber-web result for these volume fractions, but approaches the latter for high fiber volume fractions since the percolation threshold of the fcc lattice [107] is at a much higher fiber volume fraction. Curve (3) is the Kozeny-Carman expression [94]

\[
k = \frac{(1 - \phi)^3}{cS^2},
\]

where \( S \) is the specific surface area of the web, and \( c \) is a constant in capillary-tube models but is known to depend on fiber volume fraction in fibrous materials [116]. An empirical fit to measured fiber volume fractions of these materials gives \( c = 3.5(1 - \phi)^3[1 + 57\phi^3]/\phi^{1/2} \) [115, 116]. We have used this expression to get the curve (3) from Eq. 7.6. The specific surface area \( S \) was determined from the surface area of the (straight) fibers used to construct the web by subtracting the area of the inter-fiber contacts. Because of bending of the fibers this expression
gives a lower bound for $S$, and curve (3) is expected to overestimate the permeability. This is indeed what happens (cf. Fig. 7.9).

Encouraged by the exponential behavior at intermediate fiber volume fractions of the simulated permeability curve, we have made an interpolation formula that connects this behavior with the right asymptotics in the limit $\phi \to 0$. We find that the expression $k/r^2 = A[e^{Bi}\phi]^{-1}$ with $A = 5.6, B = 10.1$, fits all the simulated points very well. So far we have no theoretical arguments to support this very simple form for the permeability.

Disordered Media II: Randomly placed overlapping cylinders

In the previous section we found that the permeability of the random fiber mat has a very simple exponential dependence on the fiber volume fraction for a wide range of $\phi$. Moreover, the permeability of the disordered media is 30 to 40% higher compared to that of ordered media. This is due to the fluctuations in the pore sizes along the medium. In this section, we study the permeability of a second disordered medium in which the fibers are oriented randomly and are allowed to overlap freely. Our main objective is to see whether similar observations are still valid for such a medium. The random fiber network that is studied here is shown in Fig. 7.4.

From preliminary simulations of flow through these media it became clear that accurate results can only be obtained when cylinder radii of 6 lattice points are used for fiber volume fractions smaller than 0.5. On the other hand for $0.5 < \phi < 0.7$ cylinder radii of 12 lattice points are required to obtain satisfactory results (data not shown). Beside these accuracy restrictions, the dimension of a typical simulation cell is also determined by the fact that the fibrous medium itself is not periodic in this case (see Fig. 7.4), whereas in the flow simulations simple periodic boundaries are regularly used. This problem can be overcome by using more complicated velocity boundaries instead of periodic flow boundaries. However, if it can be shown that the edge effects due the periodic boundaries are small, the simple approach based on periodic boundaries can still be applied. To gain insight in this matter, we performed preliminary simulations for different simulation sample sizes. The sample dimension is expressed in units of the Brinkman screening length, $\alpha^{-1}$, which is defined as $\alpha^{-1} = \sqrt{k}$. The Brinkman screening length is the typical length scale in the system in which velocity disturbances caused by the single fibers decay to the bulk flow\textsuperscript{[110]}. In the remainder of this chapter we will make extensive use of this parameter for several purposes. We computed the Brinkman screening length by using Jackson and James's analytical expression for the hydraulic permeability of the cubic lattice model (see section 2). It is expected that as the simulation cell dimension is increased the edge effects become small. Moreover, it is expected that the edge effects are stronger in the dilute limit as then the permeability is relatively high. Simulations for varying cell dimensions indicate that in the dilute limit, the wall effects due to periodicity are small when the simulation cell dimension is in the order of at least $7\alpha^{-1}$. Consequently, lattices of dimensions in the order of 200x200x200 are used in the final simulations.
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Figure 7.10: The calculated dimensionless permeability $k/\rho^2$ as a function of fiber volume fraction. We have included the numerical results of Higdon and Ford for the FCC lattice and the analytical curve of Jackson and James.

In Fig. 7.10 we show the simulated permeability curve. In this figure we included the results of the ordered FCC lattice of Higdon and Ford and the analytical curve of Jackson and James [102]. We clearly see that in the dilute limit there is a very good agreement between our results and that of Jackson and James [102]. The permeability results obtained for these disordered media are also in this case higher than that of the ordered FCC lattice, which is consistent with the behavior found for the permeability of the random fiber mats. Furthermore, the computed permeability curve also shows for this medium a simple exponential dependence for a wide range of fiber volume fractions. In this case, we do not present a detailed comparison with other experimental and numerical results.

In fact the similarity between the permeability of media I and II is obvious from the behavior of both results compared to that of the FCC lattice. It is thus clear that the remarks that have been made concerning the Kozeny Carman relation, the experimental data and the analytical curve of Jackson and James are still valid for media II. In Figure 7.11 we show the permeability results obtained for the random fiber mat and the disordered media II in one graph. We clearly see
7.3 The connection between the hydraulic permeability and the geometry of the media

In the previous section we have studied the hydraulic permeability of various fibrous media. The main objective was to obtain the behavior of the permeability as a function of the fiber volume fraction. The fiber volume fraction, \( \phi \), is in principle used to characterize the geometry of the media. One of the main results is that the hydraulic permeability of disordered fibrous media has an exponential dependence on the fiber volume fraction for a large range of \( \phi \). In this chapter we explore this relation in more detail. We first argue, using scaling...
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relations, that an important control parameter for the permeability is the distance between the fibers. Then we find expressions for the fiber-fiber distance for several ordered and disordered media that have been considered in the previous chapter. Next, we correlate the previously found $k(\phi)$ functionality with the behavior of the fiber-fiber distance as a function of the fiber volume fraction. This study provides some insights in the dependence of $k$ on $\phi$.

In the next subsection, we first argue that the important parameter that controls the permeability is the fiber-fiber distance. Next, we derive expressions for the fiber-fiber distance for the different media as a function of the fiber volume fraction, $\delta(\phi)$. Finally, we study the connection between the $k(\phi)$ and the $\delta(\phi)$ behavior for various fibrous media.

7.3.1 The role of the fiber-fiber distance

We argue that an important parameter that controls the permeability of fibrous media is the fiber-fiber distance. We do this by making a direct connection between the permeability curve, the flow field, and the fiber-fiber distance. For simplicity we restrict to the case of a periodic array of cylinders. First, let us recall the hydraulic permeability curve of the periodic array of cylinders (see Fig. 7.5). In this curve we clearly see that the permeability decreases as the solid fraction is increased. However, for $\phi \approx 0.5$, there is a relatively strong decrease or a rapid down-turn in the $k(\phi)$ functionality.

To correlate this behavior with the flow field around the cylinder, we analyze the velocity along the diagonal of the simulation cell. A more detailed description of the simulation cell is shown in Fig. 7.12. In fact we are mainly interested in the effect of the cylinder surface on the flow field as a function of the solid fraction and we would like to measure the disturbances caused by the cylinder surface on the flow field. From hydrodynamics it is known that in two-dimensions there is always some interaction between the cylinder and its periodic image [4]. However, the strength of the interaction depends on the distance between the cylinder and its periodic image. As this distance becomes smaller (i.e. the fiber volume fraction increases) the interaction will be more pronounced. Some insight in this matter can be gained by inspecting the velocity along the diagonal of the simulation cell. An interesting quantity here is the $v_2$-component of velocity, $v_2$. As expected, $v_2$ is very small close to the cylinder and increases as the distance to the cylinder surface is increased. At some location it reaches its maximum. If $v_2$ reaches its maximum at a greater distance, cf the typical length scale along which velocity disturbances decay is larger, then there is a relatively stronger interaction between the cylinder and its periodic image.

In Fig. 7.13 we show $v_2$ as a function of the distance to the cylinder surface in the case of the critical fiber volume fraction, $\phi = 0.5$. It is clear that for this case the
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Figure 7.12: A 2D periodic array of cylinders. $r$ is the cylinder radius, $\delta_{sqr}$ is half cylinder-cylinder distance, $\langle v \rangle$ is the mean velocity imposed at the inlet, $d$ is the distance from the cylinder surface along the diagonal of the cell. $x_1$ and $x_2$ denote the coordinate system and $v_1$ and $v_2$ are the components of the velocity along the $x_1$ and $x_2$ axes, respectively.

length scale at which $v_2$ reaches its maximum, $d_{v_2=max}$, is approximately equal to $\delta_{sqr}$, the half distance between the cylinders. To further explore this behavior, we have determined $d_{v_2=max}$ for varying fiber volume fractions.

In Fig. 7.14 we show the ratio $\frac{d_{v_2=max}}{\delta_{sqr}}$ as a function of $\phi$. It is clear that for $\phi < 0.5$, $d_{v_2=max}$ is smaller than $\delta_{sqr}$. For higher fiber volume fractions, $d_{v_2=max} > \delta_{sqr}$. At the critical fiber volume fraction, $d_{v_2=max} \approx \delta_{sqr}$. If we now take $\delta_{sqr}$ as the typical length scale over which rapid fluctuations in the velocity field occurs, it is clear that close to the critical volume fraction there is a strong interaction between the cylinder and its periodic image. This is indeed the point where the rapid down-turn in the permeability curve starts.

These observations suggest that there is a strong correlation between the fiber-fiber distance (a geometric property) and the macroscopic permeability curve (a hydrodynamic property). Moreover, simple dimensionality analysis suggests that the hydraulic permeability is expressed in units of the square of some typical length scale [94] and by taking the fiber-fiber distance as the typical length scale in the system, the following relation for the permeability can be derived,

$$k \sim \delta_{sqr}^2.$$  (7.7)
7.3 The connection between the hydraulic permeability and the geometry of the media

Figure 7.13: The magnitude of the $x_2$ component of velocity as a function of the diagonal distance from the cylinder surface is shown. The fiber volume fraction is 0.5. The distance to where $v_2$ goes through a maximum is identified by the vertical solid line, and the distance to the simulation cell boundary, $\delta_{sq}$, is denoted by the vertical dashed line.

This scaling relation can also be derived if we consider the gap between the cylinder as a tube with radius $\delta_{sq}$. Within this approximation the mean velocity along the flow direction, $<v_1>$ is equal to [5],

$$<v_1> \sim \frac{\delta_{sq}^2}{\nu} \frac{\partial p}{\partial x_1}.$$ 

By simply comparing with Darcy's law [94], which can be written as $<v_1> = -\frac{k \partial p}{\nu \partial x_1}$, we can derive equation 7.7.

In fact this scaling relation can be intuitively understood as there should be a strong connection between the permeability and the available flux in the medium which in turn is determined by the gap between the cylinders. This connection has also been noted by Tsay and Weinbaum [117]. However, notice that this scaling relation is still very simple, because we do not include more
complicated geometrical properties of the media like the connectivity and the tortuosity [94]. Therefore we do not expect that this relation will predict the correct values for the hydraulic permeability. But we do still hope to see that the tendencies in the permeability curve are correlated with the distance between the fibers.

7.3.2 The fiber-fiber distance

Here we derive expressions for the fiber-fiber distance as a function of the fiber volume fraction. We consider the periodic array of cylinders, the BCC lattice configuration and the disordered fibrous medium used in section 8.4.4. For the periodic array of cylinders we can express the cell size \( n \) as a function of the fiber volume fraction, \( \phi = \frac{r^2}{n^2} \).
The connection between the hydraulic permeability and the geometry of the media

Figure 7.15: The flux area of the BCC lattice configuration. On the left, the upper part of the BCC cell and its periodic image is shown and on the right the flux area is depicted. The flux area is of rhombic shape with side $\frac{\sqrt{2}}{4}n$.

as follows

$$n = r\sqrt{\frac{\pi}{\phi}} \quad \text{and} \quad \delta_{sqr} = \frac{n}{2} - r.$$  

Using these relations we derive the following result for the fiber-fiber distance, for $\delta_{sqr}$,

$$\delta_{sqr} = r\left(\frac{1}{2}\sqrt{\frac{\pi}{\phi}} - 1\right). \quad (7.8)$$

To determine the fiber-fiber distance in the case of the BCC lattice configuration we consider Fig. 7.15.

In this figure we show the upper part of the BCC cell together with its periodic image. The fiber-fiber distance is now estimated using the square root of the flux area which in fact is of rhombic shape (see Fig. 7.15),

$$\delta_{bcc} \approx \frac{\sqrt{2}}{4}n - r. \quad (7.9)$$

Notice that we have included a correction factor (the second term in the r.h.s. of Eq. 7.9) in this result to take into account for the finite thickness of the fibers. For the disordered fibrous media, the estimation of the fiber-fiber distance is more complicated. Since the distances have a large spatial variation, we consider a statistical description and we use Ogston's probability distribution for the radii of spheres that fit in the gap between the cylinders [118]. It is given by,

$$\frac{dP}{dD} = \frac{2\phi}{r^2} D \exp\left(-\phi \frac{D^2}{r^2}\right). \quad (7.10)$$
Figure 7.16: Results for a periodic array of cylinders. The hydraulic permeability and the fiber-fiber distance as a function of the fiber volume fractions. The important transitions in the permeability curve is similar to that of the fiber-fiber distance curve. Dashed lines are included to illustrate the functional behavior and its transitions.

In this equation, \( \frac{dp}{dD} \) is the probability density distribution of distances, \( D \), between the cylinders. As an estimation for the fiber-fiber distance we use the mean distance,

\[
<\delta_{\text{ran}}>= \frac{r \sqrt{\pi}}{\phi^2} - r.
\]  

(7.11)

The standard deviation,

\[
\text{std} = \frac{r}{\phi^2} \left(1 - \frac{\sqrt{\pi}}{2}\right).
\]  

(7.12)

is used to characterize the spatial variation in the gap sizes [114]. Notice that this distribution has been modified to take into account the effect of the finite radii of the cylinders.

7.3.3 Results
7.3 The connection between the hydraulic permeability and the geometry of the media

Figure 7.17: Results for the BCC lattice. The hydraulic permeability and the fiber-fiber distance as a function of the fiber volume fractions. The important transitions in the permeability curve is similar to that of the fiber-fiber distance curve. Dashed lines are included to illustrate the functional behavior and its transitions.

In Fig. 7.16 we show the $k(\phi)$ and the $\delta_{sqr}(\phi)$ in the case of the periodic array of cylinders. It is evident that there is indeed a strong similarity between $k(\phi)$ and $\delta_{sqr}(\phi)$ over the entire range of fiber volume fractions. The important transitions in the permeability curve are similar to the transitions in the fiber-fiber distance curve. Although there is no clear linear relationship between $k(\phi)$ and $\delta_{sqr}(\phi)$, the scaling estimate can still be used to predict the transitions that occur in the permeability curve.

The results for the BCC lattice configuration are shown in Fig. 7.17. We observe that the scaling estimate captures the trend of the permeability curve. Even in this case, the scaling estimate can still be used to predict the transitions that occur in the permeability curve.
The results for the disordered medium are shown in Fig. 7.18. We observe that even in this case, the scaling estimate captures the trend of the permeability curve. Moreover, the estimated permeabilities are of the proper order of magnitude. The interesting observation is that the simple exponential dependence of the hydraulic permeability is very similar to the $\delta_{\text{ran}}(\phi)$ functionality. Our results suggest that the $k(\phi)$ behavior is strongly correlated with that of $\delta(\phi)$. The characteristics of the hydraulic permeability curve can therefore be at least partly explained by that of the fiber-fiber distance as a function of $\phi$.

### 7.4 The permeability of bounded fibrous media

In the previous sections we studied the hydraulic permeability of various fibrous media. We considered the functional behavior of the permeability and the fiber volume fraction for a large range of fiber volume fractions and a wide variety of fibrous media. We compared our results with existing analytical, nu-
7.4 The permeability of bounded fibrous media

Numerical and experimental data. Besides this it is shown that there is a distinct connection between the hydraulic permeability and the distance between the fibers. This connection is explored and used to explain the behavior of the permeability curve as a function of the fiber volume fraction. Although these studies already provide much relevant insight in the physics of fluid flow through fibrous media, we will additionally consider in this section another important aspect related to this topic. It is obvious that all the media studied in the previous section are unbounded. We studied configurations with periodic geometries. However, many fibrous media in practice are bounded. Typical examples are ultra-filtration, gel permeation chromatography and filtration of blood. It is therefore very important to investigate the effect of the wall boundaries on the permeability. In this section, we focus our attention on fibrous media placed between two parallel plates and calculate the $k(\phi)$ behavior as a function of the distance between the parallel plates for ordered and disordered 3D fibrous media. Our aim is to explore the effect of the wall boundaries on the hydraulic permeability and to compare the results with existing data. We therefore first study in section 8.4.1 a bi-periodic array of cylinders and next consider a disordered fibrous media in section 8.4.2.

7.4.1 A bi-periodic array of cylinders

The cell configuration for a bi-periodic array of cylinders is shown in Fig.7.19.

![Bi-periodic array of cylinders diagram](image)

Figure 7.19: A bi-periodic array of cylinders. This cylinder is placed between two parallel plates. $r$ is the radius of the cylinder and $\delta_{sq}$ is the distance between the cylinders and $B$ is the half-distance between the parallel plates.
Figure 7.20: Results for a bi-periodic array of cylinders. The hydraulic permeability as a function of the fiber volume fractions for $B = 2, 3, 5$ and $7$ Brinkman screening lengths.

In this setup a cylinder is placed between two parallel plates, the top and the bottom wall, respectively and the remaining boundaries of the simulation cell are periodic. The flow is directed from left to right. The important parameter here is the half-distance between the parallel plates, $B$, which can be expressed in terms of the Brinkman screening length, $\alpha^{-1}$, defined as $\alpha^{-1} = \sqrt{k}$. As stated in section 8.2, the Brinkman screening length is the typical length scale over which fluctuations decay to the bulk flow. It is therefore the logical choice for the unit length scale in studies aiming to explore the effect of boundaries on the permeability.

We determine the hydraulic permeability as a function of the fiber volume fraction for $B$ varying from 2 to 7 Brinkman screening lengths. The Brinkman screening length is computed using the semi-analytical results of Sangani and Acrivos (see section 8.2 and Ref. [105]).

The results are shown in Fig. 7.20. As expected, we see that the permeability of the bounded cell approaches that of the unbounded configuration as $B$ is increased. Moreover, the rate at which the permeability decreases for a specific
change in $B$, is approximately constant for all the fiber volume fractions. The percent differences between the calculated permeability and the unbounded result are 38%, 47%, 66% and 80% on average for 7, 5, 3, and 2 Brinkman screening lengths respectively. This is consistent with the notion that the bounding walls behave like an effective medium which causes a uniform reduction in $k$ over a large range of fiber volume fractions.

The literature only a few studies reported on bounded fibrous media. The most notable one is the effective medium theory of Tsay and Weinbaum [117]. They solved Brinkman’s equation [3] and derived the following equation for the permeability of bounded fibrous media,

$$k_{\text{bounded}} = k(1 - \frac{\tanh \frac{B}{\alpha^{-1}}}{B/\alpha^{-1}}),\quad (7.13)$$

where $k_{\text{bounded}}$ is the permeability of the bounded medium and $k$ is the permeability of its unbounded instance. This estimate is expected to be only valid in the dilute limit as then the Brinkman approximation is also valid [113].

In Fig. 7.21 we show the permeability as a function of the fiber volume fraction for the case $B = 5\alpha^{-1}$. In this figure we included the analytical result of Tsay and Weinbaum (Eq. 7.13). We observe a good agreement between our results and that of Tsay and Weinbaum for fiber volume fractions smaller than 0.25 (dilute limit). Similar results are found for $B$ is 2, 3 and 7 Brinkman screening lengths (data not shown). This result is important, because it confirms the range of validity of the effective medium theory of Tsay and Weinbaum which is based on several approximations and is not expected to be valid for the entire range of fiber volume fractions as noted above. Based on the connection between the permeability and the fiber-fiber distance that is discussed in the previous section, Clague et al. [114], proposed a new phenomenological estimate for the permeability of bounded media. This estimate is in good agreement with our simulation results and can be used for rapid prediction of the hydraulic permeability of bounded fibrous media (data not shown). For details we refer the interested reader to Ref. [114].

### 7.4.2 Disordered media

The results for the disordered media are shown in Fig. 7.22. To guarantee accurate results we used cylinder radii of 6 lattice points for $\phi < 0.4$, 12 lattice points for $0.4 < \phi < 0.6$ and 18 lattice points. Moreover, we performed on the order of 5 simulations for each fiber volume fraction, because in this case the bounded medium is heterogeneous due to the disorder of the medium and the relatively small simulation cell dimensions. It is clear that for the disordered medium the effect of the walls is stronger compared to the ordered case. For example, for $B = 5\alpha^{-1}$, at $\phi = 0.2$ there is a 61% difference between the calculated result
and the unbounded results. For $\phi > 0.2$, the percent difference relative to the unbounded result is approximately 75% on average. Also, unlike the ordered media, the slope in the calculated hydraulic permeabilities steepens as $B$ is reduced below 4 Brinkman screening lengths. The transition between the dilute and the intermediate regions, however, appears to occur at similar fiber volume fraction, $\phi \approx 0.2$.

Finally, we compare the hydraulic permeabilities calculated using the Lattice-Boltzmann method with the Brinkman approximation given in Eq. 7.13 (see Fig. 7.23). In this particular system, the wall to mid-plane separation, $B$, equals $5\alpha^{-1}$. The unbounded hydraulic permeabilities used in Eq. 7.13 are taken from our Lattice-Boltzmann result for the associated unbounded, disordered media presented in section 8.2 (disordered media II). In this case, it is evident that the effective medium theory of Tsay and Weinbaum [117], overpredicts the hydraulic permeabilities calculated using the LB method. Furthermore, for higher fiber volume fractions, the difference between the effective medium
7.5 Conclusions

We used the lattice-Boltzmann method on a massively parallel computer to solve the permeability of several ordered and disordered models of fibrous media. The simulations have been performed as a function of the fiber volume fraction of the media in a large range. The simulated results were found to be

theory of Tsay and Weinbaum [117] and hydraulic permeabilities calculated using the LB method is higher compared to the dilute limit. Similar behavior is observed for systems where \( B = 2 \) and \( 7 \) Brinkman screening lengths as well. As we mentioned in the previous section, Clague et al. [114], proposed a new phenomenological estimate for the permeability of bounded media, based on the connection between the permeability and the fiber-fiber distance. This estimate is also in the case of bounded disordered media in good agreement with the simulation results and can be used for rapid prediction of the hydraulic permeability of bounded fibrous media (data not shown). For details we refer the interested reader to Ref. [114].

Figure 7.22: Results for the disordered medium II. The hydraulic permeability as a function of the fiber volume fractions for \( B = 2, 5 \) and \( 7 \) Brinkman screening lengths.
in excellent agreement with available analytical, numerical and experimental data. Our results suggest an exponential dependence of permeability on fiber volume fraction in a wide range and this functionality seems to be a generic feature of fibrous porous materials, independent of whether they are random or not.

It was argued that there is a correlation between the hydraulic permeability and the distance between the fibers. This correlation was further explored and used as a possible explanation of the behavior of the hydraulic permeability as a function of the fiber volume fraction.

Finally the effect of walls on the hydraulic permeability was investigated. For various wall separation distances the hydraulic permeability is computed for a bi-periodic array of cylinders and a disordered medium as a function of the fiber volume fraction. These results were compared with the effective medium theory of Tsay and Weinbaum [117]. In the dilute limit $\phi < 0.25$ a reasonably good agreement was found for bounded ordered media. For higher fiber volume fraction the effective medium theory of Tsay and Weinbaum [117] over predicts
the permeability. Moreover, for the same wall separation distances the effect of
the walls is found to be stronger in the case of disordered media and the effective
medium theory overpredicts the hydraulic permeability.

Chapter 8

General discussion

In this thesis we studied several aspects of the lattice-Boltzmann method. In
deed, we demonstrated that the lattice Boltzmann method is a useful technique for the numerical simulation of fluid flow in complex geometries. Briefly
stated, several new ideas have been presented useful for efficient and accurate
lattice-Boltzmann simulations. These include an extension of these newly used
translatory and 3D models, generalization of lattice-Boltzmann variables, incorporating a new technique to reduce the number of time steps to
achieve stationary solutions, and generalization to the lattice-Boltzmann method at rest. Moreover, we studied the benchmark case of the large oscillation
method. Finally, the transport properties of some models of disordered
random media have been studied in detail. We compared the lattice-Boltzmann results with existing experimental and numerical data and made a direct comparison between the results obtained with the lattice-Boltzmann method and the geometry of the media. The conclusions we stated at the end of each chapter and also be found in the summary of the thesis.

In this chapter, we believe that some interesting ideas have appeared as
search topics to be studied in the near future. To this end we have summarized the recent developments of this field.

The lattice-Boltzmann method is a powerful tool in the simulation of complex fluids and in the extension of lattice-Boltzmann models to new
applications. Nevertheless, there are several fundamental issues that need to be
addressed. The following suggestions are quite natural steps to progress:

1. Application of different formulations of LBM to more-realistic criteria in
   address three-dimensional problems. In recent years, several studies have
   been reported for extending the lattice-Boltzmann model to realistic and
   more-realistic criteria. All these efforts including those reviewed are the
to applied to rather simple geometries. The challenge now is to apply these
techniques to realistic effect. Important issues like, prin type, active media,
Hydraulic Permeability of Fibrous Media

Figure 7.23: Results for disordered medium II. The hydraulic permeability as a function of the fiber volume fractions for $\theta = 3$ Brinkman screening lengths. The effective medium theory result of Gao and Weinbaum [117] is also included in the figure.

In excellent agreement with available analytical, numerical and experimental data, our results suggest an exponential dependence of permeability on fiber volume fraction in a wide range and this functionality seems to be a generic feature of fibrous porous materials, independent of whether they are random or not.

It was argued that there is a correlation between the hydraulic permeability and the distance between the fibers. This correlation was further explored and used as a possible explanation of the behavior of the hydraulic permeability as a function of the fiber volume fraction.

Finally, the effect of scale on the hydraulic permeability was investigated. For various well-arranged disordered, the hydraulic permeability is computed for a periodic array of cylinders and a disordered medium as a function of the fiber volume fraction. These results were compared with the effective medium theory of Gao and Weinbaum [117]. At the dipole length $\theta = 0.25$, a reasonably good agreement was found for selected ordered media. For higher fiber volume fractions, the effective medium theory of Gao and Weinbaum [117] over predicts