
by

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Abstract

The study of fluid flow in porous media is important in many fields from oil recovery and carbon sequestration to fuel cells. An important area still under investigation is the relationship between the porous microstructure and the permeability of a material since accurate permeability estimations are required for predictive continuum models of flow and mass transport through porous media. Tortuosity is another important parameter used in continuous permeability relationships to relate permeability to porosity and other microstructural properties of porous media such as pore connectivity. The focus of this research is to provide foundational tools to characterize porous media flow transport properties such as permeability and tortuosity. To achieve this goal, this thesis is divided into two parts: First, a numerical-based approach (lattice-Boltzmann model) was developed in-house to simulate fluid flow in porous media. This numerical tool was used to determine the permeability of two structured simulated porous domains. The lattice-Boltzmann model was also used in a stochastic model to investigate the impact of the geometric properties of the grains (such as grain aspect ratio) on the tortuosity-porosity relationships in porous media. In the second part, an analytical approach was proposed and used to investigate the tortuosity-porosity relationships in fractal geometries.
From the permeability study, it was found that the predictability of the Kozeny-Carman equation (a commonly-used permeability relationship) can be improved with a modified KC parameter that is an algebraic function of porosity. From the numerical stochastic tortuosity study, it was found that tortuosity exhibits an inverse relationship with the porosity that can be expressed in logarithmic form. Furthermore, the adjusting parameters ($a$ and $b$) were calculated in the tortuosity-porosity correlation of $\tau = a - b \ln(\phi)$. It was found that tortuosity increases with increasing grain aspect ratio. From the analytical tortuosity study, it was found that the analytical tortuosity-porosity relationships in the studied fractal geometries are linear and the tortuosity has an upper bound at the limiting porosity ($\phi = 0$ for the Sierpinski carpet). These tools and observations provide the capability for predicting continuous permeability and tortuosity correlations that can be used in large-scale continuum modelling of fluid flow in porous media.
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1 Introduction

1.1 Background and Motivation

Characterizing the flow and transport properties in porous media is a critical component for addressing problems in many areas of engineering and science, such as groundwater hydrology [1], oil and gas recovery [2], carbon sequestration [3], membrane separations [4] as in fuel cells [5], etc. These varied applications cover a vast range of length scales from the kilometer scale in oil and gas recovery to the centimeter and millimetre scales in membrane separations or to the micron scale for micro-fluidic devices. All these processes are, however, ultimately governed by pore-scale phenomena, which occur at the scales of microns. Figure 1.1 illustrates a carbon sequestration process in a saline aquifer-based reservoir and the disparity that exists between the length scales.

Figure 1.1 Schematic of a carbon sequestration process and the substantial disparity among the length scales.

In the carbon sequestration process shown above, saline aquifers are geological porous formations that are saturated with brine and can extend over tens of kilometers. Cap rocks are formations with low permeabilities situated at the top of the storage zone and hinder the upward migration of the injected CO\textsubscript{2}. Due to buoyancy forces, the injected CO\textsubscript{2} can travel upwards up to tens of meters before reaching the cap rock. Therefore, modelling of reservoirs such as the one
shown above, would involve simulations of large porous domains. It should be noted that the fluid flow simulations in such domains are ultimately affected by the pore-scale features of the formations.

Such a significant difference in length scales makes the simultaneous solution of macroscopic and microscopic numerical modelling of porous media highly challenging. Therefore, at the continuum scale (i.e. macroscopic) a porous material is typically assumed to be a homogeneous material described by spatially averaged properties. Such spatially averaged properties are highly dependent on the pore-scale structure of the porous formations. Therefore, a relationship describing this dependence is required for macroscopic simulations. Such relationships can be obtained through pore-scale investigations. Pore-scale investigations usually fall within one of the following three categories: analytical, numerical, and experimental, each of which will be further discussed and compared in this thesis.

A key goal of pore-scale studies is to relate a variety of structural properties (e.g. porosity) of porous materials to flow and transport properties (e.g. permeability and tortuosity) through macroscopic relationships. These relationships can then be used in continuum-scale modelling of porous formations (e.g. oil reservoirs, etc).

1.2 Permeability

The permeability ($K$) of a porous medium is a measure of its hydraulic conductivity towards fluid flow through its pore space when subjected to an external driving force (pressure gradient).

1.2.1 Significance of Permeability Relationships

The relationship between permeability and the microstructure of a porous material is an essential relationship, as it impacts fluid transport within the porous medium according to the Darcy’s law [6,7] or some more advanced models [8,9]. Therefore, it can influence the efficiency of any flow processes. Such permeability relationships are important for a wide range of applications ranging from resin transfer moulding [10,11], biomedical engineering [12,13], recovery of oil
and gas and groundwater treatment [14,15], to filter separation modelling [16,17], and fuel cell simulations [5,18].

For example, permeability relationships are critical in the oil and gas industry as an accurate estimate of this property is needed to effectively evaluate and exploit potential resources [19]. The permeability of an oil or gas reservoir is important, for example, when determining optimal injection rates or production rates. Permeability predictions are similarly important in carbon sequestration as high-permeability sandstones provide desirable capacity for carbon dioxide (CO$_2$) storage, while low-permeability cap rocks above the storage sites are needed to confine injected supercritical CO$_2$ [20]. Permeability relationships are also important for studying the subsurface flow of water. For example, for soil to be suitable for agricultural use, it must have sufficiently high permeability to prevent waterlogging. On the other hand, it must have a sufficiently low permeability to retain moisture and thus foster plant growth. Therefore, thorough investigations of permeability relationships are required [21-25] for accurate modelling of the flow transport in any of the above situations.

It should be mentioned that macroscopic approaches to fluid flow simulation in porous media use Darcy’s law [6,7] or more complicated models [8,9]. These macroscopic (continuum-scale) approaches require permeability as an input parameter, but permeability can vary within the porous media. Therefore, spatially-averaged continuous permeability relationships that correlate permeability with pore-scale properties such as porosity are needed for macroscopic flow simulations.

1.2.2 Darcy’s Law

Permeability is one of the most common transport properties of porous materials, and it was first introduced by Darcy in 1856 [7]. Darcy noticed that for laminar flow through saturated porous media, the flow rate ($\langle u \rangle$) is linearly proportional to the applied pressure gradient ($\frac{dp}{dx}$). He introduced permeability as part of the proportionality constant in Darcy’s law given below:

$$\langle u \rangle = -\frac{k}{\mu} \frac{dp}{dx},$$

(1.1)

where $\mu$ and $K$ are dynamic viscosity of the working fluid and the permeability of the porous
medium, respectively. It has been shown by numerous experimental investigations [6,8] that if the flow rate through a porous medium is raised, pressure drop becomes no longer proportional to fluid velocity. It is generally admitted that this deviation from Darcy’s law with increasing fluid velocity is due to a more prominent role of inertial forces. It must be emphasized that, although inertial forces dominate viscous forces in turbulent flow, caution must be taken not to identify a deviation from Darcy’s law with the onset of turbulence. Turbulence occurs at $Re$ values at least one order of magnitude higher than the $Re$ at which deviation from Darcy’s law occurs. In other words, the flow can be laminar but do not comply with Darcy’s law.

### 1.2.3 Methods of Permeability Calculations

Bulk transport properties such as permeability can be quantified by a variety of methods: experimental, analytical, and numerical.

Most experimental methods of permeability prediction involve the application of a constant pressure gradient across the porous medium from which the average flow velocity is determined from the measured fluid flow-rate. The permeability of the medium is subsequently determined using Darcy’s law [7]. Many of the earlier studies of permeability in porous media were conducted experimentally [26-29] including the first work by Darcy in 1856 [7]. Figure 1.2 shows a schematic of Darcy’s experimental setup, which has been the basis for many permeability-related experimental studies since.
In analytical methods, the general approach is to represent the porous medium with an idealized structure and then to solve the Stokes equations, or similar equations, for a particular structure. For example, fibrous porous materials can be idealized as matrices of rods (structured geometries). For such porous materials, analytical methods can be divided into three categories depending on the structure of the matrix and the flow direction: (i) flow parallel to an array of parallel rods [30-34], (ii) flow normal to an array of parallel rods [32,35-37], and (iii) flow through three-dimensional (3D) arrays [38,39].

Permeability predictions can also be conducted numerically. In principle, if the structure of a medium is known, one can compute the permeability of the medium by solving the Navier-Stokes or Boltzmann equations, which describe the fluid flow through the medium. Once the steady-state velocity field is calculated for a given pressure gradient, the permeability can be determined using Darcy’s law [7]. For example, Koponen et al. [40] used the lattice-Boltzmann modelling (LBM) to calculate the permeability of a random 3D fibre web as a function of its porosity. Pinela et al. [41] used a commercial finite-volume-based program, FLUENT to solve Navier-Stokes equations and to calculate the permeability of porous structures composed of regularly placed overlapping solid circles with constant radius in the porosity range of $\phi \in$
A detailed description on a numerical approach (LBM) for permeability prediction is provided in Chapter 2.

1.3 Tortuosity

Tortuosity is a measure of complexity of porous media structures and can often be realized as elongation of streamlines (hydraulic tortuosity):

\[
\tau = \frac{\langle L_h \rangle}{L_s},
\]

where \(L_s\) is the straight-line length across the porous medium in the direction of the macroscopic flow direction and \(\langle L_h \rangle\) is the average effective flow path length taken by the fluid (average length of particle pathways). The concept of tortuosity was first introduced by Carman in 1937 [42] to match the analytical permeability results, calculated based on the primitive bundle of capillary tubes model, to experimental data. Tortuosity is still used in (more advanced) continuous permeability relationships to relate permeability to porosity and other pore-scale properties of porous media such as pore connectivity, etc [43]. Tortuosity, in addition to being used in permeability relationships, has other practical significances. For instance, in the context of carbon sequestration, it has been found that rock formations with high tortuosities can trap more CO\(_2\) than less tortuous formations, through a process called residual trapping [21]. Additionally, due to the increased interfacial area between CO\(_2\) and water in more tortuous formations, dissolution rates are increased [22]. Such practical significances of tortuosity in addition to its role in relating permeability to porosity have made tortuosity an important parameter to be investigated.

Tortuosity can be used to characterize various aspects of porous media for example, their hydraulic or electrical conductivity. Therefore, depending on their application and the method of determination [44], there are several tortuosity definitions [44-49]: geometric, hydraulic, electrical, and diffusive. These several tortuosity definitions along with their variances and common applications will be discussed more thoroughly in Chapter 3.
Constitutive tortuosity models can be produced in a variety of ways: Experimental [50-52], numerical [47,53-56] and analytical [57,58]. A more detailed discussion of tortuosity calculations is provided in Chapters 3 and 4.

1.4 Fractals

Naturally-occurring porous media, such as sedimentary rock, rarely consist of mono-sized particles, but rather tend to consist of large distributions of particle sizes (poorly-sorted porous media). Nonetheless, most investigations of tortuosity in the literature (including our studies in Chapters 2 and 3) involve porous media consisting of mono-sized (same-sized) particles, such as the analytical studies by Yun et al. [59], Yu & Li [60], and Jian-Long et al. [61] or the numerical studies by Koponen et al. [53,54] and Matyka et al. [47]. Figure 1.3 shows a structured and a stochastic representation of porous media with mono-sized particles.

![Figure 1.3 Porous media composed of mono-sized spherical particles: (a) structured, (b) stochastic.](image)

One way to represent the porous media with complex and large distribution of particle sizes is to use fractals [62-66]. Katz and Thompson [64] are among the first investigators who presented experimental evidence indicating that the pore spaces in a set of sandstone samples conform to fractal geometries.
In this thesis, fractal geometries were used to provide insight into poorly-sorted porous media, and a novel analytical approach was presented and applied to characterize tortuosity-porosity relationships in such geometries. A detailed review of the applied analytical approach and the fractal geometries are presented in Chapter 4.

1.5 Research Gap

The three topics mentioned above: permeability, tortuosity, and the concept of fractals in porous materials have proven highly useful for understanding flows in porous media; however, in particular, there are some gaps that have not been addressed in the literature.

a) Existing continuous permeability-porosity relationships are not predictive. One such relationship is the commonly-used semi-empirical Kozeny-Carman (KC) equation that features a material-specific fitting parameter, $C_{KC}$, which is generally treated as a constant coefficient. In this work, the predictability of this relationship was improved by proposing a modified functional form for $C_{KC}$. Details of this contribution are discussed in Chapter 2.

b) The impact of micro-scale geometric properties of the individual grains (such as grain aspect ratio) on the tortuosity-porosity relationships has not been extensively studied. In this thesis, it was shown that the grain aspect ratio in 2D porous media composed of rectangular grains impacts the adjusting parameters in the previously reported logarithmic tortuosity-porosity correlation, $\tau = a - b \ln(\phi)$. Separate tortuosity-porosity relationships were calculated for each of the three grain aspect ratios. Details related to this study are covered in Chapter 3.

c) The Sierpinski carpet is a commonly used fractal [67-69] with a long history of application to natural porous media [70,71] and has been frequently used for analytical studies of flow in porous media. However, to the best of author’s knowledge, there is only one analytical work [67] that has studied the tortuosity-porosity relationship in such structure. In this thesis, a novel analytical approach was proposed that led to a markedly different trend for the Sierpinski carpet tortuosity-porosity relationship presented by the previous analytical work [67]. A tortuosity-porosity correlation for a circular-based Sierpinski carpet was also
obtained. The tortuosity obtained from both geometries exhibited linear relationships that was is in agreement with the trend proposed by previous numerical [53] and experimental works [69].

1.6 Contributions

My thesis is focused on the characterization of flow transport properties such as permeability and tortuosity within porous media. This involved the development of a single-relaxation time (SRT) LB model to calculate permeability. Furthermore, a multiple-relaxation time (MRT) lattice-Boltzmann (LB) model and an analytical approach were developed to calculate tortuosity within various porous media.

My contributions are as follows:

- Improved permeability predictability of KC equation by calculating new KC parameters for two simulated porous structures: periodic arrays of a) staggered parallel infinite cylinders and b) spheres. The proposed KC parameters ($C_{KC}$) are functions of porosity to ensure permeability estimation improvement for a wide range of porosity:

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- Performed a parametric study on the impact of grain aspect ratio on the tortuosity-porosity relationships of two-dimensional (2D) porous media composed of rectangular particles. Separate tortuosity-porosity relationships were presented for each grain aspect ratio by calculating the adjusting parameters in the previously reported tortuosity-porosity correlation, $\tau = a - b \ln(\phi)$

  Submitted as: A. Ebrahimi Khabbazi, J. Hinebaugh and A. Bazylak. Determining the impact of rectangular grain aspect ratio on tortuosity-porosity correlations of two-dimensional stochastically generated porous media, Physics of Fluids (Submitted in June 2015)
Investigated the relationships between tortuosity and porosity within two deterministic fractal geometries by presenting and applying a novel mathematical approach on a deterministic Sierpinski carpet and a slightly altered version of the Sierpinski carpet with a generator that has a circular inclusion.


My PhD research also resulted in several conference contributions [72-76].

1.7 Organization of the Thesis

This thesis is organized into five chapters. The introductory background and motivations are presented in Chapter 1, along with an overview of the contributions of the thesis. Chapter 2 is focused on permeability predictions through numerical modelling (SRT LBM). A detailed description of the SRT LBM is also presented. New functional forms of KC parameter ($C_{KC}$) are determined for the two porous structures of: periodic arrays of a) staggered parallel infinite cylinders and b) spheres. Chapter 3 is focused on tortuosity calculations through numerical modelling (MRT LBM). The impact of the geometric properties of the individual grains, (such as grain aspect ratio) on the tortuosity-porosity relationships in porous media using stochastic numerical modelling is investigated. This impact is quantified by fitting our tortuosity data to the previously reported logarithmic tortuosity-porosity correlation, $\tau = a - b \ln(\phi)$ and calculating new adjusting parameters. As a result, spatially-averaged continuous tortuosity-porosity relationships are provided for 2D stochastically generated porous media composed of rectangular grains with distinct aspect ratios. The minimum number of required stochastic simulations is determined in each case. Chapter 4 is focused on analytical calculation of tortuosity in two deterministic fractals (a Sierpinski carpet and a circular-based Sierpinski carpet). A novel mathematical approach for calculating tortuosity is presented in this chapter. Conclusions and a road map for future work are provided in Chapter 5.
2 Developing a New Form of the Kozeny-Carman Parameter for Structured Porous Media through Lattice-Boltzmann Modelling

2.1 Abstract

The semi-empirical Kozeny-Carman (KC) equation is a commonly-used relationship for determining permeability as a function of porosity for granular porous materials. This model features a material-specific fitting parameter, $C_{KC}$, which is generally treated as a constant coefficient. Recent studies, however, have shown that $C_{KC}$ is not constant and could be a varying function of porosity. LBM was used to calculate the absolute permeability of two simulated porous structures: periodic arrays of a) staggered parallel infinite cylinders and b) spheres. Various functional forms of $C_{KC}$ was then identified and for each form, a regression analysis was performed in order to fit the function to the permeability values determined from the LB simulations. From this analysis, optimal fitting parameters were extracted for each function that minimized the error between permeability values obtained from the KC model and the LB simulations. All linear and non-linear functional forms proposed in this work improve the predictability of the KC model. An algebraic function for $C_{KC}$ provided the most accurate prediction of the KC porosity-permeability relationship for the geometries examined.

2.2 Introduction

The study of flow in porous media is of crucial importance in many fields, including geophysics and soil science [3,77-81]. An important area still under investigation is the relationship between the porous microstructure and the permeability of a material [82-84]. This is an essential relationship, as it impacts fluid transport within the porous medium and can influence the efficiency of any flow process. For example, in carbon sequestration, high-permeability sandstones provide desirable capacity for carbon dioxide (CO$_2$) storage, while low-permeability cap rocks above the storage sites are needed to confine injected supercritical CO$_2$ [20]; therefore

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a thorough investigation of permeability is required [21-25].

There is a direct relationship between permeability and porosity of porous media [42,85-87]. The empirical Kozeny-Carman (KC) model [88] is a permeability-porosity relationship for granular porous media (Equation 2.1) that is commonly used to estimate permeability values for the modelling of fluid flow in various porous materials [62,63,89]. It has the form of:

$$ K = \frac{1}{C_{KC}} \cdot \frac{\phi^3}{S^2 \tau^2}, $$

(2.1)

where $\phi$ is the porosity, $S$ is the specific surface area, $\tau$ is the tortuosity, and $C_{KC}$ is the Kozeny-Carman constant (an empirical parameter). $C_{KC}$ is material dependent and accounts for variations in permeability between porous materials having the same porosity, but varying microstructures. However, this model has many limitations, which have been addressed with a variety of modifications, as summarized in a review by Xu and Yu [85]. For instance, the limitation of the KC model in estimating permeability at low porosities has been improved by Mavko and Nur [89]. To address the same limitation, Bourbiè et al. [90] suggested a variable porosity power law, which improved the permeability estimation at low porosities. Their model had the form $K = C \phi^n d^2$ where $n$ depends on porosity, with $n = 3$ for high porosities ($\phi \gg 0.3$) and $n \approx 8$ for low porosities ($\phi < 0.05$), where $C$ is a fitted permeability factor, and $d$ is the characteristic length. Panda and Lake [43] included the particle size distribution in the model, and Koponen et al. [54] used the effective permeability to improve the permeability prediction accuracy of the KC model. In addition, recent studies have revealed that $C_{KC}$ is, in fact, not constant and can instead vary with porosity, even for the same material [85].

Increasing the accuracy of $C_{KC}$ can further improve the accuracy of the KC model for predicting transport properties in porous materials. However, using a bulk permeability value to model flow within large-scale porous material should be approached with caution. This is due to the structural heterogeneity inherent in most porous materials, such that the volume-averaged porosity varies from region to region [91,92]. Pore-scale flow patterns are determined, in part, by the local microstructure, which in turn affects the macroscopic permeability. As a result, the accuracy of large-scale transport models of porous media (such as geologic reservoirs) can be improved with information from pore-scale flow analysis. However, multi-scale modelling that includes simultaneous resolution of reservoir and pore-length scales is computationally complex.
and expensive. Experimental determination of local permeability values can be expensive and time-consuming, and assigning an accurate universal permeability function to a particular class of porous materials remains a challenge. An alternative approach is to numerically simulate fluid transport at the microscale and use the results to inform appropriately partitioned simulations at the reservoir-scale.

A variety of numerical schemes are available for simulating flow in porous media at short length scales [93-96]. These include pore-network modelling (PNM), Navier-Stokes (NS) based computational fluid dynamics (CFD) techniques, and LBM. PNMs have attractive features (computational efficiency and capability of handling large domain sizes), but it is difficult to produce a topologically-equivalent network for certain classes of rocks with this method [25]. Another drawback of PNM includes the inability to resolve the velocity and concentration gradients within a single pore. CFD and LBM both can be employed to resolve the in-pore gradients; however, they differ from each other in various aspects. Some major differences are as follows:

- **NS equations** are second-order partial differential equations (PDEs); however, Boltzmann equation (LBE) is derived from a first order PDE, i.e. the Boltzmann equation.
- The convection operator of the NS equations is a nonlinear term, where all the terms of the LBE are linear due to the lattice Bhatnagar–Gross–Krook (BGK) simple collision operator.
- In the LBM, pressure is calculated using an algebraic equation of state, while CFD solvers for the incompressible NS equations need to solve the Poisson equation for the pressure, which is an elliptic second order PDE and involves global data communication. In contrast, data communication in LBM is always local which, which makes the LBM highly parallelizable. Only adjacent lattice nodes are considered for the computation of local distribution functions [97,98].

Significant advancements have been made through the application of LBM in the study of transport in porous media, specifically in areas such as single-phase flow in reconstructed porous domains [99], modelling of evaporation [100], binary fluid flows [101], heat transfer [102,103] and multiphase flows [104-107].
In this investigation, a novel methodology for rapidly and accurately evaluating various forms of the KC equation and its parameter, $C_{KC}$, is presented and demonstrated through LBM of fluid flow within two geometries: $i$) a staggered array of infinite parallel cylinders and $ii$) a periodic array of spheres. The work presented here provides a valuable method for obtaining permeability-porosity relationships needed for informing coupled mass and momentum equations, such as the Brinkman equation solution in reservoir-scale modelling [108].

2.3 Numerical Method

2.3.1 Lattice-Boltzmann Modelling

In this study, a single-relaxation time (SRT) LBM was employed to simulate single phase flow in porous geometries, which includes a 2D representation of a staggered array of parallel fibres and a 3D representation of a body-centred cubic (BCC) array of spheres. These geometries have been broadly studied in the literature [36,37,87], providing opportunities for validation for this methodology. The approach presented here can be applied to representative elementary volumes at the pore scale to inform reservoir scale modelling. The SRT LBM consists of a discretized Boltzmann equation to approximate the compressible NS equations in the nearly-incompressible limit [109]. For the discretization to be accurate, a low Mach number condition must be satisfied [110,111], as is the case here ($Ma \approx 10^{-5}$).

The LB method involves an iterative sequence of propagations and collisions of fictitious particles at the lattice nodes of a discretized domain. The mass density of each non-solid node is defined by a set of scalar particle distribution functions (PDF; $f$ in Equation 2.2, below), each of which is related to a lattice velocity unit vector. At each time step, the PDFs are shifted to neighboring nodes according to their unit velocity vector through the propagation process (also known as streaming). Following each streaming step, a collision step is performed, whereby the value of each PDF is updated by applying an algebraic collision operator. In its simplest form, the collision operator is based on the BGK approximation [112].

Streaming and collision of the fictitious particles are encapsulated in the LB equation, as shown
in Equation 2.2 [113]:

\[
f_i(\vec{x} + c_i \vec{e}_i \Delta t, t + \Delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau_R} \left[f_i(\vec{x}, t) - f_{ieq}(\vec{x}, t)\right],
\]

(2.2)

where \( c_i = \frac{\Delta x}{\Delta t} \) is the magnitudes of discrete lattice velocities, \( \Delta x \) is the lattice spacing, and \( \Delta t \) represents the time step in lattice units (equal to unity here). \( \tau_R \) is the dimensionless relaxation time, \( e_i \) are the velocity basis vectors, and \( f_i \) is the probability distribution function. \( f_{ieq} \) is the corresponding equilibrium distribution function, given by Equation 2.3 [114]:

\[
f_i^{eq} = \rho w_i \left[ 1 + \frac{3}{e^2} e_i \vec{u} + \frac{9}{2 e^4} (e_i \vec{u})^2 - \frac{3}{2 e^2} \vec{u} \cdot \vec{u} \right],
\]

(2.3)

where \( \vec{u} \) denotes the velocity field, \( \rho \) represents the density in lattice units, and \( w_i \) are the weight coefficients. The corresponding equilibrium distribution is a low Mach-number truncated Maxwell-Boltzmann distribution [115]. In Equation 2.2, the left-hand side represents the streaming step, wherein the PDFs are shifted based on their velocities, and the right-hand side describes the collision operator. In this study, the D2Q9 model (two dimensions with nine directional velocities; Figure 2.1) was used for 2D simulations and D3Q19 for 3D modelling [114]. For the D2Q9 lattice, \( w_i = \frac{1}{9}, \frac{4}{9} \) and \( \frac{1}{36} \), whereas for D3Q19, \( w_i = \frac{1}{3}, \frac{1}{18} \) and \( \frac{1}{36} \) in Equation 2.3.

![Figure 2.1 Schematic of the D2Q9 lattice employed to discretize the computational domain.](image)

Macroscopic quantities such as density, velocity, and pressure can be determined from the distribution function \( f_i(\vec{x}, t) \) [98]:

\[
\rho = \sum_i f_i,
\]

(2.4-a)

\[
\rho \vec{u} = \sum_i e_i f_i,
\]

(2.4-b)

\[
P = \rho c_s^2,
\]

(2.4-c)

where \( c_s \) denotes the speed of sound in lattice units (equal to \( 1/\sqrt{3} \)), and \( P \) denotes the pressure.
The kinematic viscosity \( \nu \) is given by:

\[
\nu = \delta x^2 \frac{\partial \nu_l}{\partial t},
\]

where \( \nu_l \) is the kinematic viscosity in lattice units, \( \nu_l = (\tau_R - 0.5) c_s^2 \) [98].

### 2.3.2 Permeability Calculations

The numerical model of fluid flow within a porous material can be used in combination with Darcy’s law (Equation 2.6) to calculate permeability of the porous medium of interest.

\[
\langle u \rangle = -\frac{K}{\mu} \nabla P,
\]

where \( \langle u \rangle \) denotes the volume-averaged flow velocity, \( K \) is the permeability of the porous medium under investigation, \( \mu \) is the dynamic viscosity of the fluid, and \( \nabla P \) represents the pressure gradient vector. To avoid inaccuracies due to eddies, Darcy’s law is only accurate in the limit of viscous (or creeping) flow (pore-scale Reynolds numbers \( Re < 1 \)) [116]. \( Re < 0.1 \) for all the simulations presented here. All computations were performed in MATLAB (R2010b).

### 2.3.3 Model Validation

To determine appropriate grid spacing, a mesh-refinement study was performed on the 2D fibrous geometry. The ideal lattice spacing was determined to be 144 lattices nodes in each direction (length and width) for the range of fibre radii studied (30-165 \( \mu m \)). The numerical model was then validated with Gebart’s analytical solution for permeability of a quadratic (square) fibre arrangement (Figure 2.2), assuming parabolic flow.

![Figure 2.2 Computational domain employed for validation: (a) Schematic of quadratic fibre distribution in the geometry used by Gebart [87]. (b) Schematic of unit cell.](image-url)
Gebart performed a combined theoretical, numerical, and experimental study of the permeability of ordered arrays of fibres and presented the following permeability-porosity relationship in the limit of closed-packed fibres [87,117]:

\[
\frac{K}{R^2} = C_G \left( \sqrt{\frac{1-\phi_c}{1-\phi}} - 1 \right)^{\frac{5}{2}},
\]

(2.7)

where \( R \) is the fibre radius (\( \frac{K}{R^2} \) is the non-dimensionalized permeability), \( \phi \) is the porosity, and \( \phi_c \) is the critical porosity below which flow does not occur (i.e. percolation threshold). \( C_G \) is a proportionality constant, also known as the geometric factor, which Gerbart calculated to be \( C_G = \frac{16}{9\pi\sqrt{2}} \) for the quadratic fibre arrangement. Gebart showed that the analytically-determined permeability was in agreement with a finite difference solution of the NS equations, for porosity values up to 0.65. To facilitate our numerical validation, the geometric factor and critical porosity employed by Gebart was used: \( C_G = \frac{16}{9\pi\sqrt{2}} \) and \( \phi_c = 1 - \frac{\pi}{4} \) [87].

### 2.3.4 Geometry

Transport phenomena in some structures can be efficiently modelled in 2D with significant computational savings and without compromising accuracy. Perpendicular flow over arrays of infinite parallel fibres is an example of a 2D simulation that is representative of the 3D case. There are, however, situations where 3D modelling is required, such as when the geometry and flow fields are not symmetric. In this study, two separate geometries were investigated: a) a staggered array of parallel fibres (2D), and b) a 3D BCC array of spheres, which cannot be accurately modelled in 2D.

The staggered array of parallel fibres were represented by a 2D domain consisting of staggered arrays of identical disks with radius, \( R \), (Figure 2.3(a)). The fibres are arranged in a periodic pattern so that only a single unit cell with periodic boundary conditions is required (Figure 2.3(b)).
Figure 2.3 Schematic of the staggered parallel fibre geometry: (a) Cross-section of fibres (black) and void space (white) and (b) a unit cell (computational domain). The pixilation observed in this figure is representative of the numerical resolution of the computational domain.

The size of the computational domain was chosen to be $480 \, \mu m$ in both length and width. The centre-to-centre distance between two adjacent solid circles was constant over the domain and set to $340 \, \mu m$. This was the same characteristic length employed by Kang et al. [118] in their pore-scale study of reactive transport involved in geologic CO$_2$ sequestration. The same characteristic length has also been employed here in order to facilitate future comparison with the above-mentioned study. Porosities were varied by changing the radius of the fibres. To remain consistent with the 2D structure, the size of the 3D domain (Figure 2.4) was also set to $480\mu m \times 480\mu m \times 480\mu m$. 
2.3.5 Model Assumptions and Boundary Conditions

The underlying motivation for this work is to determine the permeability of deep saline aquifers for CO₂ sequestration, where CO₂ is injected into geological porous formations. One method of CO₂ sequestration entitled “surface dissolution” involves the CO₂ saturation of extracted brine, followed by the injection of the saturated solution into geological formations. In this work, a CO₂-saturated brine solution at 65°C with a salinity of 85000 ppm (NaCl) was modelled [119]. Despite this assumption, the results presented are general, since the Reynolds number is sufficiently low ($Re \ll 1$). In these conditions, permeability is found to be independent of the fluid properties such as, viscosity, density and pressure gradient [116]. A density of 1.041 g/cm³ and a dynamic viscosity of 0.6025 cP were employed. To generate creeping flow, a constant pressure gradient boundary condition of 0.19 Pa was imposed between the inlet and outlet. Periodic and bounce-back boundary conditions were employed at the side boundaries and the surface of the solid materials, respectively. The bounce-back scheme, equivalent to the no-slip boundary condition, was implemented via the direct reflection of fictitious particles impacting a solid boundary [120].

Care must be exercised when using SRT LBM, as the permeability of the porous medium could
become unrealistically dependent on the kinematic viscosity, $\nu$ [121]. Since the kinematic viscosity is a function of the relaxation time, $\tau_R$, (Equation 2.5), an informed choice of $\tau_R$ is essential. By selecting a suitable $\tau_R$ value, the $\tau_R$ dependence in SRT LBM simulations can be alleviated. Note that a $\tau_R$ value that is too low can lead to non-physical system properties, whereas if it is too high, the system will not converge. Pan et al. [93] reported that the results obtained using SRT LBM are less dependent on the relaxation time for $\tau_R$ near unity. Therefore, in this study, the relaxation time was set to 1. It should be noted that a multiple-relaxation time approach (MRT) may be employed to mitigate this problem [122]. This method is more robust than the SRT method, but comes at the cost of increased complexity.

To ensure that the simulation of a single unit cell is an appropriate choice for the computational domain, various domain sizes were examined. It was found that the permeability calculated from a single unit cell with periodic boundary conditions is identical to that calculated for larger domains consisting of up to five unit cells, in both the horizontal and vertical directions. Based on this result, simulations were carried out on a single unit cell throughout this study.

Figure 2.5 shows the LBM-derived velocity field distribution within the porous media with a staggered array of infinite parallel cylinders previously employed by Gebart [87]. The velocity distribution calculated here demonstrates the ability of LBM to resolve gradients at the pore-scale, and as expected this distribution is parabolic.
To compare our permeability results from LBM to those from Gebart’s analytical solution, the dimensionless permeability was defined as follows:

\[ K_{ND} = \frac{K}{R^2} \]  

(2.8)

where \( K_{ND} \) is the non-dimensionalized permeability. Figure 2.6 illustrates the close agreement between the permeability-porosity relationship determined from the LB simulations and Gebart’s analytical solution.

Figure 2.6 Non-dimensionalized permeability as a function of porosity: comparing single-phase LBM to Gebart’s analytical relationship [87].
2.4 Results and Discussion

In the following section, the results of the LB simulations for the two examined geometries are presented. First, the model used to compute the tortuosity, which is then used to determine the permeability from the KC equation (Equation 2.1) is discussed. It is important to note that the final fitting parameters in the permeability relationships will depend on the definition of tortuosity used. Next, the functional forms of $C_{KC}$ that will be used to modify the KC equation are presented. Finally, the permeabilities obtained from the simulations to modify the KC relationship (Equation 2.1) by determining functional expressions for the $C_{KC}$ parameter are compared.

2.4.1 Tortuosity Calculation

In this study, tortuosity, $\tau$, is computed as the ratio of the average of the actual path lengths (as determined from the LB simulations) to the length of the system in the direction of the macroscopic flux [53]. This is given by Equation 2.9 [56]:

$$\tau = \frac{\sum_{i,j} U_{mag}(i,j)}{\sum_{i,j} |U_x(i,j)|},$$

(2.9)

where, $U_x$ is the $x$-direction velocity component, and $U_{mag}$ is the velocity magnitude:

$$U_{mag}(i,j) = \sqrt{U_x(i,j)^2 + U_y(i,j)^2},$$

(2.10)

for all lattice nodes $i,j$ in the system. This method was chosen as it accounts for both the microscopic flow and the geometry in the tortuosity calculation [53,56]. However, the main advantage of this method is that it does not require streamline calculations, which is a sophisticated, time-consuming and error-prone task, especially in realistic 3D geometries. Instead, it allows for calculation of the streamline tortuosity directly from the velocity field. Therefore, one can compute the tortuosity of practically any fluid flow system in which the velocity field is determined, whether numerically, analytically or experimentally.

It is important to note that the final expression for $C_{KC}$ will depend on the definition of tortuosity used. Other methods have been used to compute tortuosity [48,53,56]. One such description is the ratio of the shortest continuous path between any two points in the pore space to the distance
between the same two points on a straight line in the direction of the mean flow [53]; however, this method only considers the geometry, and does not account for the complexity of the flow or transport mechanisms.

### 2.4.2 Functional Forms

To improve the accuracy of the KC equation in predicting the porosity-permeability relationship for flow in porous media, alternate forms of the KC parameter were considered. Davies and Dollimore [123] and Kyan et al. [124] found that $C_{KC}$ first decreases with porosity, at low porosities, then increasing at higher values. Davies and Dollimore [123] suggested a rational form for $C_{KC}$ for sedimenting sphere beds and found that the specific geometry under consideration would determine the order of the rational function. Kyan et al. [124] proposed a more detailed rational function for fibrous materials, which incorporated the viscous friction factor. For their specific porous geometries, they found a minimum in $C_{KC}$ near $\phi = 0.85$. Happel and Brenner [125] reported experiments on a variety of structured materials and showed that $C_{KC}$ may be a monotonically increasing function of porosity. All of the behaviors described above can be modelled using exponential, power-law, logarithmic or algebraic functions.

To improve the predictability of the KC equation for describing the porosity-permeability relationship for flow in porous media, five alternative functional forms for the $C_{KC}$ parameter (used in Equation 2.1) were examined. In addition to the conventionally-used constant $C_{KC}$ (Equation 2.11-a), the five functional forms are listed below (Equations 2.11-b–2.11-f):

$$C_{KC} = A,$$  
(2.11-a)

$$C_{KC} = A\phi + B,$$  
(2.11-b)

$$C_{KC} = A\phi^B,$$  
(2.11-c)

$$C_{KC} = A \log B \phi + C,$$  
(2.11-d)

$$C_{KC} = A(\phi - C)^B, B \in N,$$  
(2.11-e)

$$C_{KC} = A|\phi - C|^B + D, B \in R,$$  
(2.11-f)

where $A$, $C$, and $D$ are real fitting parameters, and $B$ is either natural (Equation 2.11-e) or real (Equation 2.11-f). The permeability-porosity relationship determined for each functional form is compared to that determined from the LB simulations. These are all compared with the results
using the constant KC parameter (Equation 2.11-a).

Each functional form was evaluated by comparing it to the LB results using a nonlinear regression analysis employing the Generalized Reduced Gradient (GRG2) algorithm [126]. To this end, the permeability and tortuosity values obtained from the LB simulations were used to determine optimal fitting parameters for the $C_{KC}$ functions that minimize the error in permeability between the simulated values and those calculated from Equation 2.1. The error function used in the regression analysis to determine the algebraic fitting parameters was the sum-squared difference between log-values of the computed and simulated permeabilities. The GRG2 algorithm was implemented using the Microsoft Excel Solver (Microsoft Excel, version 14.0).

2.4.3 KC Parameter for Staggered Parallel Fibres

The LB model was applied to a 2D porous structure consisting of a staggered array of identical disks (representing infinite parallel fibres in 3D) to find a suitable expression for $C_{KC}$. In the KC equation, specific surface area, $S$, is calculated as the solid phase surface area per unit volume of the unit cell.

The non-dimensionalized permeability obtained from the LB simulations is compared to those calculated from the KC equation (Equation 2.1) with two forms of $C_{KC}$ in Figure 2.7. The calculated non-dimensionalized permeability values were determined using two forms of the KC parameter. First, $C_{KC}$ was assumed constant, as in the original KC model [127]. The best-fit value for this was found to be 2.409. However, this form of the KC parameter failed to reproduce accurate permeability values for the entire porosity range considered.
Figure 2.7 Dimensionless permeability values obtained from LB simulations, compared to values estimated from the KC model for the parallel-cylinder structure (Figure 2.3(b)), using two forms of $C_{KC}$: constant $C_{KC}$ (dotted line) and a functional form of $C_{KC}$ (solid line).

The KC value used in the original model was $C_{KC} = 2$, which is comparable to the fitted value of 2.409. This discrepancy in $C_{KC}$ can be attributed to variations between the geometries used. In the original model [87], the porous medium was formed of $N$ identical parallel tubes through a solid block, whereas in our model, the flow is around solid parallel fibres. The model with constant $C_{KC}$ does not provide accurate results. For instance, there is an error of 40% in the permeability prediction at a porosity of 0.42, as can be seen from the deviation between the dotted line and LBM data points in Figure 2.7.

A non-linear algebraic function of porosity was found to provide an appropriate relationship (Equation 2.11-f), where, $A, B, C$ and $D$ were determined to be 5420, 5.6, 0.6 and 3.38 respectively. This functional form for $C_{KC}$ was derived for an approximate porosity range of $\phi \in (0.25 - 0.97)$. Figure 2.7 demonstrates an improved fit of the model using the algebraic form in Equation 2.11-f (solid line), as opposed to the constant-value $C_{KC}$ (dotted line). The functional form reduces the error from 40% to 8% in permeability prediction at a porosity of 0.42. The fitted values obtained for $A, B, C$ and $D$ in Equation 2.11-f depend on the method used to calculate the tortuosity.
2.4.4 Determination of KC Parameter for BCC Array of Spheres

For the study involving a 3D domain, a staggered array of spheres was employed, which is similar to the packed-bed-of-beads geometry used in an early extension of the original KC equation [42]. In that study, a value of $C_{KC} = 5$ was used. Due to the similarity between the geometries, it was expected a similar value for $C_{KC}$ for our BCC structure. The best fit-value for $C_{KC}$ found for the LB simulations was 5.63, using a constant $C_{KC}$ value. Figure 2.8 shows the dimensionless permeability values obtained from the numerical simulations and from the KC equation for the BCC unit cell. As can be seen from the dotted line, a constant $C_{KC}$ value is not an appropriate choice, as the discrepancy between the LBM results and the KC model reaches 26% at a porosity of 0.42.

![Figure 2.8 Dimensionless permeability values obtained from LB simulations, compared to estimated values from the KC model for the BCC geometry (shown in Figure 2.4). Three alternate forms of $C_{KC}$ were used: constant $C_{KC}$ (dotted line), linear function of porosity (dashed line), and third-order polynomial form (solid line).](image)

As shown above, the KC model with constant $C_{KC}$ for the BCC structure was more accurate than for the infinite parallel cylinder geometry discussed above. The predictability of the KC model for the BCC case was further improved by using a linear expression (Equation 2.11-b) for $C_{KC}$. This improvement is shown in Figure 2.8 (dashed line). For example, the discrepancy in the permeability prediction of the KC model at 0.42 porosity decreased to 4% when a linear function of porosity (Equation 2.11-b) was employed for $C_{KC}$. The linear form of the KC parameter
(Equation 2.11-b) utilized to improve the predictability of the KC model. The fitting coefficients $A$ and $B$ were found to be 9.63 and 0.02, respectively. This functional form for $C_{KC}$ was derived for an approximate porosity range of $\phi \in (0.34 - 0.83)$.

Permeability estimations by the KC model were further enhanced by adopting a higher-order polynomial, though the improvement was only moderate. The linear form of $C_{KC}$ provides sufficient accuracy, without increasing the complexity or error introduced with more variables. This was not the case for the staggered array of parallel cylinder geometry, as various types of functions were examined in an effort to reproduce the pore-scale numerical results. The reason for the complexity in the parallel cylinder $C_{KC}$ expression was the significant variation of permeability values with porosity. This large variation is mainly due to the arrangement of solid space in parallel-cylinder structure, as opposed to the BCC geometry. For instance, in the BCC geometry, there is a pathway for fluid particles even if the spheres are in contact, while this is not the case for the infinite parallel-cylinder geometry. To capture permeability values for a wide range of porosity, a highly-nonlinear function of porosity was required for the parallel-cylinder geometry, as opposed to a simple linear expression for the BCC case (Equation 2.11-b).

In this work, further evidence that the $C_{KC}$ parameter is not constant has been provided, and instead is a function of porosity, as previous studies have suggested [85,128]. An efficient numerical approach that can be used to rapidly evaluate various forms of the KC relationship has been validated and applied. This numerical approach will be a useful tool for researchers, as experimental approaches for determining permeability are often expensive and time-consuming compared to numerical schemes [25]. The LB model used for this investigation presents a rapid method of determining an appropriate $C_{KC}$ for porous materials.

### 2.5 Conclusions

To determine the proper form of the KC parameter for a specific material, many permeability measurements must be performed over a large range of porosities. Since such experiments are often costly and time-consuming, a numerical approach was developed to characterize alternate forms of the KC equation. In this study, an SRT LB model of single-phase flow within porous media was presented and validated with an analytical permeability-porosity relationship [87].
Both the staggered array of infinite parallel cylinders and the body-centred cubic (BCC) array of spheres required a functional form for the KC parameter to be accurately determined over the range of porosities considered. The LB model developed for this investigation is a valuable tool for calculating the $C_{KC}$ parameter for a variety of porous media. For the application of carbon sequestration, which may involve heterogeneously structured geologic formations, the methodology presented here can be employed to determine the permeability-porosity relationship for various locally-homogeneous regions throughout the reservoir. In future studies, micro-CT images of the porous medium of interest can be incorporated into the LB simulations.
3 Determining the Impact of Rectangular Grain Aspect Ratio on Tortuosity-porosity Correlations of Two-dimensional Stochastically Generated Porous Media

3.1 Abstract

Stochastic numerical modelling is a powerful tool for estimating bulk transport properties of porous media, such as tortuosity. However, stochastic numerical modelling has not been used extensively to investigate the impact of the geometric properties of the individual grains, (such as grain aspect ratio) on the tortuosity-porosity relationships in porous media. The impact of grain aspect ratio on the tortuosity-porosity relationships of 2D porous media composed of rectangular particles was determined by calculating the adjusting parameters in the previously reported logarithmic tortuosity-porosity correlation, \( \tau = a - b \ln(\phi) \). These adjusting parameters were then obtained by calculating average tortuosity values with grain aspect ratios of \( \in \{1, 2, 3\} \) and a porosity range of \( \in [0.55 - 0.95] \). A minimum of 6, 8 and 10 stochastic simulations were also determined for grain aspect ratios of \( \in \{1, 2, 3\} \), respectively, to be required to calculate these average tortuosity values in laminar flow (\( Re \ll 1 \)). The minimum number of required stochastic simulations is highly valuable for the efficient numerical determination of tortuosity-porosity relationships.

3.2 Introduction

Permeability and effective diffusivity are valuable material properties for predictive continuum models of flow and mass transport through porous media. When empirical values for these properties are not available, estimates can be made based on porosity and tortuosity values. Tortuosity, \( \tau \), provides a means of measuring the complexity of fluid pathways through a porous material and has been strongly correlated to material porosity [54,129]. Therefore, tortuosity has been applied in numerical models for science and engineering applications ranging from oil

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recovery and carbon sequestration to fuel cells [118,130-133].

There are several definitions of tortuosity in the literature [44-49], depending on characterization needs, ranging from the determination of electrical conductivity to hydraulic conductivity. Several tortuosity definitions along with their variances and common applications are discussed below to emphasize the importance of implementing tortuosity definitions with care.

The geometrical tortuosity, $\tau_g$, can be defined as the ratio of the average length of the geometric flow paths, $\langle L_g \rangle$, to the length of the medium in the direction of macroscopic flux, $L_s$, [44]:

$$
\tau_g = \frac{\langle L_g \rangle}{L_s}, \quad (3.1)
$$

while the hydraulic tortuosity, $\tau$, is defined as the ratio of the average effective flow path length taken by the fluid, $\langle L_h \rangle$, to the straight-line length across the medium, $L_s$ [55]:

$$
\tau = \frac{\langle L_h \rangle}{L_s}, \quad (3.2)
$$

Geometric pathways include the shortest paths consisting of straight lines touching and passing by grains with close tangents (Figure 3.1(a)), whereas in reality, fluid particles are expected to travel through smoothed streamlines [44,46]. Therefore, $\tau$ is always greater than $\tau_g$.

Furthermore, geometrical tortuosity is commonly based on geometric parameters, such as particle size, shape, and arrangement.

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Figure 3.1 Example schematic of a (a) geometric and (b) hydraulic flow path: Note that the hydraulic length ($L_h$) is greater than the geometric length ($L_g$).

Hydraulic tortuosity accounts for the hydrodynamics of the flow within porous formations (Figure 3.1(b)). Hydraulic tortuosity is used to determine the permeability of porous media. For
example, in the subsequent and often cited Kozeny-Carman relationship, the permeability is expressed as a function of tortuosity [54,134]:

\[ K = \frac{1}{C_{KC}} \cdot \frac{\phi^3}{S^2 \tau^2} \quad (3.3) \]

where \( K \), \( C_{KC} \), \( \phi \), and \( S \) are permeability, Kozeny-Carman constant (shape factor), porosity, and specific surface area, respectively.

The electrical tortuosity is defined as [135-137]:

\[ \tau_e = \left( \frac{\langle L_e \rangle}{L_s} \right)^2 \quad (3.4) \]

where \( \langle L_e \rangle \) is defined as the average path length for electronic flow. However, an alternate definition of the electrical tortuosity is the ratio of the conductivity of a porous medium saturated with an electrolyte to that of the free electrolyte [138]. Electrical tortuosity can play an important role in determining electrical resistivity of a given formation. Similar to the former definition of electrical tortuosity, diffusive tortuosity, \( \tau_d \), can be defined [49] as:

\[ \tau_d = \left( \frac{\langle L_d \rangle}{L_s} \right)^2 \quad (3.5) \]

where \( \langle L_d \rangle \) is the average length of the diffusive pathway of a chemical species. Diffusive tortuosity can also be defined as the ratio of the diffusion coefficient of the given species in free fluid to its value in porous media [45,46,139-141]. Diffusive tortuosity is used when diffusion is the dominant transport mechanism in the porous media, such as in the case of gas diffusion layers in polymer electrolyte membrane fuel cells.

In the literature, hydraulic tortuosity calculations have been conducted using experimental [50-52], analytical [57,58] and numerical methods [47,53-56]. Experimental-based parametric investigations pose challenges due to cost and time limitations as well as restrictions to probing in-situ phenomena at the microscale. Analytical models, while highly insightful, are typically constrained to a particular class of structured domains. For example, Du Plessis and Masliyah [57] derived an analytical model particularly for isotropic granular media. Contrary to analytical and experimental methods, numerical models can be used to determine tortuosity values for wide ranges of porous media classes and with computational and temporal cost effectiveness.
Another advantage of pore-scale numerical modelling is the inherent high resolution representation of the pore-scale structure. Modelling the fluid flow within stochastic porous media has gained significant popularity. For instance, Koponen et al. [53,54], Nabovati et al. [56], Matyka et al. [47], and Duda et al. [55] numerically modelled 2D stochastically generated domains and performed hydraulic tortuosity calculations. Stochastically generated domains were used to capture the inherent heterogeneity in porous formations. These previous studies demonstrated high variability in tortuosity values for each porosity due to the stochastic structures and reported mean tortuosity values. However, the minimum number of stochastic domains (i.e. grain arrangements) needed for obtaining conclusive average tortuosity results has yet to be determined. It is important to note that this minimum number of domains may be related to the smallest representative domain size needed for predictive mass transport models. Studies are also needed to understand the applicability of 2D stochastic modelling-based tortuosity values to experimentally derived correlations.

Koponen et al. [53] used lattice gas cellular automaton to investigate flow in a 2D porous medium consisting of stochastically distributed mono-sized solid rectangles with unrestricted overlapping. They found that the hydraulic tortuosity was linearly correlated to the porosity given by

$$\tau = 1 + 0.8(1 - \phi).$$

(3.6)

Although their model was capable of capturing flow path tortuosities, they later found that their suggested linear tortuosity-porosity relationship was not representative near the percolation threshold. They then proposed the following relationship for the porosity range of $\phi \in [0.4 - 0.5]$ [54]:

$$\tau = 1 + \alpha \frac{(1-\phi)}{(\phi - \phi_c)^\beta},$$

(3.7)

where $\alpha$ and $\beta$ are adjusting parameters being $\alpha = 0.65$ and $\beta = 0.19$, and $\phi_c = 0.33$ is the percolation threshold.

Matyka et al. [47] used LBM to determine the tortuosity-porosity relationship for fluid flow in 2D porous media constructed with freely overlapping solid squares for an approximate porosity
range of $\phi \in (0.45 - 0.95)$. They used a periodic boundary condition to reduce the finite-size effects and fit their tortuosity results with the frequently used logarithmic form of [51,142-145]:

$$\tau = 1 - P\ln(\phi), \quad (3.8)$$

where they found a value of 0.77 for $P$, the adjusting parameter.

Nabovati et al. [56] used a similar geometry to perform grain aspect ratio ($AR$) analysis for $AR = 0.5, 1$ and 2 with LBM. They reported a good agreement with Koponen et al. [53] and suggested a third-order polynomial function to fit their simulation results for the average tortuosity in terms of porosity. Nabovati et al. [56] concluded that higher grain aspect ratios would increase the tortuosity values for the same porosity. This increase in tortuosity values at higher grain aspect ratios has also been experimentally shown by Comiti and Renaud [51] using porous media consisting of plates (parallelepipedal particles of low thickness-to-side ratio) with aspect ratios of $AR = 2.27, 4.78,$ and 9.8. They also found that tortuosity-porosity correlations were strongly dependent on the grain aspect ratio. In summary, numerical models provide valuable, complementary tools to experimental and analytical methods for determining material tortuosity.

While past work has provided significant insight into the porosity-tortuosity relationships exhibited by a variety of porous materials, the impact of grain aspect ratio on tortuosity has yet to be fully characterized. Specifically, the impact of grain aspect ratio, $AR > 2$ on tortuosity values for 2D porous media has not been compared to experimental work presented by [51]. The applicability of 2D numerical models for tortuosity determinations should also be evaluated through direct validation with experimental measurements.

In this study, an LBM-based 2D stochastic model was used to simulate irregular porous media to determine the impact of grain aspect ratio on tortuosity-porosity relationships. The impact of grain aspect ratio on the tortuosity-porosity relationships of 2D porous media composed of rectangular particles was determined by calculating the adjusting parameters ($\alpha$ and $b$) in the previously reported tortuosity-porosity correlation of $\tau = a - b.\ln(\phi)$. These adjusting parameters were then calculated by calculating average tortuosity values with grain aspect ratios of $AR \in \{1,2,3\}$ and a porosity range of $\phi \in [0.55 - 0.95]$. A sensitivity study was performed to determine the impact of the number of stochastic simulations on the average tortuosity, and
the applicability of our model was evaluated through direct comparisons with experiments reported in the literature.

3.3 Numerical Method

LBM was used to solve 2D fluid velocity domains at the pore scale, from which hydraulic tortuosities were determined. Simulation domains were created from stochastically placed rectangular grains with fixed aspect ratios \( AR \in \{1, 2, 3\} \) over a porosity range of \( \phi \in [0.55 - 0.95] \). Tortuosity was calculated for multiple stochastically generated domains for each aspect ratio and porosity. A sensitivity study was performed to determine the impact of the number of stochastic simulations on the average tortuosity.

3.3.1 Lattice-Boltzmann Modelling

In this work, a multiple-relaxation-time (MRT) LBM was implemented in MATLAB for single-phase fluid flow simulations in 2D stochastic porous media at the pore scale. The following LB equation with the MRT collision model was used:

\[
f(x_j + c\delta t, t_n + \delta t) = f(x_j, t_n) - M^{-1} \hat{S} [m - m^{eq}(\rho, u)](x_j, t_n),
\]

where \( f, c, \delta t, \hat{S}, m, \rho \) and \( u \) are distribution function, lattice discrete velocity set, time step, relaxation rate matrix, moments, macroscopic density and velocity, respectively. The matrix, \( M \), is a map of the distribution functions and its moments as follows:

\[
m = M f.
\]

The MRT LBM methodology was chosen since the results are independent of the choice of the relaxation time (viscosity-independent results), compared to the single-relaxation-time (SRT) method [93]. For a complete description of the MRT LBM developed for this study, the reader is directed to [146,147] (also see Appendix II for an outlined implementation of MRT matrices).
3.3.2 Geometry, Model Assumptions and Boundary Conditions

3.3.2.1 Geometry

The computational domain consists of 2D porous media composed of stochastically placed, freely overlapping solid rectangles that were assumed to simulate geometric irregularities of porous media found in nature [47,53,54].

Porosity was adjusted by changing the number of solid rectangles in the domain. Since rectangle overlap was allowed, the porosity was prescribed with high precision (±1%). The porosity of the medium was calculated as the ratio of the number of the lattice sites in the fluid region to the total number of the lattice sites.

The locations of the grains were prescribed with a pseudo-random number generator from a standard uniform distribution [148] on an interval represented by the domain size. This random placement of grains led to a high number of possible grain arrangements (stochastic configurations) for a given porosity. For instance, Figure 3.2 shows how four configurations can be constructed (without overlapping) to construct porous media with different grain locations, yet identical porosities and grain aspect ratios (\(\phi = 0.95\) & \(AR = 1\)).

![Figure 3.2 Possible configurations of a 2D porous medium with a porosity of 0.95, grain aspect ratio of 1, and non-overlapping square grains.](image)

The number of possible stochastic configurations can increase with increasing numbers of grains. The number of grains in the domain increases as the porosity decreases. When overlapping is allowed, higher number of grains may be required to produce the same porosity compared to the...
case where overlapping is not allowed. Table 3.1 presents the minimum number of grains required to construct a porous medium with a desired porosity for each distinct grain aspect ratio. The number of grains contained in the domain reflects the relative number of possible grain arrangements (stochastic domains), each of which comes with a distinct tortuosity value.

Table 3.1 Minimum number of grains required for each porosity and grain aspect ratio combination.

<table>
<thead>
<tr>
<th>Porosity</th>
<th>Minimum number of grains required&lt;sup&gt;a&lt;/sup&gt;</th>
<th>AR = 1</th>
<th>AR = 2</th>
<th>AR = 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.95</td>
<td>5</td>
<td>6</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>0.90</td>
<td>10</td>
<td>12</td>
<td>11</td>
<td></td>
</tr>
<tr>
<td>0.80</td>
<td>20</td>
<td>23</td>
<td>22</td>
<td></td>
</tr>
<tr>
<td>0.70</td>
<td>30</td>
<td>34</td>
<td>32</td>
<td></td>
</tr>
<tr>
<td>0.60</td>
<td>40</td>
<td>45</td>
<td>43</td>
<td></td>
</tr>
<tr>
<td>0.55</td>
<td>45</td>
<td>51</td>
<td>48</td>
<td></td>
</tr>
</tbody>
</table>

<sup>a</sup> Min # of grains = \( \lceil (1 - \phi) \times \frac{A_{\text{tot}}}{A_{\text{grain}}} \rceil \), where \( A_{\text{tot}} \) and \( A_{\text{grain}} \) are domain and grain areas in terms of number of lattice sites

The coefficient of variation (\( CV \)) was used as a normalized measure of tortuosity variability for various porosities and grain aspect ratios. \( CV \) is defined as:

\[
CV = \frac{\sigma}{\mu},
\]

where \( \sigma \) is the standard deviation of the tortuosity values for a given porosity and grain aspect ratio, and \( \mu \) is the mean of those tortuosity values, which are given by:

\[
\sigma = \sqrt{\frac{\sum (\tau - \mu)^2}{n-1}},
\]

and

\[
\mu = \frac{\sum_{i=1}^{n} \tau_i}{n},
\]

for any number of samples (i.e. stochastic configurations), \( n \).
3.3.2.2 Model Assumptions

The Reynolds number (on the order of $10^3$) was constant throughout all simulations to enforce a creeping flow condition where the hydraulic tortuosity was independent of the fluid properties such as, viscosity, density and pressure gradient [116]. The size of the grains was chosen in a way to keep the total area of each individual grains nearly constant relative to the size of the domain (see Table 3.2). This effort is made in order to isolate the effect of only the porosity and grain aspect ratio on tortuosity.

<table>
<thead>
<tr>
<th>Grain Aspect Ratio</th>
<th>Grain Dimensions ($x \times y$)</th>
<th>Grain Area</th>
<th>Domain Dimensions ($x \times y$)</th>
<th>Domain Area</th>
<th>Grain/Domain Area Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10 × 10</td>
<td>100</td>
<td>100 × 100</td>
<td>10000</td>
<td>0.010</td>
</tr>
<tr>
<td>2</td>
<td>8 × 16</td>
<td>128</td>
<td>120 × 120</td>
<td>14400</td>
<td>0.009</td>
</tr>
<tr>
<td>3</td>
<td>9 × 27</td>
<td>243</td>
<td>160 × 160</td>
<td>25600</td>
<td>0.009</td>
</tr>
</tbody>
</table>

In Table 3.2, the dimensions of the grains and domains that were used in this investigation are reported in terms of number of lattice sites. As shown in Table 3.2, the resolution of the domains was increased with increasing grain aspect ratio. The domain resolution (number of lattice sites) for each grain aspect ratio was determined after mesh sensitivity studies were performed (see Section 3.3.6). For each porosity, stochastic simulations for each of three distinct grain aspect ratios (i.e., $AR = 1, 2, \text{ and } 3$) were performed and analyzed.

3.3.2.3 Boundary Conditions

The following boundary conditions were implemented: Periodic boundary conditions were applied on side walls of the domain, perpendicular to the direction of the inlet flow. No-slip solid wall boundary conditions were set at the surfaces of the grains using the bounce back method [109,149]. Pressure boundary conditions were used at the inlet and outlet. The pressure difference between the inlet and outlet was prescribed to ensure a low-Mach number (i.e.
\( Ma \ll 1 \) and low Reynolds number (i.e. \( Re \ll 1 \)) fluid flow for the LB model and to minimize inertial effects [150].

Narrow pores and flow passages posed convergence challenges for pore-level numerical simulations, such that fluid flow could not be solved when these narrow passages were resolved with an insufficient number of nodes. According to Nabovati [151], at least three fluid nodes were required across flow passages in order for LBM to accurately capture the fluid flow behavior. This condition limits the effectiveness of numerical techniques at lower porosities, particularly when the domain is dominated by narrow flow passages. In this study, 0.55 was the porosity value above which our simulations converged for all simulated grain aspect ratios. To address the issue with narrow flow passages, a standard numerical mesh refinement procedure was implemented. At the end of each simulation, the inlet and outlet flow rates were confirmed to be within 1% of each other, indicating that mass was conserved throughout the entire domain.

3.3.3 Convergence Criteria

The LB method involves an iterative approach for solving the flow equations. Once the LBM iteration was started, the temporal evolution of the velocity field was monitored until it reached steady state. The LBM iteration was terminated once the summation of residual velocities at all lattice nodes fell below \( 10^{-4} \), determined through:

\[
\sum_{i,j} \frac{u(i,j) - u_{old}(i,j)}{u(i,j)} < 10^{-4}, \tag{3.14}
\]

where \( u(i,j) \) and \( u_{old}(i,j) \) are the flow velocity at node \( (i,j) \) at the current and previous time steps, respectively. Beyond this threshold residual velocity, tortuosity values did not change.

3.3.4 Model Validation

In addition to ensuring mass conservation (see Section 3.3.2.3), the MRT LBM algorithm employed in this study was validated as follows: First, a simulation of Poiseuille flow between two parallel plates, similar to the work of Durst et al. [152] was performed. The entry length obtained from our MRT model was in agreement with the experimental results by Durst et al. [152]. Furthermore, a developing velocity profile obtained using the MRT model was validated
with the velocity profile obtained from our previously developed and validated SRT model [153]. A complete description of the SRT LBM is available in our previous work [153]. In another validation step, the results from the MRT LBM were verified with the experimental results reported by Kueny et al. [154] for a flow over backward-facing step. The velocity profiles and the size of the separation region were in agreement with those reported by Kueny et al. [154]. For further details on these model validation studies, one may refer to the Appendix.

### 3.3.5 Tortuosity Calculations

In this study, hydraulic tortuosity, \( \tau \), was defined as the average elongation of fluid streamlines [55]. The streamline tortuosity is expressed as the ratio of the average fluid velocity magnitude to the average fluid velocity along the macroscopic flow direction (Equation 3.15). [55,56]:

\[
\tau = \frac{\sum_{i,j} U_{\text{mag}}(i,j)}{\sum_{i,j} |U_x(i,j)|},
\]

where \( U_x \) is the \( x \)-direction velocity component, and \( U_{\text{mag}} \) is the velocity magnitude defined as:

\[
U_{\text{mag}}(i,j) = \sqrt{U_x(i,j)^2 + U_y(i,j)^2},
\]

for all lattice nodes \( i, j \) in the system. This method was particularly useful since the velocity field information was readily available after solving the fluid flow through LBM.

### 3.3.6 Mesh-independence Study

Mesh-independence studies were performed to determine appropriate grid spacing for various grain aspect ratios (as stated in Section 3.3.2.2.). The mesh studies were all performed for a porosity of 0.55 for \( AR = 1, 2, \) and 3. The appropriate lattice spacing was determined so that the tortuosity changes were less than 0.001 as the number of lattice sites was increased by increments of 20. Table 3.2 shows that the grain/domain area ratio was maintained constant by considering larger grains when increasing the domain size. Table 3.2 includes the domain dimensions in terms of the used number (after mesh-independence study) of lattice sites across domains for various grain aspect ratios.
3.4 Results and Discussion

In this section, the following will be presented: 1) a sample visualization of the calculated velocity and streamlines within 2D stochastic domains, 2) the sensitivity analysis for calculating the minimum number of stochastic configurations, 3) the impact of the grain aspect ratio on tortuosity, and 4) the applicability of this work to experimental measurements relevant to an industrial application (pulp and paper industry).

3.4.1 Velocity Field and Streamlines

Figure 3.3 shows the velocity field and the flow streamlines for two sample porous media, both of which have a porosity of 0.85. The porous media in Figure 3.3a consist of grains with $AR = 3$ while the porous media in Figure 3.3b consist of square grains with $AR = 1$. The hydraulic tortuosity values were calculated to be 1.23 and 1.11 for grain aspect ratios of $AR = 3$ and 1, respectively.
Figure 3.3 Example velocity distribution fields and flow streamlines within stochastically generated 2D porous media with porosity $\phi = 0.85$ and: (a) $AR = 3$, (b) $AR = 1$ for rectangular grains. Tortuositities of domains (a) and (b) were calculated to be 1.23 and 1.11, respectively.

These tortuosity values may indicate that higher grain aspect ratios lead to increases in hydraulic tortuosity. However, since the geometries were generated stochastically, more geometries of each grain aspect ratio should be studied for verification.

3.4.2 Minimum Number of Stochastic Configurations

Variability was observed in calculated tortuosity values due to the stochastic nature of domain generation. Figure 3.4 shows that the $CV$ for tortuosity increased with decreasing porosity. The $CV$ was used to evaluate the minimum number of stochastic simulations needed to calculate a representative tortuosity value. In order to determine the minimum number of required stochastic domains, the distribution of tortuosity values around the mean tortuosity was calculated at each porosity and grain aspect ratio. Wider distributions in tortuosity values indicated a higher number of required stochastic domains.
Figure 3.4 Coefficient of variation (CV) of tortuosity values as a function of porosity for 2D porous media constructed with freely overlapping rectangular grains.

Figure 3.5 shows the results of the study that was performed to determine the minimum number of stochastic configurations with a porosity of 0.55 for three distinct grain aspect ratios. A minimum of 6, 8 and 10 stochastic configurations were required to provide a representative average tortuosity value for grain aspect ratios of 1, 2 and 3, respectively. The convergence criterion was the point where the average tortuosity fell below 1%.
Since a porosity of $\phi = 0.55$ exhibited the highest $CV$ (Figure 3.4), the minimum number of stochastic simulations for this porosity was applied to all cases of $\phi > 0.55$ as a conservative estimate. The only exceptions were for domains with $\phi = 0.90$ and 0.95, for which three configurations were averaged (where the variation of average tortuosity varied by less than 1%).
3.4.3 Effect of Porosity and Grain Aspect Ratio on Tortuosity

Figure 3.6 illustrates the effect of porosity and grain aspect ratio on tortuosity. Tortuosity values increased with decreasing porosity, and tortuosity approached unity as the porosity approached 1.0. Tortuosity also increased with increasing grain aspect ratio, which reflected the emergence of longer particle pathways compared to those in porous structures with lower grain aspect ratios (Figure 3.3). It was also observed that the spread in tortuosity values was more prevalent at lower porosity values, indicating that the impact of aspect ratio on tortuosity is more significant at lower porosities.

![Graph showing relationship between tortuosity and porosity](image)

Figure 3.6 Relationship between tortuosity and porosity for 2D stochastically generated porous media with rectangular grains of varying aspect ratio.

The consequence of this result is that numerical fluid flow simulations based on porous media characterizations are particularly sensitive to the accuracy of the characterization method, with minor inaccuracies leading to significant changes in tortuosity calculations.
3.4.4 Applicability of 2D Model

The applicability of our 2D stochastic modelling results to the results of previous experiments [51] with similar porous media was examined. The tortuosity values obtained from the MRT LBM were fit to tortuosity-porosity relations of the following general logarithmic form:

\[ \tau = a - b \ln(\phi), \]  

(3.17)

where \( a \) and \( b \) are adjusting parameters. Below are the explicit logarithmic tortuosity-porosity correlations that were found to describe the numerical tortuosity values for a porosity range of \( \phi \in (0.55 - 0.95) \):

\[ \tau = 1.01 - 0.37\ln(\phi), \text{ for } AR = 1 \]  

(3.18-a)

\[ \tau = 0.99 - 0.80\ln(\phi), \text{ for } AR = 2 \]  

(3.18-b)

\[ \tau = 0.98 - 1.16\ln(\phi), \text{ for } AR = 3 \]  

(3.18-c)

The correlations stated above are also shown in Figure 3.6. As shown in Equations 3.18, it was found that \( a \sim 1 \) for all three examined aspect ratios, which is in agreement with Equation 3.8 [51,142-145]. The value of \( b \) was also found to agree with the adjusting parameter, \( P \), from Equation 3.8. \( P \) values are the experimentally-determined adjusting parameters of the \( \tau - \phi \) correlation, and \( b \) values are the adjusting parameters for the numerically-determined \( \tau - \phi \) correlations. The \( b \) values reported in Equations 3.18 correspond to the experimentally
determined \( P \) values by Comiti and Renaud [51] (in the range 0.86 to 3.2) for porous media
consisting of parallelepipedal particles of low thickness-to-side ratios with distinct aspect ratios
(for \( AR = 2.27, P = 0.86; \text{ for } AR = 4.78, P = 1.66; \text{ and for } AR = 9.8, P = 3.2 \)). For example, the \( P \) value for \( AR = 2 \), can be linearly extrapolated to \( P = 0.78 \) based on the near-linear relationship
that exists between the \( P \) and \( AR \) values reported by Comiti and Renaud [51]. The \( P \) value of
0.78 agrees with the \( b \) value of 0.80 (Equation 3.18-b) that was calculated for \( AR = 2 \) by fitting
Equation 3.17 to the numerical tortuosity values presented here.

Experimentally-determined \( P \) values reported by Comiti and Renaud [51] as well as the
numerically-determined \( b \) values from the present work are shown in Figure 3.7. This figure
shows that \( b \) and \( P \) values exhibit a near-linear correlation with grain aspect ratio. It can also be seen that \( b \) and \( P \) values are in agreement over the overlapping range of grain aspect ratio.
Figure 3.7 Relationship between the experimentally-determined adjusting parameters \( P \) reported by Comiti and Renaud [51] and grain aspect ratio as well as the relationship between the numerically-determined adjusting parameters \( b \) from the present work and grain aspect ratio. The dashed lines connecting the data points are only intended to show the trend and do not represent a linear fit.

Based on the agreement between the adjusting parameters in Equations 3.18 and the adjusting parameters suggested by Comiti and Renaud [51], the tortuosity calculated from 2D stochastic modelling of porous media with freely overlapping rectangles provides realistic simulations of porous media with fixed beds of parallelepipedal particles of low thickness-to-side ratio. Such porous media are relevant to the pulp and paper industry such as wood chips that are used for paper pulp synthesis [51].

3.5 Conclusions

In this study, the impact of grain aspect ratio on the tortuosity-porosity relationships in porous media was investigated using an MRT LBM based analysis. To determine the impact of grain aspect ratio on the tortuosity-porosity relationships, average tortuosity values in 2D stochastically generated porous media composed of rectangular particles were calculated. It was shown that tortuosity exhibits an inverse relationship with the porosity that can be expressed in logarithmic form. The adjusting parameters in the tortuosity-porosity correlation of \( \tau = a - \)
\( b. \ln(\phi) \) were calculated. It was also demonstrated that the effect of aspect ratio on the tortuosity diminishes as the porosity approaches unity. Therefore, it is expected that accurate characterization of porous media in terms of the grain aspect ratio becomes critical in predicting tortuosity and resolving fluid flow in low porosity formations.

In addition, it was shown that the tortuosity values from the 2D stochastic domains were in agreement with the results reported by Comiti and Renaud [51], and therefore expected to be applicable to similar domains such as fixed beds packed with parallelepipedal particles of low thickness-to-side ratio, such as wood chips used in the pulp and paper industry. It was also determined that a minimum of 6, 8 and 10 stochastic simulations were required to calculate the average tortuosity values in laminar flow \((Re \ll 1)\) simulations of our 2D domain for aspect ratios of 1, 2 and 3, respectively. The work presented here provides a methodology for porous media researchers to numerically determine tortuosity-porosity correlations that can be validated with experimentally derived measurements. The methodology presented in this work provides a useful tool for material designers to tailor the particle arrangements of particles for prescribing desired tortuosity parameters.
4 Analytical Tortuosity-porosity Correlations for Two Deterministic Fractal Geometries

4.1 Abstract

Naturally-occurring porous media, such as sedimentary rock, rarely consist of mono-sized particles, but rather tend to consist of wide distributions of particle sizes (poorly-sorted porous media). In this study, deterministic fractal geometries including a Sierpinski carpet and a slightly altered version of the Sierpinski carpet with a generator that has a circular inclusion were used to provide insight into the poorly-sorted porous media found in sedimentary rock. The relationships between tortuosity and porosity within these fractals were investigated by presenting and applying a novel mathematical approach. A new correlation between the tortuosity, $\tau$, and porosity, $\phi$, was found within this Sierpinski carpet ($\tau = \frac{3}{2} - \frac{\phi}{2}$), which agrees well with previous empirical observations reported in the literature. An analytical tortuosity-porosity correlation was also found within a circular-based Sierpinski carpet ($\tau = \left(1 - \frac{4}{\pi}\right)\phi + \frac{4}{\pi}$), which is to the best of the author’s knowledge, the first tortuosity-porosity relationship proposed for the circular-based Sierpinski carpet.

4.2 Introduction

Tortuosity, $\tau$, is a parameter frequently utilized in continuum models during estimates of effective flow and transport properties within porous media [54,134]. The concept of tortuosity was first introduced by Carman [42] in 1937 as a parameter that describes the average elongation of microscopic fluid flow (particle) pathways in porous media with respect to free flow [55]. In the subsequent and often cited Kozeny-Carman relationship, tortuosity is used to determine the permeability, $K$, of porous media, as follows [54,134]:

$$K = \frac{1}{C_{KC}} \cdot \frac{\phi^3}{S^2 \tau^2}, \quad (4.1)$$

where $C_{KC}$, $\phi$, and $S$ are the Kozeny-Carman constant (shape factor), porosity, and specific surface area, respectively [155].

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In the literature, most investigations of tortuosity involve porous media consisting of mono-sized (same-sized) particles, such as the analytical studies by Yun et al. [59], Yu & Li [60], and Jian-Long et al. [61] or the numerical studies by Koponen et al. [53,54] and Matyka et al. [47]. However, natural granular porous media (e.g. sedimentary rocks) are rarely mono-sized [44]. It is noteworthy to mention that even though the structures studied by Koponen et al. [53,54] and Matyka et al. [47] were constructed by monosized particles, overlapping was allowed, which could potentially lead to structures of a narrow range of sizes, especially in low porosity systems. In addition to granular porous media, sometimes fibrous porous materials (e.g. filters and insulating materials) have wide distributions of fibre diameter (poorly-sorted). Figure 4.1 shows the schematic of a mono-sized medium and a poorly-sorted granular porous medium. Figure 4.2 shows a scanning electron microscopy (SEM) image of a granular rock sample (Pink Dolomite) which exhibits wide distributions of particle sizes.

![Figure 4.1 Schematic of a (a) well-sorted sedimentary rock versus (b) a poorly-sorted sedimentary rock.](image-url)
Evidence suggests that natural porous media can be described as a fractal [62,64,156]. There is even stronger support that surfaces of rock grain and of whole rock samples are fractal [157,158]. Therefore, in the field of porous media, many researchers have used fractals to generate poorly-sorted porous structures to characterize natural porous media properties or to simulate fluid flow within porous formations [67-69,159-163]. A fractal is a structure that contains repeating patterns at every length scale (generation). In theory, fractals can be infinitely self-similar meaning that they can contain a particular geometric shape (square, circle, etc) in an infinite range of length scales. Therefore, they can be useful in representing porous materials that contain wide distributions of particle sizes at various length scales. For instance, the $n^{th}$ generation of a fractal can represent porous media that contain grains of $n$ distinct sizes.
The Sierpinski carpet (Figure 4.3a-c) is a commonly used fractal [67-69] with a long history of application to natural porous media [70,71]. The Sierpinski carpet is expected to represent rock formations particularly at higher generations (lower porosities) where the fractals are less sparse. Therefore, the fractal can act as an appropriate benchmarking domain for modelling transport in porous media consisting of wide distributions of particle sizes [71]. Feranie and Latief [69] applied a square full-walk technique to calculate tortuosity in a 2D fractal model of porous media constructed of randomized Sierpinski carpets. They reported good agreement with previous work [53,164] for the porosity range of $\phi \in (0.3, 0.7)$. Feranie and Latief [69] focused their study on porous media containing grains of 2 to 4 distinct sizes. Li and Yu [67] estimated tortuosity through a deterministic Sierpinski carpet using an analytical method and generated the following exponential relationship between tortuosity and porosity:

$$
\tau = \left(\frac{19}{18}\right)^{\frac{\ln(\phi)}{\ln(8/9)}}.
$$

(4.2)
An advantage of their model is that it can be applied over a full range of porosities (Sierpinski carpet generation: $n \in \{0, 1, 2, \ldots, \infty\}$). Although Li and Yu’s [67] results diverge from the linear [53,69] or close-to-linear [165] tortuosity-porosity correlations found by other researchers, theirs follows the concave trend suggested by many of the works discussed by Ghanbarian et al. [44].

Ghanbarian et al. [44] suggested that the bounds of tortuosity should be 1 at $\phi = 1$ and should approach infinity as the porosity approaches some critical value (limiting porosity, which is 0 for the Sierpinski carpet).

In another study, Lue et al. [68] found the following logarithmic relationship between tortuosity and porosity for the Sierpinski carpet:

$$\tau = 0.946 - 0.408 \ln(\phi).$$

Four generations of the Sierpinski carpet ($n \in \{2, 3, 4, 5\}$ or $\phi \in (0.55 - 0.79)$) were considered in their modelling efforts due to the computational limitations. While previous work provided great insight into the tortuosity-porosity relationships for low-generation Sierpinski carpets, new insight is needed for materials that exhibit wider distributions of particle sizes (high-generation Sierpinski carpet). Since the Sierpinski carpet only features square grains, the effect of grain shape on the tortuosity-porosity correlation requires further investigation.

An analytical approach for determining tortuosity relationships can be particularly beneficial for high generations ($n > 6$) of fractals where mesh-based numerical approaches can become computationally prohibitive. High-generation fractal geometries can be equivalent to the porous media containing grains or pore spaces with substantial variances in size. Figure 4.3 shows an example of the first 3 generations ($n = 0, 1, \text{and} 2$) of such geometries, though one can imagine higher generations can be used to represent wider distributions of particle sizes. For instance, at $n = 5$, the smallest grain is a factor of $1.5 \times 10^{-4}$ the size of the largest grain in the domain. While non-uniform numerical meshes could be applied, at the higher generations required for low porosity domains, the substantial disparity in length scales could make the numerical models prohibitively computationally expensive [166]. Therefore, an analytical model is crucial for tortuosity estimation, particularly when wide distributions of particle sizes exist within the porous media.
In summary, an accurate analytical method is required to study the tortuosity-porosity correlations in high-generation fractals (porous media with wide distributions of grain sizes). New correlations are needed to improve estimates of effective flow and transport properties within such low-porosity formations. Furthermore, it is still unknown how the shape of the grain may affect the tortuosity-porosity relationships in a Sierpinski carpet type of structure (where the Sierpinski carpet structure is fixed and only the square grains in the structure are replaced by other shapes such as circles).

In this study, a new analytical approach was proposed and applied to calculate the tortuosity of flow within a 2D deterministic Sierpinski carpet. Furthermore, the proposed approach was applied to calculate the tortuosity of the flow in a round-grained version of the Sierpinski carpet, the circular-based Sierpinski carpet. In both cases, a linear correlation with a distinct slope between tortuosity and porosity was found that aligned well with other work [53,69,165].

4.3 Methodology

In this section, the construction process of the used porous media (the Sierpinski carpet and the circular-based Sierpinski carpet) is presented followed by a description of the proposed analytical method with detailed mathematical derivation steps:

4.3.1 Geometry

The two geometries used in this study are a Sierpinski carpet (Figure 4.3a-c) as well as a slightly altered version of the Sierpinski carpet with a generator that has a circular inclusion, hereafter called the circular-based Sierpinski carpet (Figure 4.3d-f). Figure 4.3a-c shows the construction of the first three generations \((n = 0, 1, \text{ and } 2)\) of the Sierpinski carpet. The 0\(^{th}\) generation, which is also called the initiator of the Sierpinski carpet, is an empty square (Figure 4.3a). If the 0\(^{th}\) generation is divided into 9 equal square sections and the central section is filled with a solid square, then the 1\(^{st}\) generation is formed (Figure 4.3b). If this process is continued recursively for the 8 remaining empty squares in the 1\(^{st}\) generation, the 2\(^{nd}\) generation is formed (Figure 4.3c). Higher generations are similarly generated by replicating this process, which can be continued
indefinitely. The circular-based Sierpinski carpet is also constructed by following the same rules as in the Sierpinski carpet generation; however, instead of fully filling the central square with solid material, a circle is inscribed. Figure 4.3d-f shows the construction of the first three generations of the circular-based Sierpinski carpet.

4.3.2 Analytical Model

The analytical tortuosity calculations that follow are proposed as an alternative approach to that presented by Li and Yu [67] for the deterministic Sierpinski carpet. It should be noted that hydraulic tortuosities have not been calculated in our work. Instead, analytical tortuosities have been calculated, where straight pathways follow the direction of the macroscopic flux touching and tracing around the grain boundaries and passing through pore space. In reality, fluid particles are expected to travel through smoothed streamlines. The simplifying assumptions in our method can be summarized as below:

(i) the fluid is considered to be arbitrarily compressible,
(ii) vortex generation within the porous media is neglected.

According to the definition of the analytical tortuosity given above, there are some expected deviations from the hydraulic tortuosity values. Assumption (i) leads to a comparative underestimation of tortuosity due to artificially straight flow paths in the void regions; the flow far from the solid particles would have had some curvatures due to the streamlines around the solid particles in a hydraulic simulation. Assumption (ii), on the other hand, leads to an overestimation of tortuosity; the neglected vortices would have made a portion of the pores inaccessible to incoming fluid particles, resulting in less tortuous flow paths (it should be noted that the particles in the recirculation regions are not considered in tortuosity calculations because they do not enter or exit the domain). Matyka and Koza [167] showed that the hydraulic tortuosity is lower than the analytical prediction, which led us to expect that the overestimating effect of Assumption (ii) dominates the counteracting underestimating effect of Assumption (i). It should be noted that the straight flow paths resulted from Assumption (i) may not be physical. Nonetheless, as discussed above, since Assumption (i) and (ii) have counteracting effects on the tortuosity values, it is expected that the tortuosity values calculated using the presented analytical approach are physically representative.
Analytical tortuosity of a single particle pathway is given by:

$$\tau = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \frac{L_{pi}}{L},$$

(4.4)

where $L_{pi}$ is the length of the $i^{th}$ particle pathway, $L$ is the length of the domain, and $\frac{L_{pi}}{L}$ is the tortuosity of the $i^{th}$ particle pathway. The overall tortuosity of the domain is, however, calculated as the weighted average of tortuosities over an infinite number of particle pathways. Based on this definition with the assumption of laminar flow, the tortuosity is equal to unity ($\tau_0 = 1$) within the initiator ($0^{th}$ generation) of the Sierpinski carpet.

### 4.3.3 Sierpinski Carpet

Figure 4.4 illustrates the analytical derivation of the tortuosity within the 1st generation of the Sierpinski carpet.

The 1st generation of the Sierpinski carpet was segmented into three equally-sized sections. Since each section constitutes of 1/3 of the total area, the overall tortuosity of the 1st generation of the Sierpinski carpet can be expressed as:

$$\tau_1 = \frac{1}{3} \tau_u + \frac{1}{3} \tau_{1m} + \frac{1}{3} \tau_l,$$

(4.5)

where $\tau_u$, $\tau_l$, and $\tau_{1m}$ represent the tortuosities of the upper, lower and the middle sections of the 1st generation of the Sierpinski carpet. According to Assumption (i) stated earlier, the flow within the upper and lower 1/3 of the Sierpinski carpet (as represented by flow along path $AB$ in
Figure 4.4) was straight, and the tortuosity in the upper and lower sections are approximated to be $\tau_0$ (unity). As a result, $t_1$ can be written as:

$$t_1 = \frac{2}{3} \tau_0 + \frac{1}{3} \tau_{1m}. \quad (4.6)$$

The middle section, however, can be divided further into three more sections: one central and two outer sections as shown in Figure 4.4. Therefore, the tortuosity in the middle section, $\tau_{1m}$, can be written as:

$$t_{1m} = \frac{2}{3} \tau_{1m0} + \frac{1}{3} \tau_C, \quad (4.7)$$

where $\tau_{1m0}$ and $\tau_C$ represent the tortuosity in the middle outer and the central sections of the 1st generation of the Sierpinski carpet. Due to the geometric similarity between the middle outer sections and the 0th generation of the Sierpinski carpet, the tortuosity in these sections are approximated with $\tau_0$. The tortuosity in the middle section can be expressed as:

$$t_{1m} = \frac{2}{3} \tau_0 + \frac{1}{3} \tau_C. \quad (4.8)$$

This is the point where our approach diverges from the earlier method presented by Li and Yu [67] as they considered:

$$t_{1m} = \frac{7}{6} t_1. \quad (4.9)$$

Combining Equations 4.6 and 4.8 will result in the following expression for the overall tortuosity of the 1st generation:

$$t_1 = \frac{8}{9} \tau_0 + \frac{1}{9} \tau_C. \quad (4.10)$$

Similarly, for the 2nd generation, the tortuosity in the upper, lower and the middle outer sections can be approximated with $t_1$ and written as:

$$t_2 = \frac{8}{9} t_1 + \frac{1}{9} \tau_C. \quad (4.11)$$

In a similar fashion, it follows that the overall tortuosity for the nth generation is:

$$t_n = \frac{8}{9} t_{n-1} + \frac{1}{9} \tau_C, \quad (4.12)$$

which is a recursive expression that can also be written as:
\[ \tau_n = \frac{8}{9} \tau_{n-2} + \frac{1}{9} \tau_c + \frac{1}{9} \tau_c. \] (4.13)

If the expression inside the bracket is further expended, it leads to the following formula for the \( n^{th} \) generation tortuosity:

\[ \tau_n = \left( \frac{8}{9} \right)^n \tau_0 + \frac{1}{9} \tau_c \left[ \left( \frac{8}{9} \right)^{n-1} + \left( \frac{8}{9} \right)^{n-2} + \cdots + \left( \frac{8}{9} \right)^0 \right]. \] (4.14)

Since \( \tau_0 = 1 \):

\[ \tau_n = \left( \frac{8}{9} \right)^n + \frac{1}{9} \tau_c \sum_{i=0}^{n-1} \left( \frac{8}{9} \right)^i. \] (4.15)

The summation term in Equation 4.15 can be expressed as:

\[ \sum_{i=0}^{n-1} \left( \frac{8}{9} \right)^i = -9 \left[ \left( \frac{8}{9} \right)^n - 1 \right]. \] (4.16)

Combining Equation 4.15 and 4.16 results in \( \tau_n \), written as a function of the generation number, \( n \):

\[ \tau_n = \left( \frac{8}{9} \right)^n + \tau_c \left( 1 - \left( \frac{8}{9} \right)^n \right). \] (4.17)

The porosity of a material can also be calculated as the weighted average of the porosities of its sections:

\[ \phi_n = \left( \frac{8}{9} \right)^n + \frac{1}{9} \phi_c \sum_{i=0}^{n-1} \left( \frac{8}{9} \right)^i. \] (4.18)

Therefore, the porosity of the Sierpinski carpet fractal and the circular-based Sierpinski carpet can be calculated using the following expression:

\[ \phi_n = \left( \frac{8}{9} \right)^n + \phi_c \left( 1 - \left( \frac{8}{9} \right)^n \right), \] (4.19)

where \( \phi_c \) is the porosity of the central section. After a set of algebraic manipulations of Equations 4.17 and 4.19, a general form of the tortuosity-porosity correlation can be found for the fractals with Sierpinski carpet structure:

\[ \tau_n = \frac{1 - \tau_c}{1 - \phi_c} (\phi_n - \phi_c) + \tau_c. \] (4.20)
As defined above, the tortuosity in the central section, $\tau_C$, can be expressed as the average tortuosity values (over an infinite number of particle pathways around the central grain). Due to the square grain in the Sierpinski carpet, this is equivalent to the average value of the most and least tortuous flow paths in this section (CD and EF in Figure 4.4), which is $\tau_C = \frac{2+1}{2} = \frac{3}{2}$. For the Sierpinski carpet fractal, $\phi_C$ is zero, as the entire centre cell is occupied by the square grain. Substituting $\tau_C$ and $\phi_C$ into Equation 4.20 results in the following expression for overall tortuosity for the $n^{th}$ generation (valid for $\phi_n \in [0,1]$):

$$\tau_n = \frac{3}{2} - \frac{\phi_n}{2}.$$  \hspace{1cm} (4.21)

By substituting $\phi_C$ of the Sierpinski carpet (Equation 4.19), the porosity of such porous media takes on the following form:

$$\phi_n = \left(\frac{8}{9}\right)^n,$$  \hspace{1cm} (4.22)

### 4.3.4 Circular-based Sierpinski Carpet

Using the same analogy for the circular-based Sierpinski carpet, the tortuosity of the $n^{th}$ generation of the circular-based Sierpinski carpet will follow the same form as Equation 4.20. To calculate the tortuosity in the central section, $\tau_C$, however, the average tortuosity (over the most and least tortuous flow paths in the central section) cannot be simply used as it was done for the Sierpinski carpet analysis. Instead, an infinite number of particle pathways travelling around the central grain must be considered to calculate the average tortuosity.

![Figure 4.5 Schematic of particle pathways through the 1st generation of the circular-based Sierpinski carpet.](image_url)
Due to symmetry, the tortuosity of the central section of the circular-based Sierpinski carpet, \( \tau_C \), can be calculated by integrating the tortuosity function (Equation 4.23) of the ABC flow path shown in Figure 4.5 from 0 to \( R \). The tortuosity function of the ABC flow path is given by:

\[
\tau_C(\theta) = \frac{\overline{AB} + \overline{BC}}{R} = \frac{R(1-\cos(\theta)) + R(\frac{\pi}{2} - \theta)}{R} = \left(1 + \frac{\pi}{2}\right) - (\theta + \cos(\theta)),
\]

where \( \theta \) is the angle \( \angle BOD \) as described in Figure 4.5. To obtain the tortuosity of the central section, this function has to be integrated along the vertical direction over \( 0 < \chi < R \) with equal vertical steps. According to Figure 4.5, angle \( \theta \) can be expressed as:

\[
\theta = \sin\left(\frac{\chi}{R}\right),
\]

thus, combining Equations 4.23 and 4.24 leads to the following expression for the tortuosity of any arbitrary particle pathway in the central section of the circular-based Sierpinski carpet:

\[
\tau_C(\chi) = \left(1 + \frac{\pi}{2}\right) - \left[\sin\left(\frac{\chi}{R}\right) + \cos\left(\sin\left(\frac{\chi}{R}\right)\right)\right].
\]

Integrating \( \tau_C(\chi) \) over \( 0 < \chi < R \) will result in the following expression for the average tortuosity in the central section of the circular-based Sierpinski carpet:

\[
\tau_C = \int_0^R \tau_C(\chi) d\chi = 2 - \frac{\pi}{4}.
\]

Furthermore, one can show that the porosity of the central section in the circular-based Sierpinski carpet is:

\[
\phi_C = \frac{4R^2 - \pi R^2}{4R^2} = 1 - \frac{\pi}{4}.
\]

Substituting \( \tau_C \) from Equation 4.26 and \( \phi_C \) from Equation 4.27 back into Equation 4.20, the tortuosity-porosity correlation for the circular-based Sierpinski carpet is given by:

\[
\tau_n = \left(1 - \frac{4}{\pi}\right) \phi_n + \frac{4}{\pi}.
\]

Furthermore, after substituting \( \phi_C \) of the circular-based Sierpinski carpet (Equation 4.19), the porosity of the \( n^{th} \) generation of the circular-based Sierpinski carpet takes on the following form:

\[
\phi_n = 1 - \frac{\pi}{4} \left(1 - \left(\frac{8}{9}\right)^n\right).
\]
It should be noted that both of the above calculated tortuosity-porosity correlations (Equations 4.21 and 4.28) are applicable across generations of their respective geometries, i.e. \( n \in \{0, 1, 2, \ldots, \infty\} \). As a result, their range of validity is \( \phi \in (0,1] \) for the Sierpinski carpet and \( \phi \in \left(1 - \frac{\pi}{4}, 1\right] \) for the circular-based Sierpinski carpet. Note that \( \phi = 0 \) and \( 1 - \frac{\pi}{4} \) are the limiting porosities for the Sierpinski carpet and the circular-based Sierpinski carpet, where the limits occur when \( n \to \infty \).

4.4 Results and Discussion

In this section, the obtained tortuosity-porosity correlations will be compared with existing tortuosity-porosity relationships in the literature. Two relationships similar to the linear correlations calculated here have been previously reported by other researchers [53,69,165]:

\[
\tau = 1 + p(1 - \phi), \tag{4.30}
\]

\[
\tau^2 = 1 + q(1 - \phi), \tag{4.31}
\]

where \( p \) and \( q \) are adjusting parameters. Equation 4.30 was proposed by Feranie and Latief [69] for the tortuosity in randomized Sierpinski carpets (RSCs) with \( p = 0.799 \) for the porosity range of \( \phi \in (0.3 - 0.7) \). The same form of tortuosity-porosity correlation (Equation 4.30) was one of the suggested correlations by Koponen et al. [53] after they solved the flow equations for a porosity range of \( \phi \in [0.5, 1] \) for randomly placed squares with free overlapping using Lattice Gas Automata (LGA). Equation 4.31 was determined empirically by Iversen and Jørgensen [165] for sandy \( (q = 2) \) or clay-silt \( (q = 3) \) sediments over the porosity range of \( \phi \in (0.4 - 0.9) \). It should be noted that even though the work by Iversen and Jørgensen [165] was based on diffusive tortuosities, it should be reasonable to use their results for the verification of analytical (straight-line based) tortuosity values. According to Ghanbarian et al. [44], in the Sierpinski carpet (as employed in this work), the straight-line based tortuosity will match the diffusive tortuosity under the assumptions of steady state and established concentration gradient conditions.

Regression analyses were performed to find the suitable \( p \) and \( q \) that fit to our analytical model. Since \( p \) is the adjusting parameter in the linear tortuosity-porosity correlation (Equation 4.30)
and our analytical approach also led to a linear tortuosity-porosity correlation, one can use any number of generations of the analytical results (> 2) in the regression analysis to calculate the exact value of $p$ for both geometries. As for $q$, we used 8 and 12 generations of the analytical results in the regression analyses for the Sierpinski carpet and the circular-based Sierpinski carpet, respectively. These numbers of generations were selected since $q$ is the adjusting parameter for the Equation 4.31 that has been reported by Iversen and Jørgensen [165] to be only valid over the approximate porosity range of $\phi \in (0.4 - 0.9)$. Our nonlinear regression analyses involved the Generalized Reduced Gradient (GRG2) algorithm [168]. The error function for the GRG2 algorithm was defined as the square root of the sum-squared difference between the tortuosity values from the present study and those generated by Equations 4.30 and 4.31. Implementing the regression analysis for the Sierpinski carpet, it was found that Equations 4.30 and 4.31 provided a satisfactory fit with $p = 0.500$ and $q = 1.122$. Meanwhile, $p = \frac{4}{\pi} - 1$ and $q = 0.583$ were found to provide satisfactory fit for the circular-based Sierpinski carpet. $p$ and $q$ are adjusting parameters obtained by fitting the previously reported tortuosity-porosity correlations [53,69,165] to our analytically derived tortuosity values. The coefficient of determination was found to be 1 for Equation 4.30 for both the Sierpinski carpet and the circular-based Sierpinski carpet. However, the coefficients of determinations were found to be 0.9997 and 0.9992 for Equation 4.31 for the Sierpinski carpet and the circular-based Sierpinski carpet, respectively.

Our tortuosity-porosity correlations (Equations 4.21 and 4.28) are in agreement with the two aforementioned correlations (Equations 4.30 and 4.31): each correlation follows a linear trend (as in Equation 4.21, 4.28, and 4.30) or a close-to-linear trend (as in Equation 4.31). The difference between our analytically-determined adjusting parameters and those from previous studies can be attributed to (i) the differing geometry of pore spaces used in each study and (ii) the simplifying assumptions used in our analytical model. Figure 4.6 provides a comparative view of the tortuosity values obtained by the present analytical model (Equation 4.21) for the Sierpinski carpet with those correlations stated above (Equations 4.30 and 4.31) [69,165].
Figure 4.6 Analytical tortuosity values of the Sierpinski carpet from present study versus tortuosity values obtained from previous correlations [69,165] with new adjusting parameters determined through regression analysis.

Figure 4.7 provides a comparative view of the present analytical model (Equation 4.28) for the circular-based Sierpinski carpet with previous empirical correlations reported by other researchers (Equations 4.30 and 4.31) [69,165]. This comparison shows that the same form of tortuosity-porosity correlations proposed by other researchers [69,165] can still be applied to the Sierpinski carpet with the modified adjusting parameters. Furthermore, this agreement between our correlations and the ones reported by others [53,69,165] validates our proposed analytical approach for estimating tortuosity.
Figure 4.7 Analytical tortuosity values of the circular-based Sierpinski carpet from present study versus tortuosity values obtained from previous correlations [69,165] with new adjusting parameters determined through regression analysis.

It can be observed from Equation 4.19 that the tortuosity-porosity correlation for any deterministic fractals with Sierpinski carpet structure has a linear form. In addition, because $\tau_C$ and $\phi_C$ are constant with respect to any repeating shape, it can be expected that this linear correlation comes with a distinct slope for any other shaped repeating element in the Sierpinski carpet structure. Coefficient $p$ in Equation 4.30 can be expressed in terms of $\tau_C$ and $\phi_C$ as follows:

$$p = -\frac{1-\tau_C}{1-\phi_C} \quad (4.32)$$

As shown above, the analytical tortuosity-porosity correlations would be linear for any deterministic fractals that follow the Sierpinski carpet structure regardless of the shape of the grains (square, circle, etc). This linearity of the analytical tortuosity-porosity correlations may be counter-intuitive when compared to some tortuosity-porosity correlations presented by Ghanbarian et al. [44] where tortuosity approached infinity as porosity approached a critical value. This discrepancy can be attributed to two possible reasons:

(i) The structured nature of the Sierpinski carpet: e.g. however much solid is added to the domain, the solids do not overlap or touch each other. Therefore, pathway deviations are local and insignificant. Figure 4.8 provides an example of a highly structured porous
material that illustrates how the tortuosity does not approach infinity when the porosity approaches its limiting value \((\phi = 0)\).

(ii) The simplified tortuosity definition and underlying assumptions associated with the analytical model (Section 4.3.2).

![Diagram](image)

Figure 4.8 An illustration of a highly structured porous media (where tortuosity does not approach infinity when \(\phi \to 0\))

We, however, expect that reason (i) is the dominating factor: Matyka and Koza [167] demonstrated that analytical tortuosity provides an overestimation of hydraulic tortuosity; therefore, an upper bound is expected for hydraulic tortuosity values since an upper bound was observed for the analytical tortuosity values calculated in this work.

Figure 4.9 provides a comparative view the analytical tortuosity-porosity correlations for the Sierpinski carpet with the circular-based Sierpinski carpet where the limiting porosities for both geometries are also reflected.
As it can be observed, the dashed line representing the tortuosity-porosity correlation for the Sierpinski carpet covers the entire porosity range of $\phi \in (0, 1]$. This range for the circular-based Sierpinski carpet is $\phi \in \left(1 - \frac{\pi}{4}, 1\right]$. The lower bounds in both cases indicate the limiting porosities as Equation 4.18 reduces to $\phi_C$ when $n \to \infty$. The limiting porosity and the tortuosity-porosity correlation both vary with the shape of the grain (square to circle), despite the identical location of the grains in the porous structures (same configurations).

### 4.5 Conclusions

In this study, a new analytical approach was proposed and applied to calculate tortuosity-porosity correlations in the Sierpinski carpet ($\tau_n = \frac{3}{2} - \frac{\phi_n}{2}$). A tortuosity-porosity correlation was also obtained for the circular-based Sierpinski carpet ($\tau_n = \left(1 - \frac{4}{\pi}\right) \phi_n + \frac{4}{\pi}$) applicable for the infinite generation, which would have been computationally prohibitive to obtain numerically. From Equations 4.21 and 4.28, it is evident that the tortuosity obtained from both geometries exhibited linear relationships. This observation is in agreement with the trend proposed by Koponen et al.
[53] and Feranie and Latief [69]. However, our findings starkly contrast the trend for the Sierpinski carpet tortuosity presented by Li and Yu [67].

In this work, it was also shown that the limiting porosity and the tortuosity-porosity correlations in the porous media of the same structure could be impacted by the shape of the grains. Nonetheless, the linear trend in tortuosity-porosity correlations remained unaffected by the shape of the grain.

It was shown how the tortuosity values calculated from a 2D analytical model for the Sierpinski carpet fractal and the circular-based Sierpinski carpet follow a similar correlation (linear or close-to-linear) proposed by previous researchers. The corresponding adjusting parameters were then calculated for each structure.

The present model is a conceptual tool which can provide profound insights on how estimates of effective flow and transport properties for continuum models of low-porosity fractal formations can be determined. As an extension to this study, it would be helpful to investigate how the tortuosity values from a 3D analytical model compare to previous studies. Additionally, it would be interesting to show the dependence of the tortuosity-porosity correlation adjusting parameters on the rotation of the entire Sierpinski carpet or the individual grains.
5 Conclusions and Recommendations

In this thesis, LBM and a novel analytical approach were developed for determining continuous permeability-porosity and tortuosity-porosity relationships in porous media. The numerical tool has the advantage of being applied to complex domains and boundary conditions. The numerical model is also a powerful tool for stochastic and parametric studies because the geometry of the digitally-constructed medium can be varied rapidly and arbitrarily. However, capabilities of numerical modelling are limited to the available computational resources and therefore, challenges may arise when encountering geometries with substantial disparity in length scales. Conversely, analytical tools proved to be highly capable of handling such domains with substantial disparity in length scales.

5.1 Conclusions and Contributions

In Chapter 2, the permeabilities of two simulated porous structures: periodic arrays of a) staggered parallel infinite cylinders and b) spheres were calculated using LBM. Using the numerically calculated permeabilities, $C_{KC}$ was modified to enable the KC equation to produce permeability values that closely matched the numerical values. It was found that an algebraic function for $C_{KC}$ provided the most accurate prediction of the KC equation for the geometries examined.

In Chapter 3, stochastic numerical modelling was performed to investigate the impact of the geometric properties of the individual grains (such as grain aspect ratio) on the tortuosity-porosity relationships in porous media. It was found that:

- tortuosity exhibits an inverse relationship with the porosity that can be expressed in logarithmic form.
- tortuosity increases with increasing grain aspect ratio.
- the effect of grain aspect ratio on the tortuosity diminishes as the porosity approaches unity. Therefore, it is expected that accurate characterization of porous media in terms of the grain aspect ratio becomes critical in predicting tortuosity and resolving fluid flow in low porosity formations.
• a minimum of 6, 8 and 10 stochastic simulations were required to calculate the average tortuosity values in laminar flow ($Re \ll 1$) simulations of the simulated 2D domains for aspect ratios of 1, 2 and 3, respectively.

In Chapter 4, a novel analytical approach was proposed and implemented to investigate the relationships between tortuosity and porosity within the Sierpinski carpet and the circular-based Sierpinski carpet. It was found that the tortuosity-porosity correlations in such deterministic fractals are linear and the tortuosity has an upper bound in the limiting porosity. Additionally, it was found that the value of the limiting porosity and the slope of the linear tortuosity-porosity correlation could be impacted by the shape of the grain.

In summary, LBM was used in this thesis to study the fluid flow in various forms of porous media to characterize transport properties such as permeability and tortuosity. This highly-parallelizable numerical tool has the capability to be used for larger and more complex geometries. Additionally, a novel analytical approach was introduced and implemented to characterize tortuosity in fractal geometries. These methodologies can be further utilized to improve continuous permeability-porosity and tortuosity-porosity relationships for other forms of porous media. These continuous relationships are critical for continuum-scale fluid simulations in porous materials.

5.2 Future Work

The following areas of research are recommended for future work:

• Reconstructed porous domains from computed tomography (CT) images could be used in LBM. Domains reconstructed from CT images have the potential to be more representative of the porous material under investigation.

• Parametric studies could be performed using the stochastic modelling approach presented in Chapter 3. One could determine the impact of parameters, such as: grain shape, grain orientations, etc. on transport properties (tortuosity, permeability, etc.). This study can also be extended to incorporate 3D domains.
The analytical approach presented in Chapter 4 for calculating tortuosity in fractals can be further modified and improved based on the results of the numerical tools. One may use regression analysis to define new adjusting parameters to the analytical correlations by fitting the analytical correlations to the numerical results. As mentioned earlier, numerically modelling fractals becomes increasingly difficult as the generation number increases (due to the substantial disparity in length scales). Therefore, one can only typically use the first few generations of a fractal for the regression analysis (to inform analytical correlations). An analytical model modified via a regression analysis could be representative for high generations of the fractals.
References


[168] Lasdon L, Waren A. Generalized reduced gradient software for linearly and nonlinearly constrained problems. Austin, Texas, USA: Graduate School of Business, University of Texas; 1977.
Appendix I

This appendix is intended to provide more data for validation purposes in order to help in the reproduction of the work:

Case 1. Poiseuille flow between two parallel plates

In the first validation step, a simulation of Poiseuille flow between two parallel plates was performed, similar to what Durst et al. [152] have performed. For the validation purposes, the developing velocity profile was obtained from our MRT model and compared it to the one obtained from our previously published SRT method [153]. An excellent agreement between these two models was demonstrated in Figure A-1 and Figure A-2. Secondly, the entry length calculated from our MRT model was compared to the model proposed by Durst et al. [152].

The parameters used in the MRT model are presented in the table below:

<table>
<thead>
<tr>
<th>Physical properties</th>
<th>Relaxation parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain length, $n_x = 400$</td>
<td>$s_1 = 0$</td>
</tr>
<tr>
<td>Domain height, $n_y = 41$</td>
<td>$s_2 = s_3 = \frac{1}{\tau}$</td>
</tr>
<tr>
<td>Inlet Velocity, $U_{in} = 0.02$</td>
<td>$s_4 = 0$</td>
</tr>
<tr>
<td>Density, $\rho_{out} = 1.0$</td>
<td>$s_5 = s_7 = \frac{(2\tau - 1)}{8\tau - 1}$</td>
</tr>
<tr>
<td>Relaxation time, $\tau = 0.8$</td>
<td>$s_6 = 0$</td>
</tr>
<tr>
<td>Reynolds number, $Re = 7.8$</td>
<td>$s_8 = s_9 = \frac{1}{\tau}$</td>
</tr>
</tbody>
</table>
Figure A-10. Developing velocity profile computed by the MRT LBM.

Figure A-11. Developing velocity profile computed by the SRT LBM.

As shown in Figures A-1 and A-2, and as it was expected from the literature, the maximum velocity occurred at the centreline and it reached to 1.5 times of the inlet velocity (according to the analytical solution for Poiseuille problem between two parallel plates) at its fully developed
condition. The maximum velocity was used as a measure to determine the entry length. Based on a widely-used criterion, entry length is defined as where the maximum (centreline) velocity reaches to 99% of its analytical value for fully developed flow. Beyond the entry length, the flow is called fully-developed. Figure A-3 shows how the entry length was calculated in our model.

![Figure A-12. Centreline velocity development along the channel.](image)

Durst et al. [152] has proposed the equation below for the entry length:

\[
\frac{L_e}{D} = \left[ (0.631)^{1.6} + (0.0442 \, Re)^{1.6} \right]^{1/6},
\]  

(A-1)

where \(L_e, D\) and \(Re\) are entry length, height of the channel (spacing between two parallel plates) and the flow Reynolds number, respectively. Durst et al. [152] (Equation A-1) estimates a value of \(\frac{L_e}{D} = 0.77\) and our MRT LBM predicts a value of \(\frac{L_e}{D} = 0.81\) for the entry length of the channel.

Case 2. Flow over backward-facing step

The second case in our validation process was a flow over backward-facing step. This flow is widely used for validation purposes by numerical modellers. At this step, our results obtained from the LB simulations was compared with the ones measured experimentally by Kueny et al. [154]. Figure A-4 shows the geometry used in our simulations as well as setup used in the experiment performed by Kueny et al. [154]. Tables A-2 and A-3 list experimental conditions in Kueny’s experiment and simulation parameters in our MRT model.
Figure A-13. Schematic of the backward-facing step used in our model.

Table A-4. Experimental conditions used by Kueny et al. [154]

<table>
<thead>
<tr>
<th>Channel/flow parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upstream height $h$</td>
<td>2cm</td>
</tr>
<tr>
<td>Downstream height $H$</td>
<td>3cm</td>
</tr>
<tr>
<td>Step Height $hs = H - h$</td>
<td>1cm</td>
</tr>
<tr>
<td>Maximal velocity $U_{Max}$</td>
<td>7.23 cm/s</td>
</tr>
<tr>
<td>Reynolds number $Re = \frac{U_{Max} hs}{v}$</td>
<td>50</td>
</tr>
</tbody>
</table>

Table A-5. Numerical model parameters

<table>
<thead>
<tr>
<th>Upstream Channel Length, $T_x$</th>
<th>100</th>
<th>Inlet Velocity, $U_{in}$</th>
<th>0.111</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step Height, $T_y$</td>
<td>30</td>
<td>Density, $\rho$</td>
<td>1.0</td>
</tr>
<tr>
<td>Domain length, $n_x$</td>
<td>370</td>
<td>Relaxation time, $\tau$</td>
<td>0.8</td>
</tr>
<tr>
<td>Domain height, $n_y$</td>
<td>92</td>
<td>Reynolds number, $Re$</td>
<td>50</td>
</tr>
</tbody>
</table>
Numerical model parameters were set to replicate the experimental conditions, such as $Re = 50$:

$$Re = \frac{u_{Max} h_s}{v} = \frac{\frac{2}{3}U_{h_0} h_s}{\frac{1}{3}(\tau - 0.5)} = \frac{\frac{2}{3}(0.111)(3.0)}{\frac{1}{3}(0.8 - 0.5)} \approx 50.$$ (A-2)

Figure A-5 shows the velocity profiles for the flow over the backward-facing experiment with $Re = 50$ which is in agreement with the experimentally-determined representative velocity profiles obtained by Kueny et al. [154] (Figure A-6).

![Figure A-14. Velocity profile for the flow with $Re = 50$.](image)
Figure A-15. Velocity profile (Re = 50) from the experimental work by Kueny et al. [154].
In addition to the velocity profile, a comparison between the streamline patterns obtained from the LB model and the ones reported by Kueny et al. [154] was performed. Figures A-7 and A-8 show an excellent agreement between the numerical and experimental results. For example, the dimensionless length of the separation region is calculated to be approximately 3 in both numerical and experimental studies presented here:

**Figure A-7.** Streamline patterns (Re = 50) obtained by the MRT LBM.

**Figure A-8.** Streamline patterns (Re = 50) from the experimental work by Kueny et al. [154].

**Summary**

A multiple-relaxation time (MRT) lattice-Boltzmann model (LBM) was developed and validated with two experiments: (i) Poiseuille flow between two parallel plates, and (ii) laminar flow over backward-facing step. In the first case, the developing velocity profile of a Poiseuille flow
between two parallel plates was shown. It was shown that the maximum centreline velocity was equal to its analytical value \( \left( \frac{3}{2} U_{in} \right) \). Furthermore, the entry length obtained from the LB simulations was compared to the entry length estimated by an empirical equation proposed by Durst et al. [152] and the results showed agreement \( \frac{L_e}{D} = 0.81 \) from the LBM vs. \( \frac{L_e}{D} = 0.77 \) from the empirical equation). In the second experiment, the velocity profiles and the streamline patterns obtained from our numerical method were compared to the ones from an experimental study by Kueny et al. [154]. An excellent agreement between the results was observed. For instance, the dimensionless length of the recirculation zone was found to be equal to approximately 3 in both studies.
Appendix II

This Appendix is intended to provide implementations of the LBM method in various case scenarios. In general, an LB model goes through the following steps:

- Initialize the variables, do the unit conversion
- Initialize the domain using the macroscopic parameters
- Calculate equilibrium from initialized macroscopic domain
- Initialize $f$ values on each node
- Perform collision on each node
- Perform streaming on each node
- Set boundary conditions
- Calculate macroscopic parameters on each node
- Calculate $f^{eq}$ on each node
- If not converged, repeat steps from collision step …

Below is my detailed step-by-step implementation of SRT LBM for D2Q9:

1. Initialization and defining parameters

```plaintext
ex = [ 1 0 -1 0 1 -1 -1 1 0 ]; %D2Q9 lattice parameters
ey = [ 0 1 0 -1 1 1 -1 -1 0 ];
w = [ 1/9 1/9 1/9 1/9 1/36 1/36 1/36 1/36 4/9 ];
cs = 1/sqrt(3);  % Cs sound speed

Uinitial = 0.000;  % Uinitial in lattice Units
Vinitial = 0.000;  % Vinitial in lattice Units
Rhoinitial = 1.0;  % Rhoinitial in lattice Units
Tau = 0.80;  % Tau - Relaxation time

Gx = 1e-4;  % Body force in lattice units in x direction
Gy = 0;  % Body force in lattice units in y direction
dx = 1e-4;  % dx is 1 in lattice units, which is equal to 1e-4 meters in physical units
dt = 1e-5;  % dt is 1 in lattice units, which is equal to 1e-5 seconds in physical units
Utol = 1e-4;  % Tolerance of U for convergence, if Residual is smaller than this value, the code is converged
Vtol = 1e-4;  % Tolerance of V
Uresidual = 100;  % set to a huge value for the first iteration,
Vresidual = 100;  % set to a huge value for the first iteration,
```
%define the parameters
f    = zeros(nx,ny,9);
ftemp= zeros(nx,ny,9);
feq  = zeros(nx,ny,9);
U    = zeros(nx,ny);
V    = zeros(nx,ny);
Uold = zeros(nx,ny);
Vold = zeros(nx,ny);
Rho  = zeros(nx,ny);

%%%%%%%%%%%%%%%%%%
% Initialization macroscopic parameters
U(:,:,1) = Uinitial ;
V(:,:,1) = Vinitial ;
Rho(:,:,1) = Rhoinitial ;
Uold = U ;
Vold = V ;

2. Calculating equilibrium distribution function
for J = 1 : ny
    for I = 1 : nx
        for a = 1 : 9
            feq(I,J,a) = w(a) * Rho(I,J) * ( 1.0 +
            3.0*(ex(a)*U(I,J)+ey(a)*V(I,J)) ... + 9.0/2.0*(
            ex(a)*U(I,J)+ey(a)*V(I,J))^2 ...
            - 3.0/2.0* ( U(I,J)^2 +
            V(I,J)^2 )
        end
    end
end

3. Collision step
% Body force implementation, Approach 1
g = w .* 1 .* (Gx .* ex + Gy .* ey) ./ cs^2 ; % as everything is in lattice units, dt is set equal to 1
for J = 1 : ny
    for I = 1 : nx
        if isfluid(I,J)==1
            for a = 1 : 9
                temp = f(I,J,a) - ( f(I,J,a) - feq(I,J,a) ) / Tau +
g(a) ; % Collision on each site, for each direction
                f(I,J,a) = temp ;
            end
        end
    end
end
4. Streaming step

```matlab
% set periodic boundary conditions on both sides
for J = 1 : ny
    if (J>1)
        JN = J - 1 ;
    else
        JN = ny ; % in periodic boundary condition in the y direction, the row before the first row is the last row
    end

    if (J<ny)
        JP = J + 1 ;
    else
        JP = 1 ; % in periodic boundary condition in the y direction, the row after the last row is the first row
    end

    for I = 1 : nx
        if (I>1)
            IN = I - 1 ;
        else
            IN = nx ; % in periodic boundary condition in the x direction, the column before the first column is the last column
        end

        if (I<nx)
            IP = I + 1 ;
        else
            IP = 1 ; % in periodic boundary condition in the x direction, the column after the last column is the first column
        end

        ftemp(IP,J,1) = f(I,J,1) ; % 8 distributions sitting on node(I,J) flies to 8 neighboring nodes for the next time step
        ftemp(I ,JP,2) = f(I,J,2) ;
        ftemp(IN,J ,3) = f(I,J,3) ;
        ftemp(I ,JN,4) = f(I,J,4) ;
        ftemp(IP,JP,5) = f(I,J,5) ;
        ftemp(IN,JP,6) = f(I,J,6) ;
        ftemp(IN,JN,7) = f(I,J,7) ;
        ftemp(IP,JN,8) = f(I,J,8) ;
        ftemp(I ,J ,9) = f(I,J,9) ; % the distribution at the center, (0,0), stays untouched
    end
end

f = ftemp ; % Update the distribution values
```

5. Bounce-back solid wall boundary treatment

```matlab
for J = 1 : ny
    for I = 1 : nx
        if isfluid(I,J)==0
```
temp = f(I,J,1); % directions of particles are switched to ensure zero velocity in all directions
f(I,J,1) = f(I,J,3);
f(I,J,3) = temp;

temp = f(I,J,2);
f(I,J,2) = f(I,J,4);
f(I,J,4) = temp;

temp = f(I,J,5);
f(I,J,5) = f(I,J,7);
f(I,J,7) = temp;

temp = f(I,J,6);
f(I,J,6) = f(I,J,8);
f(I,J,8) = temp;
end
end

end

6. Calculation of macroscopic parameters

Rhotemp = 0; % a temporary variable to calculate summation
MomtempX = 0;
MomtempY = 0;
for J = 1 : ny
  for I = 1 : nx
    if isfluid(I,J) == 1
      for a = 1 : 9
        Rhotemp = Rhotemp + f(I,J,a);
        MomtempX = MomtempX + f(I,J,a)*ex(a); % Momentum in x direction
        MomtempY = MomtempY + f(I,J,a)*ey(a); % Momentum in y direction
      end
      Rho(I,J) = Rhotemp; % Macroscopic density
      U(I,J) = MomtempX /Rho(I,J); % Macroscopic velocity in x direction
      V(I,J) = MomtempY /Rho(I,J); % Macroscopic velocity in y direction
      Rhotemp = 0;
      MomtempX = 0;
      MomtempY = 0;
    end
  end
end

end
Our implementation of the MRT LBM was based on the SRT LBM presented above except that the transformation matrix, $M$, relaxation rate matrix, $\hat{S}$, and the moments, $m$, were implemented as below:

\[
M = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 & -4 \\
-2 & -2 & -2 & 1 & 1 & 1 & 1 & 4 & 1 \\
1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 & 0 \\
-2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 & 0 \\
0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 & 0 \\
0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 & 0 \\
1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 0 \\
\end{bmatrix}
\]

\[
\text{invM} = \text{inv}(M) ;
\]

\[
\text{tau} = 0.8 ;
\]

\[
\text{s_e} = 1/\text{tau} ;
\]

\[
\text{s_eps} = 1/\text{tau} ;
\]

\[
\text{s_niu} = 1/\text{tau} ;
\]

\[
\text{s_q} = 8.0 \times (2-\text{s_niu})/(8-\text{s_niu}) ;
\]

\[
\text{S} = \text{diag}(\begin{bmatrix} 0.0, \text{s_e}, \text{s_eps}, 0.0, \text{s_q}, 0.0, \text{s_q}, \text{s_niu}, \text{s_niu} \end{bmatrix}) ;
\]

\[
\text{niu} = (\text{tau} - 0.5) / 3.0 ;
\]

\[
\text{zeta} = (1/\text{s_e} - 0.5) / 6.0 ;
\]

**Flow between parallel plates in MRT LBM**

Below is an implementation of the MRT LBM to model flow between parallel plates. Figure A-10 and A-12 can be obtained from the following code. Furthermore, inlet and outlet mass flow rates are calculated to ensure the continuity is satisfied:

\[
\text{clear all}
\]

\[
\text{for Uin} = 0.02 : 0.04 : 0.1
\]

\[
\text{nx} = 400 ;
\]

\[
\text{ny} = 41 ;
\]

\[
\text{ex} = \begin{bmatrix} 1 & 0 & -1 & 0 & 1 & -1 & 1 & 0 \end{bmatrix} ;
\]

\[
\text{ey} = \begin{bmatrix} 0 & 1 & 0 & -1 & 1 & 1 & -1 & 0 \end{bmatrix} ;
\]

\[
\text{w} = \begin{bmatrix} 1/9 & 1/9 & 1/9 & 1/9 & 1/36 & 1/36 & 1/36 & 4/9 \end{bmatrix} ;
\]

\[
\text{Vin} = 0 ;
\]

\[
\text{Rhoout} = 1.0 ;
\]
initial \( U = U \); 
\( V = 0.000 \); 
\( \rho_\text{initial} = \rho_\text{out}; \) 
\( \text{cs} = 1/\sqrt{3} \); 
\( G_x = 0.0 \); 
\( G_y = 0.0 \); 
\( dx = 1e^{-4} \); 
\( dt = 1e^{-5} \); 
\( U_{\text{tol}} = 1e^{-3} \); 
\( V_{\text{tol}} = 1e^{-3} \); 
\( U_{\text{residual}} = 100 \); 
\( V_{\text{residual}} = 100 \); 

\( f = \text{zeros (nx,ny,9)}; \) 
\( f_{\text{temp}} = \text{zeros (nx,ny,9)}; \) 
\( f_{\text{eq}} = \text{zeros (nx,ny,9)}; \) 
\( U = \text{zeros (nx,ny)}; \) 
\( V = \text{zeros (nx,ny)}; \) 
\( U_{\text{old}} = \text{zeros (nx,ny)}; \) 
\( V_{\text{old}} = \text{zeros (nx,ny)}; \) 
\( \rho = \text{zeros (nx,ny)}; \) 
\( \text{isfluid} = \text{ones(nx,ny)}; \) 
\( \text{isfluid}(:,:,1) = 0; \) 
\( \text{isfluid}(:,:,ny) = 0; \) 

\( M = [ \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 4 \\ -2 & 2 & -2 & 1 & 1 & 1 & 1 & 4 & -4 \\ 1 & 0 & -1 & 0 & 1 & -1 & 1 & 0 & 0 \\ -2 & 0 & 2 & 0 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 & 0 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & 0 \\ 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} ]; \) 

\( \text{invM} = \text{inv}(M); \) 
\( \tau = 0.8; \) 
\( \text{s_e} = 1/\tau; \) 
\( \text{s_\text{eps}} = 1/\tau; \) 
\( \text{s_\text{niu}} = 1/\tau; \) 
\( \text{s_q} = 8.0 * (2-s_\text{niu})/(8-s_\text{niu}) ; \) 

\( S = \text{diag([0.0, s_e, s_\text{eps}, 0.0, s_q, 0.0, s_q, s_\text{niu}, s_\text{niu}],0)}; \) 

\( \text{niu} = (\tau - 0.5) / 3.0; \) 
\( \text{zeta} = (1/s_\text{e} - 0.5) / 6.0; \) 

\( U(:,:,\) = \text{initial}; \) 
\( V(:,:,\) = \text{init}; \) 
\( \rho(:,:,\) = \text{rho}; \) 
\( \text{for J = 1 : ny} \) 
\( \text{for I = 1 : nx} \) 
\( \text{if isfluid(I,J)==0} \) 
\( U(I,J) = 0; \)
V(I,J) = 0 ;
end
end
Jx = Rho .* U ;
Jy = Rho .* V ;
e = -2 * Rho + 3.0 * ( Jx.^2 + Jy.^2) ;
eps = Rho - 3.0 * (Jx.^2 + Jy.^2) ;
qx = - Jx ;
qy = - Jy ;
Pxx = Jx.^2 - Jy.^2 ;
Pxy = Jx.*Jy ;
meq(:,:,1) = Rho ;
meq(:,:,2) = e ;
meq(:,:,3) = eps ;
meq(:,:,4) = Jx ;
meq(:,:,5) = qx ;
meq(:,:,6) = Jy ;
meq(:,:,7) = qy ;
meq(:,:,8) = Pxx ;
meq(:,:,9) = Pxy ;
for J = 1 : ny
  for I = 1 : nx
    meq_temp(1) = meq(I,J,1) ;
    meq_temp(2) = meq(I,J,2) ;
    meq_temp(3) = meq(I,J,3) ;
    meq_temp(4) = meq(I,J,4) ;
    meq_temp(5) = meq(I,J,5) ;
    meq_temp(6) = meq(I,J,6) ;
    meq_temp(7) = meq(I,J,7) ;
    meq_temp(8) = meq(I,J,8) ;
    meq_temp(9) = meq(I,J,9) ;
    feq(I,J,:) = invM * meq_temp' ;
  end
end
f = feq ;
m = meq ;
g = w .* 1 .* (Gx .* ex + Gy .* ey) ./ cs^2 ;
Loop_counter = 1 ;
while Loop_counter <100 || Uresidual > Utol
  Rhotemp = 0 ;
  MomtempX = 0 ;
  MomtempY = 0 ;
  for J = 1 : ny
    for I = 1 : nx
      if isfluid(I,J) == 1
        for a = 1 : 9
          ftemp(I,J,a) = feq(I,J,a) ;
          mtemp(I,J,a) = meq(I,J,a) ;
        end
      end
    end
  end
end
Rhotemp = Rhotemp + f(I,J,a) ;
MomtempX = MomtempX + f(I,J,a)*ex(a) ;
MomtempY = MomtempY + f(I,J,a)*ey(a) ;
end
Rho(I,J) = Rhotemp ;
U(I,J) = MomtempX /Rho(I,J) ;
V(I,J) = MomtempY /Rho(I,J) ;
Rhotemp = 0 ;
MomtempX = 0 ;
MomtempY = 0 ;
end
end

Jx = Rho .* U ;
Jy = Rho .* V ;
e = -2 * Rho + 3.0 * (Jx.^2 + Jy.^2) ;
eps= Rho - 3.0 * (Jx.^2 + Jy.^2) ;
qx = - Jx ;
qy = - Jy ;
Pxx = Jx.^2 - Jy.^2 ;
Pxy = Jx.*Jy ;
meq(:,:,1) = Rho ;
meq(:,:,2) = e ;
meq(:,:,3) = eps ;
meq(:,:,4) = Jx ;
meq(:,:,5) = qx ;
meq(:,:,6) = Jy ;
meq(:,:,7) = qy ;
meq(:,:,8) = Pxx ;
meq(:,:,9) = Pxy ;
for J = 1 : ny
    for I = 1 : nx
        tempf(1) = f (I,J,1) ;
        tempf(2) = f (I,J,2) ;
        tempf(3) = f (I,J,3) ;
        tempf(4) = f (I,J,4) ;
        tempf(5) = f (I,J,5) ;
        tempf(6) = f (I,J,6) ;
        tempf(7) = f (I,J,7) ;
        tempf(8) = f (I,J,8) ;
        tempf(9) = f (I,J,9) ;
        tempm = M * tempf' ;
        m(I,J,:) = tempm ;
    end
end

for J = 1 : ny
    for I = 1 : nx
        if isfluid(I,J)==1
            dm(1) = m(I,J,1) - meq(I,J,1) ;
            dm(2) = m(I,J,2) - meq(I,J,2) ;
            dm(3) = m(I,J,3) - meq(I,J,3) ;
            dm(4) = m(I,J,4) - meq(I,J,4) ;
        end
    end
end
\( \text{dm}(5) = m(I,J,5) - \text{meq}(I,J,5) \);
\( \text{dm}(6) = m(I,J,6) - \text{meq}(I,J,6) \);
\( \text{dm}(7) = m(I,J,7) - \text{meq}(I,J,7) \);
\( \text{dm}(8) = m(I,J,8) - \text{meq}(I,J,8) \);
\( \text{dm}(9) = m(I,J,9) - \text{meq}(I,J,9) \);

\text{temp} = \text{invM} * \text{S} * \text{dm}' + g' ;
\text{for } a = 1 : 9
\text{f}(I,J,a) = \text{f}(I,J,a) - \text{temp}(a) ;
\text{end}
\text{end}
\text{end}
\text{end}

\text{for } J = 1 : \text{ny}
\text{if } J>1
\text{JN} = J - 1 ;
\text{else}
\text{JN} = \text{ny} ;
\text{end}
\text{if } J<\text{ny}
\text{JP} = J + 1 ;
\text{else}
\text{JP} = 1 ;
\text{end}
\text{end}
\text{for } I = 2 : \text{nx}-1
\text{IN} = I - 1 ;
\text{IP} = I + 1 ;
\text{ftemp}(I,J,1) = \text{f}(\text{IN},J,1) ;
\text{ftemp}(I,J,2) = \text{f}(I,JN,2) ;
\text{ftemp}(I,J,3) = \text{f}(\text{IP},J,3) ;
\text{ftemp}(I,J,4) = \text{f}(I,\text{JP},4) ;
\text{ftemp}(I,J,5) = \text{f}(\text{IN},JN,5) ;
\text{ftemp}(I,J,6) = \text{f}(\text{IN},\text{JP},6) ;
\text{ftemp}(I,J,7) = \text{f}(\text{IP},J,7) ;
\text{ftemp}(I,J,8) = \text{f}(\text{IP},JN,8) ;
\text{ftemp}(I,J,9) = \text{f}(I,J,9) ;
\text{end}
\text{I} = 1 ;
\text{IP} = I + 1 ;
\text{ftemp}(I,J,2) = \text{f}(I,JN,2) ;
\text{ftemp}(I,J,3) = \text{f}(\text{IP},J,3) ;
\text{ftemp}(I,J,4) = \text{f}(I,\text{JP},4) ;
\text{ftemp}(I,J,6) = \text{f}(\text{IP},JN,6) ;
\text{ftemp}(I,J,7) = \text{f}(\text{IP},\text{JP},7) ;
\text{ftemp}(I,J,9) = \text{f}(I,J,9) ;
\text{Rho}(I,J) = ( \text{ftemp}(I,J,9)+\text{ftemp}(I,J,2)+\text{ftemp}(I,J,4)+ 2.0* ( \text{ftemp}(I,J,3)+\text{ftemp}(I,J,6)+\text{ftemp}(I,J,7) ) )/(1-\text{Uin}) ;
\text{ftemp}(I,J,1) = \text{ftemp}(I,J,3)+2.0/3.0* \text{Rho}(I,J)*\text{Uin} ;
\text{ftemp}(I,J,5) = 0.5 * ( \text{Rho}(I,J)*\text{Uin}/3.0 + \text{Rho}(I,J)*\text{Vin} - \text{ftemp}(I,J,2) + \text{ftemp}(I,J,4) + 2*\text{ftemp}(I,J,7) ) ;
ftemp(I,J,8) = 0.5 *( Rho(I,J)*Uin/3.0 - Rho(I,J)*Vin + ftemp(I,J,2) - ftemp(I,J,4) + 2*ftemp(I,J,6) ) ;

I = nx ;
IN = I - 1 ;
ftemp(I,J,1) = f( IN,J ,1 ) ;
ftemp(I,J,2) = f( I ,JN,2 ) ;
ftemp(I,J,4) = f( I ,JP,4 ) ;
ftemp(I,J,5) = f( IN,JN,5 ) ;
ftemp(I,J,8) = f( IN,JP,8 ) ;
ftemp(I,J,9) = f( I , J ,9 ) ;
Rho(I,J) = Rhoout ;
UofPout(J) = -1 + ( 2*(ftemp(I,J,1)+ftemp(I,J,5)+ftemp(I,J,8)) + ftemp(I,J,2) + ftemp(I,J,4) + ftemp(I,J,9) ) / Rho(I,J) ;
ftemp(I,J,3) = ftemp(I,J,1) - 2.0/3.0*Rho(I,J)*UofPout(J) ;
ftemp(I,J,6) = -Rho(I,J)*UofPout(J)/6.0 + (ftemp(I,J,4) - ftemp(I,J,2)) / 2.0 + ftemp(I,J,8) ;
ftemp(I,J,7) = -Rho(I,J)*UofPout(J)/6.0 + (ftemp(I,J,2) - ftemp(I,J,4)) / 2.0 + ftemp(I,J,5) ;
end

f = ftemp ;

for J = 1 : ny
    for I = 1 : nx
        if isfluid(I,J)==0
            tempo = f(I,J,1) ;
            f(I,J,1) = f(I,J,3) ;
            f(I,J,3) = tempo ;
            tempo = f(I,J,2) ;
            f(I,J,2) = f(I,J,4) ;
            f(I,J,4) = tempo ;
            tempo = f(I,J,5) ;
            f(I,J,5) = f(I,J,7) ;
            f(I,J,7) = tempo ;
            tempo = f(I,J,6) ;
            f(I,J,6) = f(I,J,8) ;
            f(I,J,8) = tempo ;
        end
    end
end

if mod(Loop_counter,100)==0
    Uresidual = 0 ;
    Vresidual = 0 ;

    for J = 1 : ny
        for I = 1 : nx
            if abs(U(I,J)) > 0
                Uresidual = Uresidual + abs( (U(I,J)-Uold(I,J))/ U(I,J) ) ;
            end
        end
    end
if abs(V(I,J)) > 0
    Vresidual = Vresidual + abs ((V(I,J)-Vold(I,J))/ V(I,J) );
end
end
dend
Uold = U;
Vold = V;
fprintf( ' Iteration = %i, Uresidual = %f \n', Loop_counter, Uresidual)
end
Loop_counter = Loop_counter + 1;
end
save ('Uin', num2str(100*Uin))
end

figure
hold on
box on
grid on
xlabel('U/Uin')
ylabel('Channel height')
yaxis = [1/ny:1/ny:1];
plot(U(300,:)/Uin,yaxis,'b', 'linewidth',2)

Re = Uin*(ny-2)/niu;

IMFR = 0; %Inlet Mass Flow Rate
for J = 1 : ny
    IMFR = IMFR + Rho(1,J)*U(1,J);
end
IMFR;

OMFR = 0; %Outlet Mass Flow Rate
for J = 1 : ny
    OMFR = OMFR + Rho(nx,J)*U(nx,J);
end
OMFR;

abs(OMFR - IMFR)/IMFR
Checking for continuity (i.e. $\dot{m}_{in} \approx \dot{m}_{out}$):

The reader is advised to benchmark the following data with the above code prior to endeavoring to use the code for further studies. Inlet and outlet mass flow rates were calculated for 3 distinct inlet velocities (corresponding to 3 Reynolds numbers). In all cases, it was shown that the mass was conserved ($\dot{m}_{in} \approx \dot{m}_{out}$):

| $U_{in}$ (m/s) | Re   | $|\dot{m}_{in} - \dot{m}_{out}|/\dot{m}_{in}$ |
|---------------|------|----------------------------------------------|
| 0.02          | 7.8  | $2.8 \times 10^{-6}$                        |
| 0.06          | 23.4 | $3.0 \times 10^{-6}$                        |
| 0.1           | 39   | $2.6 \times 10^{-6}$                        |

Simulation of flow in a staggered array of parallel cylinders using SRT LBM

Below is an implementation of the SRT LBM to model fluid flow in a staggered array of parallel cylinders. Figure 2.7 can be obtained from the following model. Furthermore, inlet and outlet mass flow rates are calculated for various porosities to ensure the continuity is satisfied:

```matlab
clear all
NOgrid = 3*48;
x = l*NOgrid;
y = l*NOgrid;
Radius=NOgrid/48*14.5;
Gx=NOgrid/48*48;
Gy=NOgrid/48*24;
CentreX0=0;
CentreY0=0;
ex = [ 1  0 -1  0  1 -1  1  0 ] ;
ey = [ 0  1  0 -1  1  1 -1  0 ]  ;
cs = 1/sqrt(3) ;
Uinital = 0.000 ;
Vinitial = 0.000 ;
Rhoinitial = 1.0;
RhoP = 1041.3;
RhoL = 1.0;
ROin = 1.0005;
RO = 1.0 ;
meu = 6.025e-4;
Nu = meu/RhoP;
Tau = 1.0 ;
NuL = (Tau-0.5)/3;
dx = 48e-5/NOgrid ;
dt = NuL/Nu*dx*dx;
```
Utoll = 1e-3 ;
Vtoll = 1e-3 ;
Uresidual = 100 ;
Vresidual = 100 ;

f    = zeros(nx,ny,9);
ftemp= zeros(nx,ny,9);
feq   = zeros(nx,ny,9);
U     = zeros(nx,ny);
V     = zeros(nx,ny);
Uold  = zeros(nx,ny);
Vold  = zeros(nx,ny);
Rho   = zeros(nx,ny);

U(:,:,)= Uinitial ;
V(:,:,)= Vinitial ;
Rho(:,:,)= Rhoinitial ;
Rho(nx, :,ny) = RO ;
Uold = U ;
Vold = V ;

isfluid = ones(nx,ny);
isfluid(:,1) = 1 ;
isfluid(:,ny) = 1 ;

for mm = 0 : ny/Gy
    Centrey = Centrey0 + mm*Gy;
    for nn = 0 : nx/Gx
        if (mod(mm,2)==1)
            Centrex = Centrex0+(nn-0.5)*Gx;
        else
            Centrex = Centrex0+nn*Gx;
        end
        for J = 1 : ny
            for I = 1 : nx
                if sqrt((I-(Centrex))^2+(J-Centrey)^2)< Radius
                    isfluid(I,J) = 0;
                end
            end
        end
    end
end

for J = 1 : ny
    for I = 1 : nx
        if isfluid(I,J)==0
            U(I,J) = 0 ;
            V(I,J) = 0 ;
        end
    end
end
for J = 1 : ny
    for I = 1 : nx
        for a = 1 : 9
            feq(I,J,a) = w(a) * Rho(I,J) * ( 1.0 + 3.0*(ex(a)*U(I,J)+ey(a)*V(I,J)) ... 
                + 9.0/2.0*( ex(a)*U(I,J)+ey(a)*V(I,J))^2 ... 
                - 3.0/2.0*( U(I,J)^2 + V(I,J)^2 )        ) ;
        end
    end
end

f = feq ;

Loop_counter = 1 ;

while Loop_counter <100 || Uresidual > Utol %|| Vresidual>Vtol

    for J = 1 : ny
        for I = 1 : nx
            if isfluid(I,J)==1
                for a = 1 : 9
                    temp = f(I,J,a) - ( f(I,J,a) - feq(I,J,a) ) / Tau  ; %
                    f(I,J,a) = temp ;
                end
            end
        end
    end

    for J = 1 : ny
        if (J>1)
            JN = J - 1 ;
        else
            JN = ny ;
        end
        if (J<ny)
            JP = J + 1 ;
        else
            JP = 1 ;
        end
        for I = 1 : nx
            IN = I - 1 ;
            IP = I + 1 ;
            if (I==1)
                ftemp(IP,J ,1) = f(I,J,1) ;
                ftemp(I ,JP,2) = f(I,J,2) ;
                ftemp(I ,JN,4) = f(I,J,4) ;
                ftemp(IP,JP,5) = f(I,J,5) ;
                ftemp(IP,JN,8) = f(I,J,8) ;
                ftemp(I ,J ,9) = f(I,J,9) ;
```
elseif (I==nx)
    ftemp(I ,JP,2) = f(I,J,2) ;
    ftemp(IN,J ,3) = f(I,J,3) ;
    ftemp(I ,JN,4) = f(I,J,4) ;
    ftemp(IN,JP,6) = f(I,J,6) ;
    ftemp(IN,JN,7) = f(I,J,7) ;
    ftemp(I ,J ,9) = f(I,J,9) ;
else
    ftemp(IP,J ,1) = f(I,J,1) ;
    ftemp(I ,JP,2) = f(I,J,2) ;
    ftemp(IN,J ,3) = f(I,J,3) ;
    ftemp(I ,JN,4) = f(I,J,4) ;
    ftemp(IP,JP,5) = f(I,J,5) ;
    ftemp(IN,JP,6) = f(I,J,6) ;
    ftemp(IN,JN,7) = f(I,J,7) ;
    ftemp(IP,JN,8) = f(I,J,8) ;
    ftemp(I ,J ,9) = f(I,J,9) ;
end
end
end
f = ftemp ;
for J = 1 : ny
    for I = 2 : nx-1
        if isfluid(I,J)==0
            temp = f(I,J,1) ;
            f(I,J,1) = f(I,J,3) ;
            f(I,J,3) = temp ;

            temp = f(I,J,2) ;
            f(I,J,2) = f(I,J,4) ;
            f(I,J,4) = temp ;

            temp = f(I,J,5) ;
            f(I,J,5) = f(I,J,7) ;
            f(I,J,7) = temp ;

            temp = f(I,J,6) ;
            f(I,J,6) = f(I,J,8) ;
            f(I,J,8) = temp ;
        end
    end
end
for J = 1 : ny
    if isfluid(I,J)==1
        U(1,J) = 1-1/ROin*(2*(f(1,J,3)+f(1,J,6)+f(1,J,7))+f(1,J,2)+f(1,J,4)+f(1,J,9));
        f(1,J,1) = f(1,J,3) + 2/3*ROin*U(1,J);
        f(1,J,5) = 1/2*(1/3*ROin*U(1,J) - f(1,J,2) + f(1,J,4) + 2*f(1,J,7));
\[
f(1,J,8) = \frac{1}{2}(\frac{1}{3}ROin*U(1,J) + f(1,J,2) - f(1,J,4) + 2*f(1,J,6));
\]
end

for J = 1 : ny
    if isfluid(I,J)==1
        U(nx,J) = -1 + \frac{1}{RO}*(2*f(nx,J,1)+f(nx,J,5)+f(nx,J,8)) + f(nx,J,2)+f(nx,J,4)+f(nx,J,9));
        f(nx,J,3) = f(nx,J,1) - \frac{2}{3}RO*U(nx,J);
        f(nx,J,6) = 1/2*(-1/3*RO*U(nx,J)-f(nx,J,2)+f(nx,J,4)+2*f(nx,J,8));
        f(nx,J,7) = 1/2*(-1/3*RO*U(nx,J)+f(nx,J,2)-f(nx,J,4)+2*f(nx,J,5));
    end
end

for J = 1 : ny-1
    if (isfluid(1,J)==0 && isfluid(1,J+1)==1)
        f(1,J,1) = f(1,J,3) ;
        f(1,J,2) = f(1,J,4) ;
        f(1,J,5) = f(1,J,7) ;
        f(1,J,6) = 1/2*(ROin - (f(1,J,9)+f(1,J,1)+f(1,J,2)+f(1,J,3)+f(1,J,4)+f(1,J,5)+f(1,J,7))) ;
        f(1,J,8) = 1/2*(ROin - (f(1,J,9)+f(1,J,1)+f(1,J,2)+f(1,J,3)+f(1,J,4)+f(1,J,5)+f(1,J,7))) ;
    end
end

for J = 1 : ny-1
    if (isfluid(nx,J)==0 && isfluid(nx,J+1)==0)
        f(nx,J,3) = f(nx,J,1) ;
        f(nx,J,4) = f(nx,J,2) ;
        f(nx,J,5) = f(nx,J,7) ;
        f(nx,J,6) = 1/2*(RO - (f(nx,J,9)+f(nx,J,1)+f(nx,J,2)+f(nx,J,3)+f(nx,J,4)+f(nx,J,5)+f(nx,J,7))) ;
        f(nx,J,8) = 1/2*(RO - (f(nx,J,9)+f(nx,J,1)+f(nx,J,2)+f(nx,J,3)+f(nx,J,4)+f(nx,J,5)+f(nx,J,7))) ;
    end
end
\[ f(nx, J, 6) = f(nx, J, 8) ; \]
\[ f(nx, J, 5) = \frac{1}{2}(RO - (f(nx, J, 9) + f(nx, J, 1) + f(nx, J, 2) + f(nx, J, 3) + f(nx, J, 4) + f(nx, J, 6) + f(nx, J, 8))) ; \]
\[ f(nx, J, 7) = \frac{1}{2}(RO - (f(nx, J, 9) + f(nx, J, 1) + f(nx, J, 2) + f(nx, J, 3) + f(nx, J, 4) + f(nx, J, 6) + f(nx, J, 8))) ; \]
\]
end
end

Rhotemp = 0 ;
MomtempX = 0 ;
MomtempY = 0 ;
for I = 1 : nx
  for J = 1 : ny
    if isfluid(I, J) == 1
      for a = 1 : 9
        Rhotemp = Rhotemp + f(I, J, a) ;
        MomtempX = MomtempX + f(I, J, a)*ex(a) ;
        MomtempY = MomtempY + f(I, J, a)*ey(a) ;
      end
      Rho(I, J) = Rhotemp ;
      U(I, J) = MomtempX /Rho(I, J) ;
      V(I, J) = MomtempY /Rho(I, J) ;
      Rhotemp = 0 ;
      MomtempX = 0 ;
      MomtempY = 0 ;
    end
  end
end
Ueq = U ;
Veq = V ;
for J = 1 : ny
  for I = 1 : nx
    for a = 1 : 9
      feq(I, J, a) = w(a) * Rho(I, J) * ( 1.0 + 3.0*(ex(a)*Ueq(I, J)+ey(a)*Veq(I, J)) ... 
      + 9.0/2.0*(ex(a)*Ueq(I, J)+ey(a)*Veq(I, J))^2 ... 
      - 3.0/2.0*(Ueq(I, J)^2 + Veq(I, J)^2 ) ... ) ;
    end
  end
end
Uresidual = 0 ;
Vresidual = 0 ;
for I = 1 : nx
  for J = 1 : ny
    if U(I, J) > 0
      Uresidual = Uresidual + abs( (U(I, J)-Uold(I, J))/ U(I, J) ) ;
    end
    if V(I, J) > 0
      Vresidual = Vresidual + abs ((V(I, J)-Vold(I, J))/ V(I, J) ) ;
    end
end
end
Uold = U;
Vold = V;

if mod(Loop_counter,100)==0
    fprintf(' Iteration = %i, Uresidual = %f \n', Loop_counter, Uresidual)
end

Loop_counter = Loop_counter + 1;
end
fprintf('\n END!\n\n')

UP=zeros(nx,ny);
VP=zeros(nx,ny);

UP=dx/dt*U;
VP=dx/dt*V;

close
figure
set(gca,'FontSize',15)
T=sqrt(UP.^2+VP.^2);
surface(T)
shading interp
axis equal
colorbar('FontSize',15)
save ([\'Radius\', num2str(10*runtime)])

IMFR = 0;
for J = 1 : ny
    IMFR = IMFR + Rho(1,J)*U(1,J);
end
IMFR;

OMFR = 0;
for J = 1 : ny
    OMFR = OMFR + Rho(nx,J)*U(nx,J);
end
OMFR;

abs(OMFR - IMFR)/IMFR

porosity = 0;
for J = 1 : ny
    for I = 1 : nx
        porosity = porosity + isfluid(I,J);
    end
end
porosity = porosity/(nx*ny)

dm=RhoP/RhoL*dx^3;

delta_pressure_L = (ROin - RO)/3;

delta_pressure_P = dm/(dx*dt^2)*delta_pressure_L;

Fluidnodes = 0;
Usum = 0;
for J = 1 : ny
  if isfluid(1,J) == 1
    Usum = Usum + U(1,J);
  end
end

for J = 1 : ny
  if isfluid(1,J) == 1
    Fluidnodes = Fluidnodes + 1;
  end
end

UinAVE = Usum/Fluidnodes;
UinP = UinAVE *dx/dt;
permeability1 = UinP*meu*nx*dx/delta_pressure_P

ReP = UinP*Radius*dx/Nu;
Checking for continuity (i.e. $\dot{m}_{\text{in}} \approx \dot{m}_{\text{out}}$):

The reader is advised to benchmark the following data with the above code prior to endeavoring to use the code for further studies. Inlet and outlet mass flow rates were calculated for various porosities to ensure that the mass was conserved ($\dot{m}_{\text{in}} \approx \dot{m}_{\text{out}}$) in all of the cases:

| Porosity | $|\dot{m}_{\text{in}} - \dot{m}_{\text{out}}|/\dot{m}_{\text{in}}$ |
|----------|---------------------------------------------------------------|
| 0.98     | $1.1 \times 10^{-6}$                                         |
| 0.96     | $1.0 \times 10^{-6}$                                         |
| 0.93     | $4.1 \times 10^{-7}$                                         |
| 0.90     | $2.4 \times 10^{-6}$                                         |
| 0.87     | $3.0 \times 10^{-6}$                                         |
| 0.85     | $3.2 \times 10^{-6}$                                         |
| 0.83     | $9.1 \times 10^{-6}$                                         |
| 0.78     | $2.7 \times 10^{-5}$                                         |
| 0.73     | $2.0 \times 10^{-5}$                                         |
| 0.67     | $1.4 \times 10^{-4}$                                         |
| 0.61     | $5.2 \times 10^{-4}$                                         |
| 0.54     | $4.3 \times 10^{-4}$                                         |
| 0.47     | $1.4 \times 10^{-4}$                                         |
| 0.39     | $3.3 \times 10^{-5}$                                         |
| 0.30     | $5.2 \times 10^{-4}$                                         |