Microstructure-based characterisation of permeability using a random walk model

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Abstract

Quantitative transport properties of materials are analysed using a random walk model, based on the microscopic compositional distribution of compositions in the materials. A material sample is defined on a simple-cubic lattice, with volume fractions specified for each composition on every volume-pixel (voxel). The quantitative relation between bulk permeability and fine scale anisotropy is investigated by assuming fully anisotropic and fully isotropic voxel morphology. Such study has prompted an analytic approximate formulation to estimate voxel permeability. The numerical approach has been verified on synthetic structures with known permeability. The analysis technique has been applied to a real-world rock sample, as illustrated by a case study contained within this paper. The investigations have shown that the bulk permeability is affected significantly by fine length scale anisotropy.

Key words: Random walk, material transport property simulation, heterogeneous system, isotropic and anisotropic structures, microstructures, data-constrained modelling, multi-spectrum X-ray CT.

1. Introduction

It is well established that bulk properties of materials are related to their microstructures [1]. However, quantitative modelling of the relationship between microstructures and the bulk properties is still a challenging topic. Many studies on theoretical models and numerical simulations have been carried out for characterising structure morphology in different applications, such as for predicting recrystallisation by cellular automata [2, 3], analysing cellular wall and curvature for grain growth [4], using statistical correlation functions to calculate structural descriptors of a heterogeneous material [5], and simulating the solidification process by a statistical mechanical model [6, 7]. Recently, a data-constrained modelling approach has been developed for compositional microstructures characterization [8-11].

The objective of this study is to investigate the relationship between bulk transport properties of a heterogeneous material and its fine length scale anisotropy. A random walk method is used to compute permeability defined by Darcy’s law. The random walk method, as a stochastic process
formed by successive summation of independent and identically distributed random variables, is commonly used in the field of statistical physics to model and analyse processes involving diffusion. The fundamental mathematics of the random walk approach has been extensively studied in the literature [12-14] and applications of this approach in many different fields have been presented from general physics, chemistry to biology and finance [15 - 18]. In particular, random walk models have been developed in hydraulic studies for numerical simulation of transport properties in heterogeneous porous media, such as the random walk particle tracking model [19, 20] and the continuous time random walk model [21, 22], which relates to an advective-dispersive equation.

For this analysis, a discrete random walk model is used to predict effective permeability of a heterogeneous material from 3D compositional volume fraction data. Such data can be derived using a data-constrained model (DCM) [8-11] with multi-spectrum X-ray computed tomography (CT) data. A material sample is represented as a 3D volumetric dataset with volume fractions for each composition defined on each voxel.

Our study addresses the following two problems. The first problem is to investigate the effect on bulk permeability from anisotropy variations at sub-voxel length-scales. Although material compositional volume fractions can be derived with DCM on individual voxels, the fine structure below voxel length scales at each voxel is undetermined. To evaluate such fine-scale effects, we focus our study on the two limiting cases: uniform isotropic voxels and extremely anisotropic voxels where different compositions in a voxel form layered anisotropic structures.

The second problem we consider is how to calculate the permeability for a voxel from given volume fraction and the permeability of each composition on that voxel. To solve this problem, an original multi-component voxel is thought to be subdivided to a finer grid, until each refined voxel represents a single composition (homogeneous voxel). By imposing isotropic or anisotropic structure constraints, the effective permeability on the refined system can be estimated by analytic formulae. The finer grid will then be up-scaled to a mixed grain (inhomogeneous voxel) to obtain permeability on the original voxel.

Compared to other types of methods with comparable numerical accuracy, such as the finite element method and finite difference method, the random walk method is computationally attractive with large 3D datasets. This is of particular importance in dealing with very large DCM generated microstructure datasets.

The formulation of random-walk method is presented in the next section, followed by a section on numerical simulations for isotropic and anisotropic voxels on synthetic microstructures. The subsequent section is a case study with sandstone. The article concludes with a conclusion, acknowledgments and references.

2. Random Walk Method

We start with a classical random walk problem, where a random walker (or a particle) initially starts at the origin on a \(d\)-dimensional hyper cubic grid and moves to one of its neighbouring positions with a certain probability. Starting at the origin \(0\), the displacement of a walker after \(N\) steps is

\[ \mathbf{R}_N = \sum_{n=1}^{N} \Delta \mathbf{r}_n, \]

where \(\Delta \mathbf{r}_n \{n = 1, 2, ..., N\}\) is an independent variable. Let \(\{\mathbf{R}_N\}\) be a set of all
positions in a random walk process, then $\{\mathbf{R}_N\}$ refers to a Markov chain. Following the Markov assumption, the probability of finding a random walker at $\mathbf{R}$ after $N + 1$ steps becomes [23]:

$$
P(\mathbf{R}, N + 1) = \int p(\mathbf{r}') P(\mathbf{R} - \mathbf{r}', N) d\mathbf{r}'
$$

where $p(\mathbf{r}')$ is the transition probability from state $\mathbf{R}(N)$ to $\mathbf{R}(N + 1)$.

As $N \to \infty$, using Taylor series to expand $P(\mathbf{R} - \mathbf{r}', N)$ at $\mathbf{R}$, it has been shown [23] that the limit distribution $\delta(\mathbf{R}, t)$, defined by $\delta(\mathbf{R}, N\Delta t) = P(\mathbf{R}, N)$, satisfies the diffusion equation:

$$
\frac{\partial \delta}{\partial t} = D \nabla^2 \delta
$$

with the initial condition $\delta(\mathbf{R}, 0) = \delta_0(\mathbf{R})$.

Let $< R_N^2 >= \langle \mathbf{R}_N \cdot \mathbf{R}_N \rangle$ be the mean square displacement of a walker and $t_N$ be the travelling time of the walker after $N$ steps. The diffusion coefficient in equation (2) is given by $D = \frac{< R_N^2 >}{2dt_N}$, which implies that the mean square displacement of a particle is proportional to time. Darcy’s law describes the flow of a fluid through a porous medium with a proportional relationship between the instantaneous discharge rate $q$ (flow rate per unit area), the viscosity of the fluid $\mu$, and the pressure gradient $\nabla P$: $q = -\frac{k}{\mu} \nabla P$, where $k$ is the permeability of the medium.

With similar derivations, the relative permeability or mobility can be calculated as $\sigma = \frac{k}{\mu} = \frac{< R_N^2 >}{2dt_N}$. For notational simplicity, $\sigma$ will be referred to as permeability in this paper. Using the random walk method, calculating permeability $\sigma$ is analogous to calculating the diffusion coefficient $D$.

In our numerical implementation on a simple-cubic grid, voxels are labelled sequentially with integer labels. A walker moves from its current position $i$ to one of its 6 neighbouring sites $j$ with a transition probability $p(i,j)$. At each step, the displacement will be accumulated while time is incremented by unity. To reduce statistical fluctuations, an ensemble of $M$ walkers is used for a random walk simulation. The mean square displacement of all walkers after step $N$ is proportional to time:

$$
\langle R_N^2 \rangle \sim 6\sigma t_N
$$

The maximum value of $N$ depends on the size of the simulation grid. More details will be discussed in section 3.3.

The transition probability in our problem is based on the degree of homogeneity of the composite media and the associated permeabilities of the neighbouring nodes. In our random walk algorithm, the transition probability between node $i$ and $j$ is evaluated by a relative harmonic mean of permeabilities at $i$ and $j$, denoted by [24, 25]

$$
p(i,j) = \frac{1}{6\sigma_{\text{max}}^2} \frac{2\sigma_i \sigma_j}{\sigma_i + \sigma_j}
$$

where $\sigma_i$ and $\sigma_j$ are permeability of two neighbour nodes and $\sigma_{\text{max}}$ is the maximum permeability among compositions.
3. Numerical Simulations on synthetic structures

In this section, we first examine two extreme microstructure constraints in order to estimate local permeability for an inhomogeneous voxel and then conduct the random walk simulations under these extreme structures. Asymptotic behaviour of the random walk method is also discussed in detail.

A two-component system \( C_1 \) and \( C_2 \) is considered in our numerical simulations. Each simulation was performed on a cubic grid with 1000x1000x1000 voxels. Each voxel is a mixture of fraction of component \( C_1 \) and \( C_2 \) according to their volume fractions. Assume that permeabilities of \( C_1 \) and \( C_2 \) are given as \( \sigma_{c1} \) and \( \sigma_{c2} \). Let \( \rho \) be the relative permeability between two components, i.e. \( \sigma_{c2} \equiv \rho \sigma_{c1} \). Our numerical simulations are focused on the permeability ratio \( \rho \) instead of the actual permeabilities.

3.1. Voxel permeability

To calculate the voxel permeability of a two-component inhomogeneous system, the following two extreme sub-voxel fine-structure constraints are applied on each voxel.

**Case 1: Anisotropic layered voxel structure**

In this case, we examine an extreme anisotropic structure where two components \( C_1 \) and \( C_2 \) are aligned as a stack of white layers \( C_1 \) and gray layers \( C_2 \) according to their volume fractions. It is assumed that a voxel can be subdivided into sub-voxels as shown in figure 1(a), such that each sub-voxel contains only a single component, either \( C_1 \) or \( C_2 \). The permeability at each sub-voxel now becomes predefined \( \sigma_{c1} \) or \( \sigma_{c2} \). Therefore, the random walk transition probability between sub-voxels \( i \) and \( j \) can be calculated with equation (4).

The random walk algorithm is applied to a refined cubic grid to simulate directional permeabilities \( \bar{\sigma}_\parallel \) and \( \bar{\sigma}_\perp \), where \( \bar{\sigma}_\parallel \) is the permeability for a flow parallel to the layered structure and \( \bar{\sigma}_\perp \) is the permeability for a flow perpendicular to the layered structure. The values of \( \bar{\sigma}_\parallel \) and \( \bar{\sigma}_\perp \) can be calculated explicitly as the theoretical upper \( (\sigma_{\text{upp}}) \) and lower \( (\sigma_{\text{low}}) \) values

\[
\bar{\sigma}_\parallel(i) = \sigma_{\text{upp}}(i) = \sum_{k=1}^{n} v(k, i) \cdot \sigma(k)
\]

\[
\bar{\sigma}_\perp(i) = \sigma_{\text{low}}(i) = 1/\sum_{k=1}^{n} \frac{v(k, i)}{\sigma(k)}
\]

where \( v(k, i) \) is the volume fraction of composition \( k \) at voxel \( i \), and \( \sigma(k) \) is the permeability of composition \( k \).

Similar to an isotropic system, the anisotropic permeabilities can be simulated with the random walk algorithm as

\[
\begin{align*}
\sigma_{\parallel} &= \frac{<R_\parallel^2>}{2dt} \\
\sigma_{\perp} &= \frac{<R_\perp^2>}{2dt}
\end{align*}
\]

where \( R_\parallel \) and \( R_\perp \) are walker displacement along parallel and perpendicular directions respectively.
The simulation results in figure 2 show good agreement between the random-walk simulated permeabilities (scatter dot-plots) and the theoretical calculations (solid lines). This serves as a verification of the random-walk algorithm.

On an extremely anisotropic voxel, its directional dependent permeability is given as

\[
\sigma_i = \begin{cases} 
\sigma_{\text{upp}}(i), & \text{if flow \parallel \ layered structure} \\
\sigma_{\text{low}}(i), & \text{if flow \perp \ layered structure} 
\end{cases} 
\]  

**Case 2: Isotropic uniform voxel structure**

In contrast to case 1, an isotropic uniform voxel is a uniform mixture of components \( C_1 \) and \( C_2 \), see figure 1(b). We are not aware of an explicit formula to determine the permeability for this voxel structure. The middle plots in figure 2 show that the effective permeability \( \sigma \) for the whole refined system is approximately \((2 \ast \sigma_{\text{upp}} + \sigma_{\text{low}})/3\). This suggests that the directionless effective permeability could be used as an equivalent approximation of the permeability for an isotropic structure. For purpose of comparison on an isotropic voxel, it is assumed that the permeability of an isotropic voxel is given as

\[
\sigma_i = \frac{2}{3}\sigma_{\text{upp}}(i) + \frac{1}{3}\sigma_{\text{low}}(i) 
\]  

where \( \sigma_{\text{upp}}(i) \) and \( \sigma_{\text{low}}(i) \) are defined in equation (5). The coefficients in equation (8) are selected with consideration that, for an anisotropic voxel with weak anisotropy \( \rho \approx 1 \) there is approximately 1/3 probability that the flow would be along the perpendicular direction.

**Figure 1.** Subdivide an inhomogeneous voxel of two components \( C_1 \) (white) and \( C_2 \) (gray) based on two extreme structure constraints: \( (a) \) – anisotropic layered structure, the parallel and perpendicular permeabilities are simulated along the horizontal and vertical directions as indicated by the arrow bars. \( (b) \) - isotropic uniform structure.
3.2. Inhomogeneous system bulk permeability simulation

For the extreme voxel structure configurations as discussed in the previous section, once $\sigma_i$ is calculated on each voxel using equation (7) and (8), the transition probability of a random walker can be calculated by equation (4). Simulation results for an inhomogeneous two-component system are shown in figure 3 with respect to the two structure constraints. The theoretical upper and lower bounds are plotted for comparison.

There are several interesting findings from this figure. Firstly, the voxel-level structure variation does affect the whole system permeability. The structure impact on permeability is higher as the permeability ratio $\rho$ increases. For a multi-component system with a wider range of permeabilities, fine length scale structure variation could heavily affect the effective permeability of the system.

Secondly, the isotropic and anisotropic structure constraints define a narrow range of permeability upper and lower bounds as volume fraction changes, compared to the wider theoretical range. Any microstructure in real data can be considered as a morph between the two extremes.

Thirdly, the voxel-based structure variation has less impact on permeability if the volume fraction is unbalanced (e.g. volume fraction of $C_1$ approaching 0 or 1 leads to a single component dominated system). This is important in dealing with high-resolution data since voxels in very fine scale show a homogeneous nature. The structure impact on permeability is higher if the total volume is more evenly spread through all compositions.
3.3. Asymptotic behaviour

The classical random walk theory is established in a continuous time space and an infinite domain. In practice, the random walk algorithm is applied to a discrete grid of finite domain with some boundary constraints. Therefore, we need to study the asymptotic behaviour of the presented random walk algorithm as the simulation size goes to infinity. The simulation size, denoted by $L$, refers to the dimension of a sub-cubic grid in which the simulation sits. A series of simulations were conducted as $L$ increases in order to examine the convergence of the simulation approach.

Figure 4 shows the simulation results at different scales for a synthetic isotropic system. The simulated permeability is plotted versus the inverse of simulation size in order to demonstrate the zero convergence as size tends to infinite. As shown in the figure, the trend line of the predicted permeability as simulation size increases converges to a limit that is very close to the known theoretical value calculated from equation (8).
Figure 4. Asymptotic behaviour of simulation scales. Red dots show the simulation results at different sizes (plotted as $1/L$ to demonstrate zero crossing value) for an isotropic system with $\rho = 10$ and $v_1 = 0.9$ (volume fraction of $C_1$). The trend line converges to 1.627 as $1/L \rightarrow 0$. The expected permeability for this structure configuration is 1.633, calculated by equation (8).

4. Case Study – DCM Rock Data Simulation

The presented random walk method was applied to a 3D DCM compositional volume fraction dataset of a rock sample for predicting the effective permeability. The rock sample is composed of three components: quartz ($SiO_2$), calcite ($CaCO_3$) and void. The multi-spectrum X-ray micro-CT images for the sample at 35 keV and 45 keV beam energies were acquired at Shanghai Synchrotron Radiation Facility (SSRF). The sample is represented numerically by a cubic grid with 1475 x 1450 x 320 voxels. Each voxel on the grid represents a material volume of 5.92 x 5.92 x 5.92 microns. Volume fractions for each composition on each voxel are generated with a data-constrained modelling (DCM) approach [26].

Based on the DCM generated datasets, the voxel-based permeability is calculated using equations (7) and (8) for the two different structural constraints. Since quartz is not permeable and permeability of calcite is insignificant compared to the void permeability, this three-component system is simplified to a void and non-void two-component system (permeable and non-permeable).

Figure 5 shows the limit behaviours of the random walk simulation on this rock sample associated with previously discussed two special structure configurations. The theoretical maximum and minimum are also applied to each voxel and simulation for the upper and lower bounds are shown as the top and bottom curves for a comparison. Four circles along with the attached values on the vertical axis give the limits of the random walk simulations corresponding to four specific configurations. As it can be seen, the simulated permeabilities for two extreme structures are within the theoretical upper and lower bounds. The difference between two structures is narrowed down to half of the theoretical range. Similar numerical experiments were repeated for different permeability values of void (range from 10 to $10^4$) and the simulation limits are shown in figure 6. As
expected, the simulation results are consistent with each other and the structure impact is higher if the void permeability is larger.

As discussed previously, structural variation has less impact on permeability if one compositional volume fraction tends to 0 or 1. We further analysed the void and non-void volume fraction data to generate a histogram distribution of void volume fraction in terms of the number of voxels with a particular volume fraction, see figure 7. The histogram reveals that the majority of voxels are dominated by a single component. For example, the highest bar in the figure indicates that nearly 40% of voxels contain 5% of void volume and 95% of non-void volume. Structure effect on the permeability will be heavily reduced for single component dominated voxels.

**Figure 5.** Comparison of the random walk simulation results for two extreme structure constraints with given $\sigma(\text{void}) = 10^2$. Simulations based on the theoretical maximum and minimum are plotted on the top and bottom respectively. The converging point for each case is drawn as a big circle on the vertical axis with the converging value attached.

**Figure 6.** Comparison of the random walk simulation results for two extreme structure constraints versus permeability of void region (plotted on a logarithmic scale).
Figure 7. Histogram distribution of void volume fraction. It indicates that most voxels have an unbalanced volume fraction, either higher or lower volume of void. Structure variation on such a voxel has less impact on the permeability.

The real data simulation demonstrates a quantitative approach for modelling microstructure uncertainty and characterising the structure impact on the permeability. The analysis shows that the microstructure impact on permeability can be considerably reduced if the sample is examined at very fine scale.

5. Conclusions

In this paper, we investigated the effect of fine scale anisotropy on the effective permeability for a heterogeneous system. A discrete random walk algorithm has been presented to simulate effective permeability from DCM compositional volume fraction data. Such data does not provide information about the fine structures smaller than voxel size. Even for a given synthetic data structure simulation, it is also impossible to deal with unlimited possibilities in mixture of compositions. Our investigation concentrated on extreme structure configurations in order to provide a more accurate estimation for any microstructure within extremes.

Synthetic data simulations with extreme microstructure constraints have led us to an analytic approximation to characterise the effect of microstructure morphology on the physical properties of composite materials. The synthetic numerical simulations on isotropic and anisotropic structure constraints have shown that the impact of microstructure on permeability varies with the compositional volume fractions and permeability ratio between compositions. In general, the higher the permeability ratio, the more impact the microstructure has.

Based on the directional permeability analysis, we have applied an approximate formula for calculating the permeability of a voxel with isotropic structure. For a layered anisotropic structure, an analytic formula was derived according to the direction of a flow to the orientation of the layered structure. The random walk simulations from isotropic to anisotropic structural variations provide more accurate estimations of the effective permeability for a multi-component system.
Computational efficiency and fast convergence of the random walk model make it practical in dealing with high resolution DCM datasets.

The random walk algorithm and analysis presented in this paper enables us to predict a bulk transport property from microstructure information. It provides a generic approach and should be applicable to predict other transport properties that are governed by similar equations. Extension of this classical random walk model to specific applications that incorporate other transport mechanisms and interfacial interactions will be the next stage of this work.

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