Pressure and flow statistics of Darcy flow from simulated annealing

Marise J E Westbroek\textsuperscript{1,2}, Peter R King\textsuperscript{1}, Dimitri D Vvedensky\textsuperscript{2,*} and Ronnie Schwede\textsuperscript{3}

\textsuperscript{1} Department of Earth Science and Engineering, Imperial College London, London SW7 2BP, United Kingdom
\textsuperscript{2} The Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom
\textsuperscript{3} Shell Global Solutions International B.V., Grasweg 31, 1031 HW Amsterdam, The Netherlands

E-mail: d.vvedensky@imperial.ac.uk

Received 8 July 2020, revised 7 December 2020
Accepted for publication 10 December 2020
Published 29 December 2020

Abstract

The pressure and flow statistics of Darcy flow through a three-dimensional random permeable medium are expressed as a path integral in a form suitable for evaluation by simulated annealing. There are several advantages to using simulated annealing for this problem: (i) any probability distribution can be used for the permeability, (ii) there is no need to invert the transmissibility matrix which, while not a factor for single-phase flow, offers distinct advantages for multi-phase flow, and (iii) the action used for simulated annealing, whose extremum yields Darcy’s law, is eminently suitable for coarse graining by integrating over the short-wavelength degrees of freedom. We show that the pressure and flow statistics obtained by simulated annealing are in excellent agreement with those obtained from standard finite-volume calculations.

Keywords: Darcy flow, random permeability, simulated annealing, pressure statistics, flow statistics, path integral

(Some figures may appear in colour only in the online journal)
1. Introduction

Fluid transport through porous media is a central concern for many natural, technological, and environmental processes [1–3]. Flow through geological porous media plays a key role in transporting natural resources such as water [4], heat [5], oil [6], and gas, such as CO2 sequestration [7]. Natural processes in porous biological tissue [8] include the flow of oxygen through lungs [9], the transport of cerebrospinal fluid through the brain [10], and hemodynamics through blood vessels [11]. Synthetic porous media find applications in chemical catalytic reactors [12], thermal insulation for buildings [13], and in direct-contact heat exchangers [14].

The foregoing scenarios span several areas of science and engineering and have led to the implementation of a broad range of theoretical and computational methods [1]. Foremost among these are molecular dynamics [15], lattice Boltzmann methods [16–18], fluid dynamics (computational and theoretical) [16, 19], path integral [20–22], finite-volume [23] and finite-element [24] methods, and continuous-time random walk theory [25–28]. These techniques model flow through porous media at various levels of spatial and temporal resolution, ranging from the scale of individual pores to macroscopic pressure and flow rates. This attests to the inherent multi-scale nature of flow through porous media.

The heterogeneity of pores in natural media, manifested as variations of the sizes and shapes of pores, is a key determinant of flow through such media. Significant advances in imaging techniques can reveal details of pore heterogeneity, which can be used to predict macroscopic flow parameters [29]. However, pore-scale information is not generally available over entire geological systems. In this case macroscopic permeability is inferred from other sources or geological analogues from which a probability distribution is ascertained (or assumed). Although pore-scale methods can simulate particular types of heterogeneity, there is no general methodology available for relating particular morphological pore characteristics to macroscopic flow parameters [30]. An important step in this direction would be the efficient computation of macroscopic flow with different permeability distributions that account for mesoscopic averages over the porous medium. This paper describes progress toward such an approach.

We consider the slow flow of a viscous fluid through a three-dimensional random porous medium. Under these conditions, the flow and the pressure gradient are related by Darcy’s law

\[ q = -K \nabla p. \]  

(1)

Here, \( q \) is the average velocity (‘flow’) of the fluid, \( K(x) = k(x)/\mu \), where \( k(x) \) is the permeability of the medium, where \( \mu \) is the viscosity of the fluid, and \( \nabla p \) is the pressure gradient driving the fluid flow. The effective permeability describes the medium on a ‘mesoscopic’ scale, large compared to the pore scale, but small on the scale of the macroscopic medium. Although proposed as an empirical relation by Darcy in the 1850s [31], this equation can be recovered from the Navier–Stokes equations under the stated flow conditions [19, 32]. In this paper, we focus on single-phase, incompressible flow, for which

\[ \nabla \cdot q = 0. \]  

(2)

When combined with (1), the equation for incompressible Darcy flow is

\[ \nabla \cdot (K \nabla p) = 0. \]  

(3)

In hydrocarbon recovery, this equation is solved numerically using the finite-volume method [33, 34], while the finite-element method is common in hydrology.
In previous work [22, 35], we formulated the solution to one-dimensional Darcy flow in a random porous medium as a path integral over pressure paths within the medium. In discrete form, the path integral is a tool to simulate Darcy pressure paths \( \{ p_i \} \) on a spatial lattice using Markov chain Monte Carlo methods according to the weighting \( e^{-S} \), where the ‘action’ \( S = S(\{ p_i \}) \) restricts the paths to follow Darcy’s law in the presence of quenched stochastic permeability. For reasons discussed in section 2, this path integral methodology is not readily adapted to higher dimensions. Hence, we turn to an alternative expression for the action that has the same form in one, two, and three spatial dimensions. Determining the extremum of this action, which yields Darcy’s law, utilizes simulated annealing [36, 37].

Although solving Darcy’s equation with simulated annealing is more computationally intensive than the finite-volume method, there are several advantages over this and other techniques. Simulated annealing allows any probability distribution to be used for the permeability (as does the finite-volume method). Moreover, there is no need to invert the transmissibility matrix during simulated annealing, which, while not an issue for single-phase flow, the case considered here, is advantageous for multiphase flow. On a more formal level, the action used for simulated annealing is eminently suitable for integration over the short-range degrees of freedom to derive coarse-grained permeability coefficients [38–42]. The porous medium can also be characterized as a statistically homogeneous continuum with local fluctuations in physical parameters. The resulting path integral can be averaged over parameter fluctuations to obtain large-distance parameters that describe the flow [20].

Our paper is organized as follows. The path integral formulation of Darcy flow through random porous media is reviewed in section 2. We explain why the procedure we developed previously for the numerical evaluation of path integrals in one dimension is not readily extended to higher dimensions. We provide an alternative path integral in terms of an action whose extremum yields Darcy’s law (3). Section 3 discusses computational methods, including the simulation of the permeability fields and the method of simulated annealing. Results are presented in section 4. We have calculated probability densities for the pressure, Cartesian flow components, the total flow along the \( y \)-direction, which is the main flow direction with our boundary conditions, and examine the effect of the variance of the log-permeability. Conclusions and a discussion are provided in section 5, including an assessment of the viability of simulated annealing as a computation methodology for Darcy flow, and the extension of the path integral approach to multi-phase flow.

2. Theory

2.1. Effective permeability

The effective permeability is modelled as a stochastic variable. Various such models exist [43]: we have opted for a log-normal process,

\[
K(x) = Ke^{L(x)},
\]

where \( Ke \) is the geometric mean of the permeability and \( L(x) \) is a correlated multivariate Gaussian process. The log-normal distribution is the conventional choice [44] and is one of several distributions for a strictly positive permeability [45]. More information on this process can be found in reference [22]. We emphasize, however, that the methods described below can be applied to any permeability distribution.

The definition of the geometric mean and its relation to an exponentiated arithmetic mean implies that, if the arithmetic mean \( \langle L \rangle = 0 \), then \( Ke = 1 \). We will adopt these values in our calculations because of the simplifications they afford, particularly in the probability
distribution of $L$, which is a correlated multivariate Gaussian probability distribution of the log-permeability with zero mean. The choice $\langle L \rangle = 0$ does not limit the generality of our result because the linearity of Darcy’s law enables any change in this mean, which causes a corresponding change in $K_g$, to be absorbed by rescaling the pressure and making corresponding changes to the boundary conditions.

2.2. Path integrals in higher dimensions

In an earlier paper [22], we developed a path integral for Darcy flow in one dimension. Our derivation is summarized in appendix. A path integral analogous to (A.9) in two dimensions is obtained by following the standard procedure for classical statistical dynamics [46–49]:

$$Z_{2D} = \int \prod_{ij} dp_{ij} \prod_{kl} dL_{kl} \exp \left[ -\sum_{ij,kl} L_{ij}(C_L^{-1})_{ijkl} L_{kl} \right] \times \delta \left[ \frac{\partial}{\partial x} (e^{L_{ij}} \frac{\partial p_{ij}}{\partial x}) + \frac{\partial}{\partial y} (e^{L_{ij}} \frac{\partial p_{ij}}{\partial y}) \right] \times J_{ij} \exp \left( \sum_{ij} u_{ij} p_{ij} \right).$$  \hspace{1cm} (5)

The $\delta$ function enforces the discrete form of Darcy’s law (3) in two dimensions, where we have used the notation

$$\frac{\partial}{\partial x} (e^{L_{ij}} \frac{\partial p_{ij}}{\partial x}) = e^{L_{ij}} \left( \frac{p_{i,j} - p_{i,j-1}}{\delta x} \right) - e^{L_{i,j-1}} \left( \frac{p_{i,j-1} - p_{i,j-2}}{\delta y} \right),$$  \hspace{1cm} (6)

$$\frac{\partial}{\partial y} (e^{L_{ij}} \frac{\partial p_{ij}}{\partial y}) = e^{L_{ij}} \left( \frac{p_{i,j} - p_{i,j-1}}{\delta y} \right) - e^{L_{i,j-1}} \left( \frac{p_{i,j-1} - p_{i,j-2}}{\delta y} \right),$$  \hspace{1cm} (7)

and $J_{ij}$ is the Jacobian, analogous to (A.9). We will not need the explicit form of this Jacobian in what follows, but we should point out that the calculation is not as straightforward as the one-dimensional case discussed in appendix.

The next step is to represent the $\delta$ function as the limit of exponential functions, so that the factors in (5) can be combined into a single exponential whose argument is the ‘action’. The usual procedure [46–49] is to use a functional Fourier transform of the $\delta$ function, which yields a complex action. This is useful for formal studies, such as various types of perturbation expansion [50, 51], where the complex action yields real results, despite the complex nature of intermediate calculations. But the Markov chain Monte Carlo method relies on real variables from the outset, so we must choose a representation of the $\delta$ function in terms of a real exponential. We use the well-known limit of a Gaussian probability density,

$$\delta(x) = \lim_{\tau \to 0} \left( \frac{1}{\sqrt{\pi \tau}} e^{-x^2/\tau} \right),$$  \hspace{1cm} (8)

to write (5) as
\[ Z_{2D}(\{u_{ij}\}) = \int \prod_{ij} dp_{ij} \int \prod_{kl} dL_{kl} \exp \left[ -\sum_{ij,kl} L_{ij}(C_{ij}^{-1})_{ij,kl} L_{kl} \right] \]
\times \lim_{t \to 0} \left( \frac{1}{\sqrt{t}} \exp \left\{ -\frac{1}{t} \left[ \frac{\partial}{\partial x} \left( e^{L_{ij}} \frac{\partial p_{ij}}{\partial x} \right) + \frac{\partial}{\partial y} \left( e^{L_{ij}} \frac{\partial p_{ij}}{\partial y} \right) \right] \right\} \right)^2 \]
\times J(\{L_{ij}\}) \exp \left( \sum_{ij} u_{ij} p_{ij} \right), \tag{9} \]

where we have neglected the factor of $\sqrt{\pi}$ because it cancels in calculations of correlation functions of the pressure. This expression is readily generalized to three dimensions.

Averages of pressure and correlation functions can be calculated from (9) by first generating permeability fields, then setting $t$ to some value, and finally using the Metropolis–Hastings (MH) algorithm \[52\] to minimize the discrete ‘action’ in the argument of the exponential. Successively smaller values of $t$ are chosen until there is convergence of the pressure distributions. This procedure, which requires separate calculations for each value of $t$, is not particularly efficient. In the next section, we develop a more elegant and practical approach based on simulated annealing.

### 2.3. Path integral for simulated annealing

To obtain a path integral that is applicable in higher dimensions, we write the action in continuum form as
\[ S = \frac{1}{2} \int_V K(x)(\nabla p(x))^2 dV, \tag{10} \]

where the integral is over the volume $V$ of the porous medium. The extremum of $S$ with respect to variations in the pressure is determined by adding an infinitesimal pressure $\delta p$ and imposing the condition
\[ S(p(x) + \delta p(x)) - S(p(x)) = 0. \tag{11} \]

By retaining $\delta p$ only to first order and performing an integration by parts, we obtain
\[ S(p + \delta p) - S(p) = \int \nabla \cdot (K \nabla p) \delta p dV \\
= -\int \nabla \cdot (K \nabla p) \delta p dV - \int_{\partial V} K \delta p \nabla p \cdot dS = 0. \tag{12} \]

The boundary integral can be written more suggestively as
\[ \int_{\partial V} K \delta p (\nabla p \cdot n) dS, \tag{13} \]

where $n$ is the outward unit normal to the boundary and $dS$ is the element of area along the boundary. For Dirichlet boundary conditions $p(x) = f(x)$ with a fixed function $f$ and $x \in \partial V$, so $\delta p = 0$ along $\partial V$, while for Neumann boundary conditions, $\nabla p \cdot n = 0$ over $\partial V$. In either case, the boundary integral vanishes. Because $K$ is nonzero, the variation $\delta p$ is arbitrary, and
the result must hold for any volume, the remaining factor in the integrand must vanish. Hence, the stationarity condition (11) yields

$$\nabla \cdot (K \nabla p) = 0,$$

which is Darcy’s law (3) for incompressible flow.

Simulated annealing aims to find the pressure that minimizes the action (10) for fixed permeability $K(x)$, which thereby follows Darcy’s law. The method is inspired by the process of annealing, which is a thermal treatment whereby a solid is slowly cooled until its structure is eventually frozen at its minimum free energy configuration [53].

### 3. Computational methods

As a case study, we will follow the convention for units used by the hydrology community. Darcy’s law (1) gives the relation between the effective permeability $K[L^2 T^{-1}]$, the flow $q[L T^{-1}]$ and the pressure (also known as the hydraulic head) $p[L]$. The total flow in a given direction is denoted by $Q_i[L T^{-1}] (i = x,y,z)$. More conventional units are obtained by inserting the properties of water. For example, $p = \rho gh$, where $\rho$ is the density of water, $g$ the gravitational acceleration, and $h$ the height above a reference state, now has the SI unit of Pascals (Pa).

Simulations of a three-dimensional rectangular prismatic porous medium are carried out on a grid of

$$N_x \times N_y \times N_z = 50 \times 70 \times 50$$

lattice elements, representing a domain of size

$$X \times Y \times Z = 40 \text{ m} \times 85 \text{ m} \times 25 \text{ m}.$$

The correlation lengths of the permeability field have been chosen as

$$\lambda_x = 8, \quad \lambda_y = 8, \quad \lambda_z = 5.$$

We have used Dirichlet boundary conditions along the $y$-direction, making that the main flow direction, with no-flow conditions were imposed along the other boundaries. The values of the variance $\sigma^2$ of the log-permeability, the defining feature of the six parameter sets, are given in table 1. These are the same variances used by Nowak et al [54], which enables a qualitative comparison to be made between our two approaches.

| No. | $\sigma^2$ | Color     |
|-----|------------|-----------|
| 1   | 0.125      | gray      |
| 2   | 0.25       | red       |
| 3   | 0.5        | blue      |
| 4   | 1.0        | magenta   |
| 5   | 1.75       | brown     |
| 6   | 2.5        | orange    |
3.1. Simulation of the permeability fields

The first step in the simulation of the permeability fields is the generation of the three-dimensional log-permeability field. Once the Gaussian field $L(x)$ is available, definition (4), with $K_g = 1$, is invoked to calculate the permeability field $K(x)$. To generate $L(x)$, we have made use of the circulant embedding technique [55], in which the correlation matrix $C$ of the desired field is embedded into a matrix $M$ that has a circulant or block circulant structure. Products of the square root $M^{1/2}$ with white noise random vectors are realizations of the desired random field [56, 57]. This method relies on the fast Fourier transform (FFT). For a $d$-dimensional rectangular mesh containing $N_d^2$ points, the computational requirements are those of an FFT of a vector of dimension $2N^2_d$ per realization [57].

3.2. Simulated annealing

The simulated annealing algorithm is based on the MH algorithm, a step-by-step explanation of which can be found in [52]. In the present case, simulated annealing seeks to minimize the action (10). Clearly, the minimum attainable value is zero. The algorithm consists of the following steps.

(a) Initialize a random pressure that is consistent with the boundary conditions.

(b) Execute the MH algorithm some $M \gg 1$ times. The MH algorithm lowers the value of the action $S$, but also accepts some modifications to the pressure that increase the action. It explores the entire ‘state space’ (the set of values of $S$ as a function of $p(x)$) and does not get stuck in a local minimum of the state space.

(c) After every $N_s \gg 1$ steps, check the value of $S$. When the value of $S$ starts to fluctuate around a constant value, go to step (d).

(d) Adapt the MH accept/reject criterion to ‘accept the change in the action with probability $\min(1, e^{-\delta S/T})$ for some constant $0 < T < 1$’. This is a ‘cooling step’ [58]. The state space is explored in smaller steps than was the case for the standard MH algorithm, while maintaining a constant acceptance rate. The lower the value of $T$, the smaller the steps. In our context, $T$ does not have the interpretation of a temperature, but its effect remains that of slowing down the exploration of state space.

(e) Repeat steps (c) and (d) until the action attains a critically low value $\epsilon_1$, say, $\epsilon_1 = 0.1$.

(f) Employ a modification of the MH algorithm known as the ‘greedy algorithm’, which accepts only changes to the pressure that lower the action, until $S$ dives below a second critical value $\epsilon_2$, say $\epsilon_2 = 10^{-2}$.

To expedite the simulated annealing algorithm, we made use of a technique known as over-relaxation (OR). The idea behind over-relaxation is to choose trial changes that cause significant changes to the pressure field, but only small changes to the action [59, 60]. Such strategic updates combine a thorough exploration of phase space with a high probability of acceptance. Because the action (10) is quadratic, it is possible to calculate an update that leaves the action unchanged, rendering the Metropolis accept/reject step unnecessary. The update

$$p_i^{\text{new}} = 2p_i^* - p_i^{\text{old}}$$

(18)

lies ‘on the other side’ of the minimum of the action: $p_i^*$ is the value of $p_i$ that minimizes $S$, with all other parameters kept fixed. Since the over-relaxation procedure is deterministic, we alternate between OR and regular MH steps to avoid any dependence of the pressure field on its random starting configuration. Here, we exchanged three in four Metropolis sweeps for OR sweeps.
We have used an exponential cooling scheme

$$T^{(k)} = \alpha^k T_i,$$

(19)

where $k$ indicates the cooling step. The MH algorithm was executed $M = 2000$ times for all parameters. For $\sigma^2 \leq 1$, repeating the cooling algorithm $N_s = 3000$ times was found to be a good choice. For $\sigma^2 > 1$, it was necessary to set $N_s = 6000$. To calculate empirical probability density functions for the pressure and flow, we have worked with $N = 10000$ realizations for each parameter set.

In comparing the computational efforts involved in running the FVM method and simulated annealing, we note that both require a permeability field as input. The computational cost associated with the FFT is

$$O(2N_xN_yN_z \log(N_xN_yN_z))$$

(20)

floating point operations (‘flops’). The key calculation in the FVM is a sparse matrix inversion. The sparse matrix solver UMFPACK [61] can solve such an equation in

$$O(N_xN_yN_z \log(N_xN_yN_z))$$

flops. In contrast to the FVM, the simulated annealing requires $O((N_xN_yN_z)^2)$ flops to calculate a pressure realization. One factor $N_xN_yN_z$ arises from the number of lattice sites. The number of required intermediate updates $N_{sep}$ introduces a further factor $N_xN_yN_z$. However, there are techniques whose implementation is likely to decrease the run time considerably, such as the multigrid Monte Carlo (MGMC) method [62–64] and directed sampling [65–67].

4. Results

We have calculated empirical probability densities for the pressure $p$, the flow components $q_x$ and $q_y$, and the total flow $Q_y$ and looked at the effect of the variance of the log-permeability $\sigma^2$. Based on information about boundedness, we have made parametric fits using the choices made in reference [54] for guidance.

All quantities were normalized to facilitate a straightforward interpretation. The Dirichlet boundary conditions were chosen to yield a pressure difference

$$\Delta p = 1 \text{ m.}$$

(22)

The flow components were normalized as

$$q^*_{x,y} = \frac{q_{x,y}}{K_e I_0},$$

(23)

$$Q^*_y = \frac{Q_y}{K_e I_0 A},$$

(24)

where $K_e$ is the theoretical expectation value of the permeability, $I_0 = \Delta p/L_y$ and $A = L_x \times L_z$. Computationally, the normalization was achieved by setting $K_e = 1/(I_0 A)$.

Due to correlations in the permeability, the distributions of pressure and flow are in general not expected to be Gaussian, particularly when the variance of the log-permeability is large. The pressure along the main direction takes values in the interval [0, 1] due to the Dirichlet boundary conditions. Given this constraint and the choice of stochastic model for the permeability, the log-normal distribution,
Figure 1. Pressure statistics for Darcy flow at the center of the domain for the following values of $\sigma^2$: (a) 0.125 (grey), 0.25 (red), 0.5 (blue) and (b) 1.0 (pink), 1.75 (brown), and 2.5 (orange), as listed in table 1. Squares represent the results of the finite-volume method, circles those of simulated annealing.

$$f(x) = \frac{1}{x \sqrt{2\pi} \sigma'} \exp \left[ -\frac{(\log x - \mu')^2}{2(\sigma')^2} \right], \quad (25)$$

is an obvious contender for parametric fits to the pressure.

To visualize the position-dependence of the pressure along the main axis, we show empirical probability density plots at two positions: (0.5X, 0.5Y, 0.5Z), which is the center of the domain (figure 1) and (0.5X, 0.8Y, 0.5Z) (figure 2). The two sets of figures show that the log-normal distribution is most evident near the boundary. Towards the center of the domain, the histograms bear more resemblance to the normal distribution [68], as the generalized central limit theorem predicts [69]. For a more extensive explanation of this theorem in the context of Darcy flow, see reference [22]. These boundary effects increase with the variance of the log-permeability, as can also be observed for the flow.

Like the pressure, the flow along the main axis is subject to a non-negativity constraint, which enforces a one-sided bound. The flow could be negative only in the unlikely event of flow reversal due to a locally very large permeability. The observed values for the cases considered here were non-negative. For the flow, as for the pressure, the shape of the probability density depends on the vicinity to a restricting boundary. We have evaluated the flow in the main direction at the center of the domain. The results are shown in figure 3. One can see that for high values of the log-permeability variance, the flow statistics are most clearly log-normal. This is because the boundary effects are more strongly felt for high values of $\sigma^2$, a pattern that can also be observed by comparing figures 1 and 2. The total flow in the main direction, defined as the average over a cross-section perpendicular to the $y$-axis, is conserved along the $y$-axis. The results can be seen in figure 4. When comparing figures 3 and 4, an obvious difference is that the flow statistics of the total flow approximate the Gaussian distribution more closely. The log-normal distribution tends to the normal distribution in the limit $(\sigma' / \mu')^2 \to 0$. The Gaussian appearance is a result of the averaging over a cross-section that defines the total flow.

Striking features of the transverse flow statistics are the enhanced values near zero and the long and heavy tails, with this behavior being most pronounced for large values of the variance of the log-permeability. Hence, the fits to the probabilities in figure 5 used the probability
Figure 2. Pressure statistics for Darcy flow at the point (0.5X, 0.8Y, 0.5Z) for finite-volume simulations (squares) and simulated annealing (circles) with the values of $\sigma^2$ compiled in table 1.

Figure 3. Normalized flow in the main direction $q^*$ for the values of $\sigma^2$ in table 1, measured at the point (0.5X, 0.5Y, 0.5Z). The log-normal pattern manifests itself most clearly for high values of $\sigma^2$. For these high values, the boundary effects, which dictate the log-normality, have the strongest influence on the flow statistics.

density function for the exponential power law,

$$g(x) = \frac{1}{2\sigma^2 \Gamma(1 + 1/k)} \exp \left[ -\frac{|x - \mu''|^{k}}{(\sigma^2)^2} \right],$$

which includes the Laplace ($k = 1$) and the Gaussian ($k = 2$) distributions as special cases. This choice was also made in [54]). All parametric fits for the parameters \{\mu', \mu'', \sigma', \sigma'', k\} were made using the in-built routine FindFit of Mathematica [70]. In the limit of large variance, the permeability can take a wide range of values. Thus, it will often occur that the flow either continues along its main axis, or is diverted. This behavior is reflected in the statistics by the tails of the distribution.
Figure 4. Normalized total flow in the main direction $Q_y^*$ for the values of $\sigma^2$ stated in table 1. The distribution of $Q_y^*$ resembles that of $q_y^*$ shown in figure 3. Due to the averaging over a cross-section, the distributions appear more Gaussian.

Figure 5. Statistics of the normalized flow in the $x$-direction, $q_x^*$, again for the parameter set given in table 1. The parametric fits of the exponential power distribution reflect the symmetry of the statistics about zero. The tails become heavier for greater values of $\sigma^2$. In the limit $\sigma \gg 1$, the flow either continues along the main axis or ‘hits a wall’ and reverses course. Thus, in this limit, the likelihood of small values for $q_x^*$ is very small.

5. Conclusion and discussion

The rock heterogeneities exert a significant influence on the flow, from the pore scale up to the kilometer scale. Calculation of the Darcy pressure statistics depends on an explicit description of the permeability $K$ at the mesoscopic scale. For this work, we have chosen a log-normal distribution. Simulated annealing can be used to calculate the pressure and flow statistics for any type of realization of the permeability $K$. An alternative to assuming the log-normal distribution could be the use of multiple-point statistics, a method that directly infers the necessary multivariate distributions from training images [71], or copulas, which describe the stochastic structure without reference to the corresponding marginal distributions [72].
We have shown that the action in (10) can be used to apply simulated annealing to calculate Darcy pressure and flow statistics. We have outlined our computational methods in such a way as to make them easily reproducible. Our model was a three-dimensional, bounded domain, with Dirichlet boundary conditions at two ends and no-flow boundary conditions at the remaining four. Our results for the pressure, calculated at two different points in the domain, as well as those for the local and total flow in the main and in a transverse direction behaved qualitatively as expected. Parametric log-normal and exponential power-law fits were made using Mathematica, all of which passed one-sided Kolmogorov–Smirnov tests at the 95% confidence level. At the moment, simulated annealing is not computationally competitive with the finite-volume method. Its runtime may be improved through the use of the multigrid method, however. Most promisingly, it may be possible to apply the renormalization group as an upscaling technique. Such an application would provide a different take on the problem and may enable the user to run coarse but fast simulations to capture the main characteristics of the pressure and flow statistics.

A major challenge is the extension of the present approach to multiphase flow. For two-phase flow a generalized form of Darcy’s law is used:

\[ q_i = -k_{r,i}(S_i)K \nabla p, \]  

(27)

where the subscript i represents the fluid phase (oil or water), \( k_{r,i} \) is the relative permeability, and \( S_i \) is the pore volume fraction of the fluid phase i. The two volume fractions must sum to one. The total velocity is given by the sum of the individual phase velocities:

\[ q = q_o + q_w. \]  

(28)

The rate of change of the saturation \( s \) is given by the conservation equation,

\[ \frac{\partial s}{\partial t} = g(s)q \cdot \nabla s, \]  

(29)

where \( g(s) \) is a nonlinear function. The constraint (2) still holds for an incompressible fluid. Equation (27) is similar to Darcy’s law for single-phase flow. An adaptation of the methodology outlined in this paper should be suited to the solution of (27). The hyperbolic saturation equation (29) poses more problems, in particular because its nonlinear nature leads to the formation of a shock in the solution [73]. Previous studies [74] indicate how a path integral formulation of this equation can be formed, providing an opportunity for future research.

Acknowledgments

MJEW was supported through a Janet Watson scholarship from the Department of Earth Science and Engineering and a studentship in the Centre for Doctoral Training on Theory and Simulation of Materials funded by the EPSRC (EP/L015579/1), both at Imperial College London. We acknowledge the support of the Imperial College Research Computing Service [75]. We thank Stephan Dürr for a helpful discussion.

Appendix. Path integral formulation for Darcy’s law in one dimension

In one dimension, this Darcy’s equation (3) reduces to

\[ \frac{d}{dx} \left( K \frac{dp}{dx} \right) = 0. \]  

(A.1)
Integrating this equation yields,
\[
K \frac{dp}{dx} = -q_0,
\] (A.2)
which is the one-dimensional version of (1).

The permeability follows a log-normal distribution. By writing \( K(x) = e^{L(x)} \), as in (4), \( L(x) \) then follows a multivariate normal distribution with zero mean. Equation (A.2) becomes
\[
\frac{dp}{dx} = -q_0 e^{-L}.
\] (A.3)

The continuous porous medium is now replaced by a lattice of points \( x_1, x_2, \ldots, x_N \) separated by a distance \( \delta x \). The pressure and permeability evaluated at these points are \( p_1, p_2, \ldots, p_N \) and \( L_1, L_2, \ldots, L_N \), respectively. The discretized form of (A.3) is
\[
\frac{p_i - p_{i-1}}{\delta x} = -q_0 e^{-L_i}.
\] (A.4)

This equation establishes a relation between two sets of stochastic variables: the pressures \( \{p_i\} \equiv \{p_1, p_2, \ldots, p_N\} \) and log permeabilities \( \{L_i\} \equiv \{L_1, L_2, \ldots, L_N\} \). The corresponding joint probability densities \( P \) and \( Q \) are related by
\[
P(\{p_i\}) = Q(\{L_i\}) J,
\] (A.5)
where the Jacobian,
\[
J = \det \left( \frac{\partial L_i}{\partial p_j} \right),
\] (A.6)
accounts for the transformation of variables and maintains normalization. Determining the Jacobian is a straightforward calculation, with the result that (A.5) becomes
\[
P(\{p_i\}) = Q(\{L_i\}) \exp \left( \sum_{i=1}^{N} L_i \right),
\] (A.7)
where we have omitted the constant factor \((q_0 \delta x)^{-N}\), which will cancel the same term in the denominator in expressions for averages of the pressure. We now use (A.4) to enforce the relation between the \( \{L_i\} \) and the \( \{p_i\} \) through a Dirac \( \delta \)-function:
\[
P(\{p_i\}) = \int \prod_{i=1}^{N} dL_i Q(\{L_i\}) \exp \left( \sum_{i=1}^{N} L_i \right) \delta \left( \frac{p_i - p_{i-1}}{\delta x} + q_0 e^{-L_i} \right).
\] (A.8)

Thus, we can write the generating functional \( Z(\{u_i\}) \) for connected \( n \)-point correlation functions of the pressure as
\[
Z(\{u_i\}) = \int \prod_{i=1}^{N} dp_i \int \prod_{i=1}^{N} dL_i Q(\{L_i\}) \exp \left( \sum_{i=1}^{N} L_i \right) \times \delta \left( \frac{p_i - p_{i-1}}{\delta x} + q_0 e^{-L_i} \right) \exp \left( \sum_{i=1}^{N} u_i p_i \right).
\] (A.9)
We now use the fact that $Q(\{L_i\})$ is a multivariate Gaussian probability density with zero mean:

$$Q(\{L_i\}) = \frac{1}{(2\pi)^{N/2}\left|\mathbf{C}\right|^{1/2}} \exp\left[-\frac{1}{2} \mathbf{L}^T \mathbf{C}^{-1} \mathbf{L}\right].$$  \hspace{1cm} (A.10)

By carrying out the integral over the $L_i$ before the integral over the $p_i$ (because the random permeability produces quenched disorder for the pressure), (A.9) reduces to

$$Z(\{u_i\}) = \int \prod_{i=1}^{N} dp_i \exp\left[-\sum_{i=1}^{N} \ln\left(\frac{p_{i-1} - p_i}{q_0 \delta x}\right) \right]$$

$$-\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \ln\left(\frac{p_{i-1} - p_i}{q_0 \delta x}\right) \left(\mathbf{C}^{-1}\right)_{i,j} \ln\left(\frac{p_{j-1} - p_j}{q_0 \delta x}\right) + \sum_{i=1}^{N} u_i p_i$$

$$\equiv \int \prod_{i=1}^{N} dp_i \exp\left[-S(\{p_i\}) + \sum_{i=1}^{N} u_i p_i\right]$$  \hspace{1cm} (A.11)

in which the action $S(\{p_i\})$ is

$$S(\{p_i\}) = \sum_{i=1}^{N} \ln\left(\frac{p_{i-1} - p_i}{q_0 \delta x}\right) + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \ln\left(\frac{p_{i-1} - p_i}{q_0 \delta x}\right) \left(\mathbf{C}^{-1}\right)_{i,j}$$

$$\times \ln\left(\frac{p_{j-1} - p_j}{q_0 \delta x}\right).$$  \hspace{1cm} (A.12)

ORCID iDs

Dimitri D Vvedensky https://orcid.org/0000-0002-4990-0208

References

[1] Sahimi M 1993 Flow phenomena in rocks: from continuum models to fractals, percolation, cellular automata, and simulated annealing Rev. Mod. Phys. 65 1393–534
[2] Vafai K (ed) 2015 Handbook of Porous Media 3rd edn (Boca Raton, FL: CRC Press)
[3] Bear J 2018 Modeling Phenomena of Flow and Transport in Porous Media (Cham: Springer)
[4] Mualem Y 1976 A new model for predicting the hydraulic conductivity of unsaturated porous media Water Resour. Res. 12 513–22
[5] Abdelaziz R, Komori F S and Carreño M N P 2016 Multiphase thermal-fluid flow through geothermal reservoirs Energy Proc. 95 22–8
[6] Orr F M Jr and Taber J J 1984 Use of carbon dioxide in enhanced oil recovery Science 224 563–9
[7] Szulczewski M L, MacMinn C W, Herzog H J and Juanes R 2012 Lifetime of carbon capture and storage as a climate-change mitigation technology Proc. Natl Acad. Sci. 109 5185–9
[8] Khaled A-R A and Vafai K 2003 The role of porous media in modeling flow and heat transfer in biological tissues Int. J. Heat Mass Transfer 46 4989–5003
[9] Miguel A F 2012 Lungs as a Natural Porous Media: Architecture, Airflow Characteristics and Transport of Suspended Particles Heat and Mass Transfer in Porous Media (Advanced Structured Materials vol 13) ed J Delgado (Berlin: Springer) pp 115–37
[10] Linninger A A, Xenos M, Zhu D C, Somayaji M R, Kondapalli S and Penn R D 2007 Cerebrospinal fluid flow in the normal and hydrocephalic human brain IEEE Trans. Biomed. Eng. 54 291–302
(11) D’Angelo C and Zunino P 2010 Robust numerical approximation of coupled Stokes’ and Darcy’s flows applied to vascular hemodynamics and biochemical transport ESAIM: Math. Modelling Numer. Anal. 45 447–76

(12) Shahamiri S A and Wierzba I 2011 Modeling the reactive processes within a catalytic porous medium Appl. Math. Modelling 35 1915–25

(13) Rashidi S, Esfahani J A and Karimi N 2018 Porous materials in building energy technologies—a review of the applications, modelling and experiments Renew. Sustain. Energy Rev. 91 229–47

(14) Mohamad A A 2003 Heat transfer enhancements in heat exchangers fitted with porous media I. Constant wall temperature Int. J Therm. Sci. 42 385–95

(15) Jin Z and Firoozabadi A 2015 Flow of methane in shale nanopores at low and high pressure by molecular dynamics simulations J. Chem. Phys. 143 104315

(16) Guo Z and Zhao T S 2002 Lattice Boltzmann model for incompressible flows through porous media Phys. Rev. E 66 036304

(17) Liu H, Kang Q, Leonardi C R, Wang H and Harting J 2016 Multiphase lattice Boltzmann simulations for porous media applications Comput. Geosci. 20 777–805

(18) Bakhshian S, Hosseini S A and Shokri N 2019 Porose-scale characteristics of multiphase flow in heterogeneous porous media using the lattice Boltzmann method Sci. Rep. 9 3377

(19) Narsilio G A, Buzzi O, Fityus S, Yun T S and Smith D 2009 Upscaling of Navier–Stokes equations in porous media: theoretical, numerical and experimental approach Comput. Geotechn. 36 1200–6

(20) Tanksley M A and Kocik J 1994 Path-integral variational methods for flow through porous media Phys. Rev. E 49 1355–66

(21) Teodorovich É V 1997 Calculation of the effective permeability of a randomly inhomogeneous porous medium J. Exp. Theor. Phys. 85 173–8

(22) Westbrook M J E, Coche G-A, King P R and Vvedensky D D 2019 Pressure statistics from the path integral for Darcy flow through random porous media J. Phys. A: Math. Theor. 52 185001

(23) Jenny P, Lee S H and Tchelepi H A 2004 Adaptive multiscale finite-volume method for multiphase flow and transport in porous media 2004 Multiscale Model. Simul. 3 50–64

(24) Hou T Y and Wu X-H 1997 A multiscale finite element method for elliptic problems in composite materials J. Comput. Phys. 134 169–89

(25) McCarthy J F 1990 Effective permeability of sandstone-shale reservoirs by a random walk method J. Phys. A: Math. Gen. 23 L445–51

(26) McCarthy J F 1990 Effective conductivity of many-component composites by a random walk method J. Phys. A: Math. Gen. 23 L749–53

(27) McCarthy J F 1993 Continuous-time random walks on random media J. Phys. A: Math. Gen. 26 2495–503

(28) Berkowitz B, Cortis A, Dentz M and Scher H 2006 Modeling non-Fickian transport in geological formations as a continuous time random walk Rev. Geophys. 44 RG2003

(29) Blunt M J 2017 Multiphase Flow in Permeable Media: A Pore-Scale Perspective (Cambridge: Cambridge University Press)

(30) Zhao B et al 2019 Comprehensive comparison of pore-scale models for multiphase flow in porous media Proc. Natl Acad. Sci. USA 116 13799–806

(31) Darcy H 1856 Les Fontaines Publiques de la Ville de Dijon (Paris: Dalmont)

(32) Whitaker S 1985 Flow in porous media I. A theoretical derivation of Darcy’s law Transport Porous Media 1 3–25

(33) Aziz K and Settari A 1979 Petroleum Reservoir Simulation (London: Applied Science Publishers)

(34) Schäfer M 2006 Computational Engineering: Introduction to Numerical Methods (Berlin: Springer) pp 77–103

(35) Westbrook M J E, Coche G-A, King P R and Vvedensky D D 2018 Evaluation of the path integral for flow through random porous media Phys. Rev. E 97 042119

(36) Kirkpatrick S, Gelatt C D Jr and Vecchi M P 1983 Optimization by simulated annealing Science 220 671–80

(37) Press W H, Teukolsky S A, Vetterling W T and Flannery B P 1992 Numerical Recipes in C: The Art of Scientific Computing 2nd edn (Cambridge: Cambridge University Press)

(38) Hristopulos D T and Christakos G 1999 Renormalization group analysis of permeability upscaling Stoch. Environ. Res. Risk Assess. 13 131–61
[39] Attinger S 2003 Generalized coarse graining procedures for flow in porous media Comput. Geosci. 7 253–73
[40] Eberhard J, Attinger S and Wittum G 2004 Coarse graining for upscaling of flow in heterogeneous porous media Multiscale Model. Simul. 2 69–301
[41] Hanasoge S, Agarwal U, Tandon K, Vianney J M and Koelman A 2017 Renormalization group theory outperforms other approaches in statistical comparison between upscaling techniques for porous media Phys. Rev. E 96 033313
[42] King P R 1989 The use of renormalization for calculating effective permeability Transport Porous Media 4 37–58
[43] Renard P and de Marsily G 1997 Calculating equivalent permeability: a review Adv. Water Resour. 20 253–78
[44] Law J 1944 A statistical approach to the interstitial heterogeneity of sand reservoirs Trans. AIME 155 202–22
[45] Jensen J L, Hinkley D V and Lake L W 1987 A statistical study of reservoir permeability: distributions, correlations, and averages SPE Form. Eval. 2 461–8
[46] Phythian R 1977 The functional formalism of classical statistical dynamics J. Phys. A: Math. Gen. 10 777–89
[47] De Dominicis C and Peliti L 1978 Field-theory renormalization and critical dynamics above $T_c$: helium, antiferromagnets, and liquid-gas systems Phys. Rev. B 18 353–76
[48] Jouvet B and Phythian R 1979 Quantum aspects of classical and statistical fields Phys. Rev. A 19 1350–5
[49] Jensen R V 1981 Functional integral approach to classical statistical dynamics J. Stat. Phys. 25 183–210
[50] Zinn-Justin J 2006 Path Integrals in Quantum Mechanics (Oxford: Oxford University Press)
[51] Özer UC, King PR and Vvedensky D D 2019 Path integral renormalization of flow through random porous media (arXiv:1911.11218)
[52] Westbroek M J E, King P R, Vvedensky D D and Dierr S 2018 User’s guide to Monte Carlo methods for evaluating path integrals Am. J. Phys. 86 293–304
[53] Du K-L and Swamy M N S 2016 Search and Optimization by Metaheuristics (Switzerland: Springer)
[54] Nowak W, Schwede R L, Cirpka O A and Neuweiler I 2008 Probability density functions of hydraulic head and velocity in three-dimensional heterogeneous porous media Water Resour. Res. 44 W08452
[55] Gneiting T, Sevciková H, Percival D B, Schlather M and Jiang Y 2006 Fast and exact simulation of large Gaussian lattice systems in $\mathbb{R}^2$: exploring the limits J. Comput. Graph. Stat. 15 483–501
[56] Nowak W, Tenkleve S and Cirpka O A 2003 Efficient computation of linearized cross-covariance and auto-covariance matrices of interdependent quantities Math. Geol. 35 53–66
[57] Dietrich C R and Newsam G N 1993 A fast and exact method for multidimensional Gaussian stochastic simulations Water Resour. Res. 29 2861–9
[58] Note that the ‘cooling parameter’ T does not have the dimensions of a temperature, as the analogy with the cooling of solids suggests
[59] Creutz M 1987 Overrelaxation and Monte Carlo simulation Phys. Rev. D 36 515–9
[60] Brown F R and Woch T J 1997 Overrelaxed heat-bath and Metropolis algorithms for accelerating pure gauge Monte Carlo calculations Phys. Rev. Lett. 58 2394–6
[61] Davis T A 2004 Algorithm 832 ACM Trans. Math. Softw. 30 196–9
[62] Goodman J and Sokal A D 1986 Multigrid Monte Carlo method for lattice field theories Phys. Rev. Lett. 56 1015–8
[63] Janke W and Sauer T 1993 Path integral Monte Carlo using multigrid techniques Chem. Phys. Lett. 201 499–505
[64] Liu J S and Sabatti C 2000 Generalised Gibbs sampler and multigrid Monte Carlo for Bayesian computation Biometrika 87 353–69
[65] Duncan A B, Lelièvre T and Pavliotis G A 2016 Variance reduction using nonreversible Langevin samplers J. Stat. Phys. 163 457–91
[66] Duncan A B, Nüsken N and Pavliotis G A 2017 Using perturbed underdamped Langevin dynamics to efficiently sample from probability distributions J. Stat. Phys. 169 1098–131
[67] Lelièvre T, Nier F and Pavliotis G A 2013 Optimal non-reversible linear drift for the convergence to equilibrium of a diffusion J. Stat. Phys. 152 237–74
[68] Ababou R, McLaughlin D, Gelhar L W and Tompson F B 1989 Numerical simulation of three-dimensional saturated flow in randomly heterogeneous porous media Transport Porous Media 4 49–565
[69] Bouchaud J-P and Georges A 1990 Anomalous diffusion in disordered media: statistical mechanisms, models and physical applications Phys. Rep. 195 127–293
[70] 2018 Wolfram Research, Inc. Mathematica v11.3 (Champaign, IL)
[71] Huysmans M and Dassargues A 2009 Application of multiple-point geostatistics on modelling groundwater flow and transport in a cross-bedded aquifer (Belgium) Hydrogeol. J. 17 1901–11
[72] Bárdossy A and Li J 2008 Geostatistical interpolation using copulas Water Resour. Res. 44 W07412
[73] Buckley S E and Leverett M C 1942 Mechanism of fluid displacement in sands Trans. AIME 146 107–16
[74] King P R and Neuweiler I 2002 Probability upscaling Comput. Geosci. 6 101–14
[75] Imperial College Research Computing Service