A rigorous pore-to-field-scale simulation methodology for single-phase flow based on continuous time random walks
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Abstract
We demonstrate a pore-to-reservoir simulation methodology and apply it to single-phase flow. Traditional numerical methods are based on the discretization of partial differential equations with known spatially-dependent coefficients, such as porosity and permeability. However, in porous media flow we do not know a priori what the governing transport equations are – for instance, single-phase transport cannot be accurately described by an advection-dispersion equation – nor do we know the reservoir properties everywhere.

We propose a different approach that does not pre-suppose the functional form of the upscaled transport equations and which automatically accounts for uncertainty in the reservoir description. Single-phase transport is modeled as a continuous time random walk. Particles make a series of transitions between nodes with a probability \( \psi(t)dt \) that a particle will first arrive at a node from a nearest neighbor in a time \( t \) to \( t+dt \). A top-down multiscale approach is used to find the flow field. At the micron scale, \( \psi(t) \) for particle transitions from pore to pore are found from modeling advection and molecular diffusion in a geologically representative network model. This \( \psi(t) \) is used to compute transport on the mm to cm scale. At larger scales, we represent the reservoir as a network of nodes connected by links. For each node-to-node transition, we compute an upscaled \( \psi(t) \) from a simulation of transport at the smaller scale. We account for small-scale uncertainty by interpreting \( \psi(t) \) probabilistically and running simulations for different possible realizations of the reservoir model. To make the number of computations manageable, \( \psi(t) \) is parameterized in terms of sub-scale heterogeneity and Peclet number, meaning that only a few representative simulations are required.

We demonstrate the methodology by finding \( \psi(t) \) for pore-scale flow and using it in a million-cell reservoir model. We show that the macroscopic behavior can be very different from that predicted by assuming that the advection-dispersion equation operates at the small scale. Small-scale structure does impact macroscopic transport; increasing the pore-level heterogeneity delays breakthrough and leads to longer late-time tails of the production since the solute spends more time in slow-flowing regions of the domain. We discuss extensions to multiphase flow and the development of a novel network-based probabilistic reservoir simulation approach.

Introduction
The conceptual framework for reservoir simulation is borrowed from traditional fluid dynamics applications where known differential equations are solved with known – albeit complicated – boundary conditions. Current research in this field – on improved discretization of the governing conservation equations, the use of unstructured grids and parallelization – reinforces the notion that the underlying principles that we use are correct – see, for instance1. However, porous media flow presents a completely distinct set of simulation challenges that we not address appropriately. First, while we use empirical approaches to describe transport and multiphase flow at the experimental, core scale, we do not know the correct form of the constitutive relationships between pressure gradient, flux and saturation on the much larger scale at which we solve the equations. The subtle interplay of heterogeneity and the length-scale-dependent balance of capillary, diffusive, gravity and viscous forces means that our conventional dispersion-and-Darcy models of flow and transport at the field scale have a somewhat dubious foundation. Second, even if we did know the governing partial differential equations, we would not know, with any certainty, the values of the coefficients in these equations. At present, we have no automatic way to incorporate our uncertainty in the description of the reservoir model into uncertainty in prediction of transport and oil recovery.

Is there a different way of looking at flow in porous media that overcomes these problems; that does not assume a priori the form of the transport equations and which can accommodate uncertainty? The approach we propose is conceptually simple and easy to implement. In this paper we will apply it to single-phase flow. We first discuss the traditional approach to modeling transport and illustrate its limitations. We then introduce continuous time random walks that we use to simulate particle movement. We perform a pore-to-core analysis of dispersion to put the methodology on a firm foundation. We then show how to upscale transport to the field scale and demonstrate that variability at every scale affects the macroscopic behavior even when the field-scale reservoir description is highly heterogeneous. Last we discuss possible extensions to multiphase flow.
Traditionally the macroscopic transport of tracer had been described by the advection-dispersion equation (ADE):

$$\frac{\partial c}{\partial t} + v \cdot \nabla c = \nabla \cdot (D \nabla c)$$  \hspace{1cm} (1)

where $c$ is the contaminant concentration, $v$ is the flow speed and $D$ is the dispersion coefficient (which, in general, is a tensor). We have assumed incompressible flow with a constant porosity. In contaminant hydrology it is often presumed that the transport can be modeled by flow in a homogenous domain with some effective $D$ assigned to accommodate the dispersion of contaminant due to small-scale heterogeneity and molecular diffusion.

Solutions to the ADE in statistically homogeneous systems produce a plume profile that is Gaussian in nature with an average displacement that scales linearly with time, $l(t) \sim t$, and a standard deviation about the mean that scales with the square root of time, $\sigma(t) \sim t^{1/2}$. However, in most cases, the macroscopic behavior of the transport cannot be described by a solution to the ADE, Eq. (1), without explicitly accounting for small-scale heterogeneity. This so-called non-Fickian or anomalous contaminant transport is observed from the laboratory to the field scales and is characterized by a slowly moving maximum concentration, a rapidly advancing leading front and a long tail of late arriving fluid. This demonstrates that we do not know the appropriate macroscopic description for the transport and hence a numerical simulation strategy based around discretization of Eq. (1) is flawed.

Continuous time random walks

We will view transport as a continuous time random walk (CTRW): particles move between a series of discrete nodes or sites with a probability $\psi(t;i,j)dt$ that a particle that first arrives at site $i$ will move to site $j$ in a time $t$ to $t+dt$. CTRWs were first introduced in the 1970s to describe electron transport in semi-conductors; more recently they have found a particularly rich application in modeling contaminant transport. Berkowitz et al. have written an excellent, recent review.

CTRW does not make any assumptions about the governing transport equations; instead physical modeling of the process of interest is used to derive $\psi$ from which the resultant macroscopic behavior can be found analytically or numerically. Anomalous transport can be elegantly described in terms of CTRW. If $\psi(t;i,j)dt$ is the probability that a particle that has just arrived at a site will move to a nearest neighbor in a time $t$ to $t+dt$, then, for many systems, at late time there is a power-law dependence of the probability: $\psi(t) \sim t^{-\beta}$ with some exponent $\beta \leq 2$. This leads to an outlet concentration that, at late time, scales as $C(t) \sim t^{-\beta}$. For $1 < \beta < 2$ we find that both the average plume displacement its standard deviation scales as $l(t) \sim \sigma(t) \sim t^{-1/\beta}$, while for $2 < \beta \leq 2$ the average displacement scales normally: $l(t) \sim t$, but the spread is still anomalous: $\sigma(t) \sim t^{1-\beta/2}$. For $\beta > 2$ the system displays Gaussian behavior.

Generally CTRW has been applied to find the ensemble average behavior of a plume in a macroscopically homogeneous domain. However, in most reservoirs the permeability distribution is described on a scale of a few meters. What is needed is a rapid simulation technique to capture the behavior for different, explicit reservoir models while capturing the effects of uncertainty in the reservoir description at smaller – below a meter – scales. CTRW has been applied to heterogeneous media, but for relatively coarsely-gridded two-dimensional systems where the solution involves the numerical inversion of a multi-dimensional Laplace transform. Here we propose a simpler approach: we simply simulate particle transport from site to site with some known $\psi(t;i,j)$ in CTRW this is equivalent to solving the master equation numerically.

We employ a multiscale methodology where, at each stage, transport is considered conceptually as a series of transitions from node to node – see Fig. 1. All the physics of the process is contained in the transit time distribution $\psi(t)$. At the very smallest scales – the pore and sub-pore level – we do know how to describe transport: it is Stokes flow in a spatially varying flow field with molecular diffusion. Hence we start at the pore scale and then describe how to upscale these results to determine transport in the field.
Pore-to-core simulation
Bijeljic et al.\textsuperscript{17} developed a pore-scale network model of dispersion. They represented a porous medium as a two-dimensional diamond lattice of throats connecting volumeless pores (nodes or sites). Each throat had a square cross-section and the distribution of throat radius matched that inferred for Berea sandstone. They then simulated transport as a series of advective and diffusive steps with physically-based mixing rules at pores. They accurately predicted the experimentally-measured dependence of longitudinal dispersion coefficient, $D_L$, on Peclet number, the ratio of advective to diffusive forces, $Pe=vI/D_m$, where $v$ is the average flow speed in the porous medium, $I$ is the throat length and $D_m$ is the molecular diffusion coefficient.

For moderate Peclet numbers $400>Pe>10$ there is an approximate power-law dependence of $D_L$: $D_L\sim Pe^\delta$ with $\delta=1.2$. As we discuss later, Bijeljic and Blunt\textsuperscript{18} provided a physical explanation for this behavior in terms of the distribution $\psi$ of pore-to-pore transit times.

We can replace a direct simulation approach that involves sub-pore-scale transport with one where particles simply hop from pore to pore with a known transit time distribution, $\psi(t;i,j)$. There are two ways in which this can be done. The first is to have the same network and measure the transit time distribution for each pore-to-pore transition. In the large $Pe$ limit, $\psi$ will tend to delta function around the advective transit time $l/v$. The flow speed $v$, however, will be different for each throat, reflecting the heterogeneity of the network.

The second way to simulate transport is to consider $\psi$ an ensemble averaged transit time distribution that accounts for all possible statistically equivalent realizations of the pore-scale structure. Since there are no systematic long-range correlations, the ensemble average network is homogeneous. However, now $\psi$ must accommodate a much wider range of transit times, even in the advective-dominated limit, since it accounts for the variation in flow speed between elements in each possible realization of the structure. This ensemble average $\psi$ is found by averaging the transit times over every pore-to-pore transition in the heterogeneous network. Bijeljic and Blunt\textsuperscript{18} found that $\psi$ was very well fit by a truncated power-law form over six orders of magnitude in time and $Pe$:

$$\psi(t) = A \frac{e^{-t/t_1}}{(1+t/t_1)^(\alpha/\beta)}$$  \hspace{1cm} (2)

where $A$ is a normalization constant, $t_1$ is an average advective transit time $= l/v$ where $l$ is the average pore-to-pore length and $v$ is the average velocity in a throat, and $t_2$ is a typical diffusive transit time $= l^2/2D_m$. This empirical form of the transit time distribution has been analyzed before in the context of CTRW\textsuperscript{10} and makes physical sense: we do not allow transit times longer than the time it would take a particle to diffuse through a stagnant throat, while for intermediate times $t_1> t > t_2$ we see an approximately power-law distribution of transit times that reflects the heterogeneity of the network. $\beta$ is a parameter that encapsulates this heterogeneity: more heterogeneous systems will have smaller values of $\beta$, representing a broader distribution of transit times. The best-fit value of $\beta$ for our simulations is 1.8.

We perform three simulations of pore-to-core transport. While the results of Bijeljic et al.\textsuperscript{17} were generated for a two-dimensional network, we are interested in three-dimensional systems. In the first simulation we use a topologically disordered network representing a sample of Berea sandstone 3 mm across with 12,349 pores and 26,146 throats. From the known hydraulic conductance of each element (pore and throat) we can compute the flow rate in the network for a given pressure drop between inlet and outlet – this is identical to what is done in conventional network modeling. We then launch 10,000 particles at the inlet face, weighted by the flux in each inlet throat and track their progress as they move in a series of discrete hops between pores. We assume that between pores the transport is represented by a one-dimensional ADE, Eq. (1), with the known velocity in the throat and where the dispersion coefficient is the molecular diffusion coefficient, $D_m = 10^{-9}$ m$^2$s$^{-1}$.

For one-dimensional solutions of the ADE we can find $\psi$ semi-analytically\textsuperscript{19}. We find the cumulative transit time distribution:

$$Y(t) = \int_0^t \psi(t')dt'$$  \hspace{1cm} (3)

where, by definition, $Y(t=\infty) = 1$. For each transition, we find a random number $z$ between 0 and 1. We then invert $Y$ to find the transit time $t_z$ such that $Y(t_z)=z$. The particle is then moved to the next pore and the time counter associated with each particle is incremented by $t_z$.

When a particle reaches a pore there may be several nearest neighbor pores to which it can move next. We can also find, analytically, the probability of transitions to each neighboring pore based on the Peclet number in each connecting throat. More details on this simulation methodology are given in\textsuperscript{19}.

We know that even in a single throat, the use of the ADE is a poor representation of the transport, since, in reality, there is a variation in velocity across the element\textsuperscript{17}. However, this does give the correct advective and diffusive limits, and we will show later, gives good macroscopic predictions of transport, since this is dominated by the variation of velocity between throats, not the variation within a throat.

During the simulation we compute the mean particle location:

$$l(t) = \bar{x}(t) = \frac{1}{N_p} \sum_{k=1}^{N_p} x_k(t)$$  \hspace{1cm} (4)

where $x_k$ is the displacement of particle $k$ from where it was launched and $N_p$ is the number of particles. The variance in location is given by:

$$\sigma^2(t) = \frac{1}{N_p} \sum_{k=1}^{N_p} (x_k(t) - \bar{x}(t))^2$$  \hspace{1cm} (5)

Then we define the longitudinal dispersion coefficient as:

$$D_L = \frac{1}{2} \frac{d\sigma^2(t)}{dt}$$  \hspace{1cm} (6)
In Fig. 2 we plot the late-time dispersion coefficient, Eq. (6), as a function of Peclet number, where Pe is varied by changing the pressure drop across the network. The results are compared to experimental results in the literature and the network studies of Bijeljic et al.\textsuperscript{17,18} It is evident that both modeling approaches predict the experimental results accurately. This comparison demonstrates that it is possible to represent transport as a series of discrete hops between nodes (pores). In this case, even though the transit time distribution between pores is not accurate, we still obtain good results, since we do model the heterogeneity of the porous medium correctly – it is the consequent distribution of velocity in different throats that dominates the behavior.

For the upscaling presented later it is convenient, in this first implementation of the method, to use cubic networks. Also shown in Fig. 2 are results using a $100 \times 100 \times 100$ cubic network but with the same Berea-derived distribution of throat radius. The throat length is 100 μm, and so this represents a sample 1 cm across. Note that the results are similar to those obtained for the topologically disordered network, except at very large Pe, indicating that for single-phase transport a regular network can be used to predict the behavior accurately, as demonstrated by other authors\textsuperscript{17,20,21}.

Our third simulation also uses a cubic network of the same size, but now we represent an ensemble averaged system that is homogeneous. Here we do not need to compute the flow field – we simply use Eq. (2) to find the transit time distribution for each pore-to-pore hop. Again this predicts the experimental data accurately. It is this approach that we will use to upscale transport later in the paper.

Note the approximate power-law behavior of the dispersion coefficient at intermediate values of Pe: $D_l \sim Pe^\beta$ with $\beta \approx 1.2$. It is possible to show that this exponent is related to $\beta$ by $\delta = 3 - \beta$ – the macroscopic dispersion is a direct consequence of the power-law distribution of throat velocities.\textsuperscript{18}

**Core-to-field-scale simulation**

It is not practical to simulate field-scale transport using a pore-scale network model. We propose an upscaling strategy that embraces the CTRW approach and where, at any scale, we represent transport as a series of transitions between discrete nodes. We consider that we have a field-scale reservoir description and we want to honor this heterogeneity explicitly. However, we will compute transport for all possible realizations of the reservoir below the grid-block scale. The approach we use borrows ideas from multiscale modeling.\textsuperscript{12-16}

First, we compute the flow field at the field-scale with known boundary conditions (wells) and initial distribution of fluids – for single-phase flow we assume that this is independent of the solute concentration. We then extract pairs of grid blocks, as represented in Fig. 3. We know the total flux across each face, $Q$. We then perform a sub-block simulation. Within each block, we represent the medium as a network of elements – at this scale this will be an ensemble-averaged, homogeneous, cubic pore-level model, described in the previous section. We find the flow rate in each throat by solving for the flow field with the known, Neumann, boundary conditions.

We then launch particles at the faces of the left-hand block in proportion to the flux across that face. We move particles from pore-to-pore as before, using Eq. (2) for the transit time distribution. The difference here is that despite the homogeneity of the network, the velocity in each element is different because of the different face fluxes, and this is accounted for in Eq. (2). When a particle moves to the right-hand block we start a clock for that particle. When it exits this block, we stop the clock. The time is the transit time for the particle to cross the block. We compute the distribution of transit times for all the particles and for different pairs of blocks.

For this example, each grid block was represented by a $50 \times 50 \times 50$ homogeneous cubic network, 5 mm across. We launched 10,000 particles into the left-hand block.

At the grid block scale, transport is advection-dominated in our examples. As a consequence, particles almost always moved macroscopically in the direction of the imposed flux. We also found that regardless of launch or exit face, or which pair of blocks we considered, the transit time distribution was exponential with the following functional form:

$$\psi_g(t) = \frac{\lambda Q}{V} e^{-\lambda Q/V}$$

where $Q$ is the flux across the face between the two blocks of interest (with units of volume per unit time), $V$ is the block volume and $\lambda$ is a dimensionless coefficient whose value we found to be approximately 5. The subscript $g$ on $\psi$ indicates
that this is the transit time distribution at the core scale, to distinguish from the pore-level ψ, Eq. (2).

This result is not surprising – when the average transport is advective-dominated there will be a typical transit time with some variation around the average that is well captured by an exponential.\(^a\) The typical transit time through a single throat is \(t/v\) where \(v\) is an average flow speed. \(v = Q/\phi A\) where \(A\) is the face area and \(\phi\) is the porosity. If a particle traverses \(n\) pores across the block, then the transit time is \(nt/v = n\phi A/Q\). Now if we take \(nL = L\), the block length in the direction of \(Q\) and \(AL = V\), we find a typical transit time of order \(\phi V/Q\) and a coefficient \(\lambda\) of order 1, which is what we find.

We demonstrate this relationship, Eq. (7), in Fig. 4 where the exponent in a best-fit to \(\psi_\phi\) in Eq. (7) is plotted against a macroscopic Peclet number \(= Q/LD_m\) which will, typically, always be much greater than 1.

In this case we did not explicitly take out pairs of blocks from the field scale model – instead we simply studied pairs of blocks in isolation with different fluxes across the faces. The reason for this is that we could find an empirical relation for the transit time distribution without having to perform a pore-scale simulation for each macroscopic block.

**Field-scale results**

For our reservoir description we chose the SPE10 model based on a North Sea oil reservoir. The model contains regions of high permeability, meandering sand channels surrounded by shaley low permeability regions with permeability varying by more than four orders of magnitude\(^b\). We used a Cartesian grid containing 1,122,000 blocks with 60×220×85 blocks. The total size of the model is 366×670×52 m. We chose two different boundary conditions. In the first we completed an injection well and a producer well at opposite corners of the model. We set the control on the injector to a flux of 800m\(^3/day\) and the producer to a bottomhole pressure of 27×10\(^5\) kPa. In the second, we injected across one face of the model and produced from the opposite face with no flow across the other faces. With these boundary conditions we first solved for the flow field and found the fluxes \(Q\) at each block face.

\[Q_1 \rightarrow Q_2 \rightarrow Q_3 \rightarrow Q_4 \rightarrow Q_5\]

Fig. 3 – The upscaling methodology. From a larger-scale simulation the flow field is computed and so the fluxes \(Q\) across each block face are known. Pairs of grid blocks are extracted from the model. Then a simulation is performed within these blocks. In this example, the sub-grid scale is a pore-level network model. As an ensemble average, the sub-grid is homogeneous. The flow rate in each element is computed using the block face, Neumann, boundary conditions: while the network is homogeneous, there is a distribution of velocity between throats because of the different fluxes at the block faces. Transport is modeled, as before, by a series of pore-to-pore transitions using Eq. (2) with the known average velocity in each element. Particles are launched along the face of the left-hand block. When a particle first enters the neighboring, right-hand block we record the time taken before the particle first exits that block. We then find this transit time distribution for all the particles, and for different pairs of blocks. At the larger scale this transit time distribution is used to represent, conceptually, a hop between two nodes indicating the centers of the grid blocks.

\[\text{Launch here} \quad \text{Link} \quad \text{Node} \quad Q \quad \text{Link} \quad \text{Node}\]

For transport, we represent the field scale as a cubic network of links (equivalent to throats) joining neighboring nodes (pores). The links join centers of adjoining blocks and the face flux \(Q\) is associated with the link, as shown in Fig. 3. We then launched 10,000 particles along the injector by a flux-weighted scheme and monitored the time taken for each to reach the producer. In the second simulation we injected particles along one face of the model and produced from the opposite face with no flow on the other faces. We compute transport as before, as a series of transitions between nodes using Eq. (7) for the transit time distribution.

While conceptually transport is node-to-node, the upscaling methodology does account for the average behavior...
of particles traversing the blocks through all possible paths. Furthermore, while the transit time is counted for transport across a block and the macroscopic simulation is, conceptually, from block center to block center, the methodology does correctly track typical transit times, since we consider movement block-to-block across specified faces.

It is remarkable to note how simple the macroscopic transit time distribution is. In theory, an ensemble-averaged macroscopic transport algorithm needs to consider a convolution integral in time that accounts for the probability of particles arriving after sampling different paths. Of course, this subtlety is blithely ignored in all petroleum upscaling applications – fortunately without significant error for single-phase flow at least.

**Fig. 5** shows the macroscopic mean particle location and standard deviation at early time for the two different boundary conditions. The mean $l(t)$ scales linearly with time, while the standard deviation $\sigma(t)$ of the particle location scales as a power-law, indicative of anomalous transport with an exponent $\beta_m \approx 1.7$. The subscript $m$ is to indicate that this macroscopic exponent can, and indeed is, different for that used to model pore-scale transport. While the boundary conditions alter the time-scale of the displacement, the scaling behavior is broadly similar for both well and face-to-face transport.

![Fig. 5](image)

**Fig. 6** shows the corresponding concentration at the producer where we find $C(t) \sim t^{-(l/\beta_m)}$ but this time the apparent exponent is $\beta_m = 1.2 \pm 0.1$. The inconsistency with the exponent from the early-time behavior indicates long-range spatial correlation in the transport; the simple characterization with a single exponent assumes statistical homogeneity in the system, which is not appropriate for this highly structured reservoir description.

The macroscopic boundary conditions do not affect the late-time behavior of the plume and so the power-law scaling is not due to near-well radial flow. Also note the highly heterogeneous nature of the field leads to breakthrough in around 100 days, while it takes over 100,000 days for all the particles to traverse the system.

![Fig. 6](image)

**What affects field-scale recovery: small or large-scale heterogeneity?**

Traditionally transport would be simulated directly on the field-scale model without any upscaling with some dispersion coefficient used to represent sub-grid-block heterogeneity. In this section we test to see if the proper incorporation of small-scale transport affects the large-scale results.

In **Fig. 6** we also show the breakthrough curves where we use $\psi$ assuming a one-dimensional ADE in each link with $D=D_m$. This is equivalent to a traditional simulation with an infinitely-resolved discretization between nodes. The late-time results are similar to those obtained using Eq. (7) for $\psi$, indicating that the large-scale heterogeneity dominates the overall behavior. This is to be expected, since the pore-scale representation of the field as a relatively homogeneous Berea sandstone contrasts with the extreme variability in the large-scale permeability. Streamline-based simulation, again assuming advective transport on the same reservoir model also gave the same macroscopic behavior with $\beta_m = 1.2 \pm 0.1$.23

However, assuming the ADE at the small scale under-predicts the breakthrough time, particularly for face-to-face transport. This is because it does not account for the fact that particles will, occasionally, encounter stagnant regions across which transport occurs only slowly by diffusion. This tends to slow down the solute as shown in previous CTRW simulations in macroscopically heterogeneous media.11
We ran one further suite of tests, where we assumed more pore-scale heterogeneity. At the pore scale we used Eq. (2) for transport in an ensemble-averaged (homogeneous) network, but now with $\beta=1.1$ and $\beta=0.5$. We re-ran the upscaling step to find an empirical form for the transit time distribution, Eq. (7). For $\beta=1.1$ Eq. (7), is still valid – see Fig. 4 – but with $\lambda=1.8$, indicating slower transport. This is to be expected: as the medium becomes more heterogeneous, particles will encounter more slow-flowing domains and this will, on average, increase the transit times.

For the most heterogeneous pore-scale network (representing, for instance, a vuggy carbonate) with $\beta=0.5$, we can no longer use Eq. (7). Instead we find, Fig. 4:

$$\psi(t) = \frac{\lambda Q P C(t)}{V} e^{-\lambda Q P \gamma \psi(t)}$$

with an exponent $\gamma=0.8$ and constant $\lambda=1.6$

Fig. 7 shows the breakthrough curves for macroscopic face-to-face transport with differing amounts of pore-scale heterogeneity. Even through the macroscopic reservoir description, captured at the meter scale with over a million grid blocks, is the same, the macroscopic behavior is very different, with breakthrough times that vary by a factor of around 4 and slightly different late-time exponents, decreasing from an apparent $\beta_m$ of 1.2 to around 1.1 as the pore-scale $\beta$ decreases. Increasing the pore-scale heterogeneity forces the solute to sample stagnant regions of the pore space more frequently. This slows down the overall transport and also leads to a very long tail in the breakthrough curve.11 Heterogeneity at all scales affects the macroscopic behavior. It is not correct to presume that simply because the meter-scale reservoir description is highly structured with more than four orders of magnitude variation in permeability it will dominate over any smaller-scale variability. Hitherto there has been no tool to see this phenomenon: a direct simulation of this pore-to-field transport would require of order a trillion cells, and using fewer cells and some effective ADE, is, as we have shown, inadequate.

$C(t)$ is a first travel-time distribution and so can be viewed as a field-scale transit-time probability $\psi(t)$. This concept can be used to define intermediate upscaling steps as described in the next section.

**Further refinements: the missing scale**

There are a number of ways in which the current methodology could be refined. The most glaring problem with the results presented here is that the pore-to-core simulations represent a sample around 1 cm across, while the field-scale grid-blocks are meter-sized. We need to include a third, intermediate core-to-grid-block upscaling step. This would involve modeling typical sub-meter-block heterogeneity at the cm scale. Then the transit time distribution across a heterogeneous representation of a meter-scale block at the core, node-to-node scale is found; it may be matched to Eq. (8), or a truncated power-law, Eq. (2), or some other functional form. To find an ensemble average, different macroscopic flux boundary conditions and small-scale realizations need to be considered. Then the field-scale simulation is performed as before. It is likely that with significant, correlated heterogeneity, the transit time distribution used at the meter (grid-block) scale would not be a simple exponential.

Another limitation of the current work is that we only consider homogeneous pore-scale networks. Ideally we would consider different networks that properly represent the differences in pore structure between blocks of different macroscopic permeability and porosity.

**Extensions to multiphase flow**

The current approach relies on using a particle tracking approach where the flux is linearly related to the solute concentration. This allows us to treat each particle independently and makes ensemble averaging easy. In multiphase flow, however, the flux from node to node is non-linearly dependent on saturation making particle tracking and ensemble averaging problematic. While it is possible to extend particle tracking to multiphase flow12, this method has yet to be fully developed. Instead, we propose that the node-to-node transport of saturation is treated as in single-point upstream weighting, but with a probabilistic distribution of putative fractional flows, representing different possible smaller-scale structure.

The advantage of this approach for general petroleum reservoir simulation is that the logic of the nodal structure does not have to be ordered and so it is easy to deal with unstructured grids representing large-scale geological features, such as faults, and to couple the reservoir transport with flow in wells and facilities.

**Conclusions**

We have proposed a pore-to-field transport simulation approach and applied it to single-phase flow accounting for advection and diffusion. We assume that transport occurs as a series of transitions between discrete sites governed by a transit time distribution.

We can predict the Peclet number dependence of dispersion coefficient at the core scale by modeling transport as a series of pore-to-pore hops. This can be done by either
explicitly representing the pore-scale heterogeneity of Berea sandstone, or by using a homogeneous network with an ensemble-averaged transit time distribution that is given by a truncated power-law.

We developed a multiscale upscaling methodology to simulate transport. We showed how to find the transit time distribution at the core scale and how to use this in macroscale simulation.

For advective-dominated transport the transit time distribution at the core scale is exponential in time, with a time-scale related to the time for a particle to advect across the block with a typical velocity.

At the field scale, with a finely-resolved highly-heterogeneous reservoir model, the overall transport behavior is anomalous with power-law scaling of the mean plume location, its standard deviation and the breakthrough curves.

The macroscopic behavior is affected by the small-scale transport even when a very heterogeneous field-scale reservoir description is used. Increasing the pore-level heterogeneity delays the particle transport, since advective trapping in slow-flowing regions becomes more common with significantly increased tailing of the breakthrough curves. It is erroneous to assume that small-scale heterogeneity is, in some mysterious way, only controlled by larger-scale geology; we are now able to perform rigorous pore-to-field simulation and it is evident that such an assumption cannot be sustained.

Future work will refine the methodology to account for cm to m scale heterogeneity and to extend it to multiphase flow.

Acknowledgements

We would like to thank the EPSRC and the Imperial College Consortium on Pore-Scale Modelling for financial support.

References


