Pore-to-field simulation of single-phase transport using continuous time random walks

Matthew E. Rhodes\textsuperscript{a,}\textsuperscript{*}, Branko Bijeljic\textsuperscript{b}, Martin J. Blunt\textsuperscript{b}

\textsuperscript{a} Chevron Energy Technology Company, Chevron North Sea Ltd., Chevron House, Hill of Babblaw, Aberdeen AB15 6XL, UK
\textsuperscript{b} Department of Earth Science and Engineering, Imperial College London, London SW7 2AZ, UK

\textbf{A R T I C L E  I N F O}

Article history:
Received 17 August 2007
Received in revised form 27 March 2008
Accepted 2 April 2008
Available online 28 May 2008

Keywords:
Single-phase transport
Upscaling
Continuous time random walk
Numerical simulation
Particle tracking

\textbf{A B S T R A C T}

We demonstrate a pore-to-reservoir simulation methodology 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 hops between nodes with a probability \( p(t) \) that a particle will first arrive at a node from a nearest neighbor in a time \( t \) to \( t + dt \). We describe transport at four scales: pore, core, grid-block, and field. At each scale the system is represented as a lattice of nodes with an appropriate transition time probability \( \psi \) derived from a simulation at the next smaller scale.

At the micron scale, we fit a truncated power-law \( p(t) \) for the distribution of transition times between pores. We use the transport algorithm of Rhodes and Blunt [Rhodes ME, Blunt MJ. An exact particle tracking algorithm for advective-dispersive transport in networks with complete mixing at nodes. Water Resour Res 2006;42:W04501. doi:10.1029/2005WR004504] on a network model representation of Berea sandstone whose results are in good agreement with experiment. This \( \psi \) is then used to calculate transport at the core scale and a \( \psi_c \) is found that accounts for cm-scale transitions. Similarly we use \( \psi_c \) to derive a meter-scale \( \psi_{gb} \) from simulations of grid-block level transport. At the field scale, we use the upscaled \( \psi_{gb} \) for calculations at the meter-scale.

We demonstrate the methodology by considering transport in a channeled sandstone reservoir, from a pore-scale representation of the microscopic structure to a million-cell field-scale geological model. Effectively we simulate transport in a model containing of order \( 10^{12} \) cells while accounting for uncertainty in the reservoir description. Heterogeneity at all scales impacts transport and tends to retard the advance of the plume with particles becoming trapped in slow-moving regions, increasing breakthrough times by up to an order of magnitude compared to those predicted using a traditional advection dispersion model.

© 2008 Elsevier Ltd. All rights reserved.

1. Motivation

The conceptual framework for transport simulation in porous media is borrowed from traditional fluid dynamics applications where known differential equations are solved with known, albeit complicated, boundary conditions. However, porous media flow presents a completely distinct set of simulation challenges. 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 concentration on the much larger scale at which we solve the equations. 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. We have no general way to incorporate uncertainty in the description of the reservoir model into uncertainty in the prediction of transport.

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? We propose to simulate transport as a continuous time random walk (CTRW) [1–3]. The approach, which is illustrated schematically in Fig. 1, allows us to extend the current CTRW framework to model transport quickly and efficiently across multiple scales. The reservoir is represented as a lattice of nodes connected by links. Transport occurs as a series of particle transitions between nodes governed by a probability distribution \( \psi(t,j) \), where \( \psi(t,j) \) is the probability that a particle first arriving at a node \( i \) will hop to a nearest neighbor node \( j \) in a time \( t \) to \( t + dt \). \( \psi \) will depend on the Darcy velocity in the link connecting \( i \) and \( j \) but the functional form will be found by simulating transport at a smaller scale. We consider there to be four distinct
Nomenclature

Symbol | Description
--- | ---
$\alpha$ | exponent of the exponential $\psi(t)$, Eq. (12)
$\alpha_1$ | dispersivity
$\beta_p$ | power law exponent in Eq. (3)
$\beta_{gb}$ | power law exponent in Eq. (14)
$\omega_1, \omega_2$ | constants in the linear scaling of $t_1$, Eq. (14)
$\zeta$ | exponent for the power law scaling of $t_2$, Eq. (14)
$\gamma$ | pore-scale exponent in $\psi_i(t)$ for $\beta_p < 1$
$v$ | flow speed
$\psi$ | transit time probability
$t_1$ | ratio of $t$ to $t_1$
$A_{ij}$ | cross-sectional area of the link connecting node $i$ to node $j$
$A$ | normalization coefficient, Eqs. (2) and (3)
$a$ | exponent which stretches the pore-scale throat distribution, Eq. (11)
$C$ | concentration
$D$ | dispersion coefficient
$D_m$ | molecular diffusion coefficient
$F_j$ | cumulative probability of particles arriving at node $j$
$G$ | normalization constant, Eqs. (4) and (5)
$L, l$ | length
$l(t)$ | average displacement of particle plume with time
$P(i,j)$ | cumulative probability of a particle jumping to node $j$
$p(i,j)$ | probability of a particle jumping to node $j$ after arriving at node $i$
$Pe$ | Peclet number
$Pe_m$ | macroscopic Peclet number ($Q/LD_m$)
$Q$ | flux into the grid block
$q$ | Darcy velocity
$t$ | time
$t_1$ | characteristic advective time
$t_2$ | characteristic cut-off time
$V$ | volume of the grid block

Subscripts

$p$ | pore
$c$ | core
$gb$ | grid-block
$m$ | macroscopic
$ij$ | labels a link connecting nodes $i$ and $j$

Scales with $\psi(t)$ that represent transitions of particles over each scale:

- Pore scale – $\mu$m – $\psi_p(t)$
- Core scale – cm – $\psi_c(t)$
- Grid-block scale – m – $\psi_{gb}(t)$
- Field scale – 100 sm – km – solved deterministically

At the three smaller scales we find an ensemble averaged $\psi$ which accounts for the range of behavior resulting from the heterogeneity that occurs at this level. At the largest scales we wish to find the transport behavior for a particular realization, but with the uncertainty due to the sub-grid-block description automatically accounted for. For the systems we simulate we find that the $\psi(t)$s which emerge are fit either by an exponential with a characteristic time $1/\alpha$ or a truncated power law with exponent $\beta$, an advective characteristic time $t_1$ and a cut-off time $t_2$:

$$
\psi = Ae^{-\alpha x}
$$

$$
\psi = Ae^{-\alpha x}\left(1 + \frac{t}{t_1}\right)^{-1+\beta}
$$

where $A$ is a normalization constant to ensure that $\int_0^\infty \psi(t) \cdot dt = 1$. We then treat the field scale as deterministic and assume a known distribution of porosity and permeability.

We first introduce continuous time random walks that we use to simulate particle movement. We perform a pore-to-core analysis of dispersion verified through comparison with experiment to put the methodology on a firm foundation. We then show how to upscale transport to the field scale and demonstrate that variability at each scale affects the macroscopic behavior even when the field-scale reservoir description is highly heterogeneous.

2. 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 $\psi(t_{i,j})$ 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 [4]; more recently they have found a particularly rich application in modeling contaminant transport [5,6]. Berkowitz et al. have written an excellent, recent review [3].

Anomalous transport can be elegantly described in terms of CTRW. For many systems, at late time, there is a power law dependence of the probability: $\psi(t) \sim t^{-1-\beta}$ with some exponent $\beta < 2$. This leads to an outlet concentration that, at late time, scales as $C(t) \sim t^{-1-\beta}$. For $1 \geqslant \beta \geqslant 0$ both the average plume displacement and its standard deviation scale as $\langle l(t) \rangle \sim \sigma(t) \sim t^\beta$, while for $2 \geqslant \beta \geqslant 1$ the average displacement scales normally: $\langle l(t) \rangle \sim t$, but the spread is still anomalous: $\sigma(t) \sim t^{1/\beta}/2$. For $\beta > 2$ the system displays Gaussian behavior [3].

Generally CTRW has been applied to find the ensemble average behavior of a plume in a macroscopically homogeneous domain [3,7]. 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 [8]. We will use a simpler approach, described below.

3. Upscaling methodology

We will simulate particle transport from node-to-node with some known $\psi(t_{i,j})$ – a real space CTRW that solves the master equation [3] numerically. We approximate $\psi(t_{i,j})$ by a $\psi(t_{Pe})$ where $Pe$ is the local Peclet number and a conditional probability $p(i,j)$ that a particle will hop to a nearest neighbor $j$ after arriving at node $i$. This is given by the analytical expressions derived by Ref. [1] which is extended to more general systems in Appendix 1.

Our method can be easily implemented. All that is required is a good random number generator [9], a robust linear solver [10,11] and a Monte Carlo sampler. We then employ a multiscale methodology [12–16] where, at each stage, transport is considered as a series of transitions from node-to-node, see Fig. 1. All
the physics of the process is now contained in the transit time distribution which we determine from simulations on a lower scale. But the question now becomes how do we find an appropriate $\psi(t)$?

4. Pore-scale simulations

At the pore scale, we can describe transport by moving particles under Stokes flow in a spatially varying flow field coupled with random molecular diffusion. Bijeljic et al. [17] developed a pore-scale network model of dispersion. They represented a porous medium as a two-dimensional diamond lattice of throats connecting volume-less pores (nodes). Each throat had a square cross-section and the distribution of throat radii matched that inferred for Berea sandstone. They then simulated transport as a series of advective and diffusive steps within the throats and physically-accelerated mixing rules at pores. They accurately predicted the experimental measured dependence of longitudinal dispersion coefficient. They then simulated transport as a series of advective and diffusive steps within the throats.

For moderate Peclet numbers $400 > Pe > 10$ there is an approximate power law dependence of $D_l$: $D_l \sim Pe^\delta$ with $\delta = 1.2$. Bijeljic and Blunt [2] provided a physical explanation for this behavior in terms of the distribution $\psi_p$ of pore-to-pore transit times.

We will replace a direct simulation approach that involves transport with one where particles simply hop from pore to pore with a known transit time distribution, $\psi_p(t; i, j)$. At the field scale we model transport deterministically as a series of transitions between conceptual nodes with the transit time distribution given by $\psi_{gb}$.

The second way to simulate transport is to consider $\psi_p$ as 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 $\psi_p$ 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 $\psi_p$ is found by averaging the transit times over every pore-to-pore transition in the heterogeneous network. Bijeljic and Blunt [2] found that $\psi_p$ was very well fit by a truncated power law form over six orders of magnitude in time and $Pe$:

$$\psi_p(t) = Ae^{-t/t_1}(1 + t/t_1)^{-1 - \delta_p}$$  \hspace{1cm} (3)

where $t_1$ 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 [7] 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 \( t_2 > t > t_1 \) we see an approximately power law distribution of transit times that reflects the heterogeneity of the network. \( \beta_p \) is a parameter that encapsulates this heterogeneity: more heterogeneous systems will have smaller values of \( \beta_p \), representing a broader distribution of transit times. The best fit value of \( \beta_p \) for our simulations is 1.8 – see Fig. 2 that shows \( \psi_p(t) \) computed for all pore-to-pore transitions using the three-dimensional Berea network described below and in the Appendix. This comparison between CTRW and pore-scale modeling was also demonstrated by Bijeljic and Blunt [2] for similar simulations in a heterogeneous network.  

We perform three simulations of pore-to-core transport. 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 [18]. From the known hydraulic conductance of each element (pore and throat) we can compute the Darcy velocity \( q_k \) in each throat connecting pores \( i \) and \( j \) for a given pressure drop between inlet and outlet: this is identical to what is done in conventional network modeling. We then calculate the probability \( p(i,j) \) that a particle landing at pore \( i \) will move to one of its neighbors [1]:  
\[
p(i,j) = \frac{G A_i q_{ij}}{\epsilon^2_s} q_j > 0 \\
p(i,j) = \frac{G A_i q_{ij}}{\epsilon^2_s} q_j > 0
\]

where \( A_0 \) is the cross-sectional area of the throat and \( G \) is a normalization coefficient such that \( \sum p(i,j) = 1 \) (see Appendix 1). We initialize the simulation by launching 10,000 particles at the inlet face, weighted by the flux,inode| in each inlet throat and track their progress as they move in a series of discrete hops between pores. When a particle arrives at a given node (pore) we generate a uniform random number \( a \) between 0 and 1. We then read from the memory \( P(i,j) \) which is given by  
\[
P(i,j) = \sum_{k=0}^{j} p(i,k) \quad k < j
\]

and then iterate \( j \) until \( P(i,j-1) < a < P(i,j) \). The particle will then take a time \( t \) to move to node \( j \) along the connecting link \( i \to j \) [1,19]. We assume that between pores the transport is represented by a one-dimensional advection-dispersion equation (ADE), with a known velocity in the throat and a molecular diffusion coefficient given by \( D = D_m = 10^{-9} \text{ m}^2 \text{ s}^{-1} \). We can find semi-analytically a solution for \( \psi_p(t;i,j) \) using the ADE (Appendix 1) which we randomly sample by defining:  
\[
F(t) = \int_0^t \psi_p(t;i,j) \cdot d\tau
\]

We choose another uniform random number \( z \) which is taken to be a point on the \( F(t) \) axis. We use \( z \) to find the corresponding time \( t \) by solving the equation \( F(t) = z \). We then track the particles until they leave the system summing the individual times taken to transit each link. This method is used to generate the results in Fig. 2.  

We know that even in a single throat, the use of a simple one-dimensional ADE with constant coefficients is a poor representation of the transport, since, in reality, Taylor dispersion occurs due to the variation in velocity across the element [20]. 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. The same method in the same network has also been used successfully to predict NMR propagators [21].  

During the simulation we compute the mean particle location:  
\[
l(t) = \bar{x}(t) = \frac{1}{N_p} \sum_{k=1}^{N_p} x_k(t)
\]

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  
\[
\sigma^2(t) = \frac{1}{N_p} \sum_{k=1}^{N_p} (x_k(t) - \bar{x}(t))^2
\]

Then we define the longitudinal dispersion coefficient as  
\[
D_L = \frac{1}{2} \frac{d\sigma^2}{dt}
\]

In Fig. 3 we plot the late-time dispersion coefficient from Eq. (10), as a function of Peclet number. The model is three-dimensional and

![Fig. 2. The ensemble average distribution of transit times \( \psi_p(t\to t_1) \) across the links in the network model of the Berea system for different Pe numbers. Solid lines show the truncated power law fit to the numerical data (Eq. (3) with \( \beta_p = 1.8 \).)](image-url)
implicitly accounts for transverse dispersion but we do not report it here. The results are compared to experimental results in the literature and the network studies of Bijeljic et al. [2,17]. 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 velocities 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. Shown in Fig. 4 are results using a 100 × 100 × 100 cubic network but with the same Berea-derived distribution of throat radius. The throat length is 200 μm, and so this represents a sample 2 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, as demonstrated previously [17,19,22].

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 and a local Peclet number – we simply use Eq. (3) 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.

**5. Effect of throat-size distribution on the ensemble average \( \psi_p(t) \)**

In this section we demonstrate the effect of the throat size distribution on the truncated power law \( \psi_p(t; Pe) \) that was obtained by Ref. [2]. If we stretch the throat size distribution of the Berea network we will make the system more heterogeneous and obtain a wider range of velocities. We use the same topologically disordered lattice and solve the ADE as before with a new pore and throat distribution given by the equation below:

\[
\frac{D_L}{D_m} = \beta_p \left( \frac{t}{t_{avg}} \right)^a
\]
velocity in each element varies because of the different face fluxes, which is accounted for in Eq. (3). When a particle enters 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 face fluxes.

At the core scale, transport was advection-dominated in our examples, with typical flow rates of order 1 m/day. 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 the imposed fluxes, the transit time distribution was exponential with the following functional form:

$$\psi_c(t) = \frac{Q}{V} e^{-Qt/V}$$

(12)

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 $\psi$ is a dimensionless coefficient whose value we found to be approximately 1.5 (see below). The subscript $c$ on $\psi$ indicates that this is the transit time distribution at the core scale, to distinguish from the pore-level $\psi_p$, Eq. (3).

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 [3]. The typical transit time through a single throat is $l/v$ 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 $nl/v = n\phi A/Q$. Now if we take $nl = L$, the block length in the direction of $Q$ and $A = V$, we find a typical transit time of order $\phi V/Q$ and a coefficient $\psi$ of order 1, which is what we find.

We demonstrate this relationship, Eq. (12), in Fig. 9 where the exponent in a best-fit to $\psi_c$ in Eq. (12) is plotted against macroscopic Peclet number $Pe_m = Q/LD_n$ which will, typically, always be much greater than 1.

**Fig. 7.** The ensemble average distribution of transit times $\psi_p(t - \tau(t))$ across the links in the network model of the Berea system when $a = 5$ for different $Pe$ numbers. Solid lines show the truncated power law fit to the numerical data (Eq. (3)) with $\beta_p = 0.5$.

**Fig. 8.** 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. 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. (3) for $\psi_p(t)$ with the known 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 face fluxes. At the larger scale this transit time distribution $\psi_c$ is used to represent, conceptually, a hop between two nodes indicating the centers of the blocks at the centimeter scale.

$\psi_c$. How we do this is illustrated in Fig. 8. For simplicity we represent our porous medium at the pore scale by a homogeneous cubic network – this, remember, is an ensemble averaged network that does predict the experimentally measured dispersion coefficient.

We consider that the core scale – defined as porous media which have a length scale of a few centimeters – is modeled by a 50 $\times$ 50 $\times$ 50 network 1 cm across. We place two such networks side by side with imposed fluxes at the face. We then launch 10,000 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. (3) for the transit time distribution. The difference here is that despite the homogeneity of the network, the

**Fig. 9.** Tests of the empirical core-scale transit-time distribution, Eq. (12). The exponent $x = xQ/V$ in the exponential relation is plotted against the macroscopic Peclet number $Pe_m = Q/LD_n$. The linear relation demonstrates that a simple transit time distribution can be used for larger-scale simulation. The upper line through the crosses is the base case for sub-scale transport in a network representing Berea sandstone ($\beta_p = 1.8$ in Eq. (3)). We find $x = 6 \times 10^{-5} Pe_m s^{-1}$. Since we perform the simulations for blocks 50 pores across, $L = 5$ mm and $V = 2.5 \times 10^{-2} m^3$, $D_n = 10^{-15} m^2 s^{-1}$ so the dimensionless constant $\gamma = 1.5$. The middle line is a parametrization of a more heterogeneous network with $\beta_p = 1.1$ and $\gamma = 0.54$. The lowest line is for a highly heterogeneous sub-grid system with $\beta_p = 0.5$. In this last case the transit time exponent varies non-linearly with Peclet number, Eq. (13), with $\gamma = 0.8$ and $\gamma = 1.6$. 

---

**Fig. 7.** The ensemble average distribution of transit times $\psi_p(t - \tau(t))$ across the links in the network model of the Berea system when $a = 5$ for different $Pe$ numbers. Solid lines show the truncated power law fit to the numerical data (Eq. (3)) with $\beta_p = 0.5$.

**Fig. 8.** 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. 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. (3) for $\psi_p(t)$ with the known 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 face fluxes. At the larger scale this transit time distribution $\psi_c$ is used to represent, conceptually, a hop between two nodes indicating the centers of the blocks at the centimeter scale.
For the most heterogeneous pore-scale model ($\beta_p = 0.5$) we find a non-linear relation between the exponent in $\psi_e$ and Pecl number.

$$\psi_e(t) = \frac{jQPe_{gb}^{w-1}}{V} e^{-\frac{t}{t_2}}$$

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

Strictly speaking an ensemble-averaged $\psi(t)$ would be the conditional probability that a particle first arrives at the face of a block and then exits in a time $t$, averaged over all possible arrival times and locations [8]. We find empirically that $\psi_e$ is a function only of time and local Pecl number; this simplifies the formulation significantly.

7. Grid-block scale simulations

We next use the $\psi_e(t)$ obtained in the previous section to produce an ensemble average $\psi_{gb}(t)$ for transport at the grid block (gb) level. To do this we first generated a geologically plausible representation of heterogeneity that will occur at this scale. We assume that the typical grid block in our system (an example of which is shown in Fig. 10) will be a relatively high porosity, high permeability (~1000 mD) sand with horizontal shale lenses interbedded between its layers. We generated 10 systems stochastically [23,24] which for computational purposes was subdivided into $100 \times 50 \times 50$ grid blocks of size 1 cm$^3$ to correspond to the core-scale blocks. This is equivalent to a geological system of size $1 \times 0.5 \times 0.5$ m which we divide in half to represent two blocks of size $0.5 \times 0.5 \times 0.5$ m placed side by side in a field scale simulation (similar to what was done at the core scale).

We then assumed the porosity, $\phi$, was distributed normally with mean 0.2 and standard deviation 0.04 while the permeability $k$ was log-normally distributed with mean $1000$ mD and a standard deviation of $200$ mD, both having a correlation length $l_x = l_y = 5l_0$ of 0.05 m. The shales were randomly located in the grid block with a permeability of 1 mD, porosity 0.01 and volume fraction 0.1. The depth of the shale bodies was taken to be 0.01 m with length in the $x$ and $y$ directions distributed uniformly ($l_x = 0.5l_y$) with a range of (0.25 m, 0.5 m). The vertical spacing between the shales $l_z$-spacing was also distributed uniformly with range (0.05 m, 0.1 m).

We repeat the procedure described in Section 6 to transport particles from node-to-node using the three values of $\lambda$ in Eqs. (12) and (13) obtained for the pore scale $\beta_p$'s used. In this case the system is locally heterogeneous and we find the distribution averaged over all simulations on the different realizations of the structure. From this study we find that again a truncated power law of the form below emerges:

$$\psi_{gb}(t) = A_t e^{-t/t_2}(1 + t/t_1)^{-\frac{1}{1+\beta_p}}$$

The parameter $\beta_{gb}$ is an exponent related to the heterogeneity at the grid block scale. $t_1$ remains a characteristic advective time given by $\omega_1 V / Q$ where $\omega_1$ is a constant which increases with the value of $\beta_p$ (see Fig. 11) while $t_2$ is now an advective cut-off time which has a power law relationship of the form $t_2 = c_2 (V/Q)^{x_2}$ where $c_2$ is a constant which increases with $\beta_p$ as shown in Fig. 12 and $x_2$ is an exponent which varies with $\beta_p$. The numerical values of these constants can be found in Table 1.

At the grid scale transport remains advection-dominated. As we now define explicit heterogeneity within our system there

---

**Fig. 10.** A realization of meter scale heterogeneity ($1 \times 0.5 \times 0.5$ m). This represents two grid blocks of size $0.5 \times 0.5 \times 0.5$ m placed side by side in the field-scale simulation.

**Fig. 11.** The advective characteristic time $t_1$ vs. the ratio of block volume to the central flux $V/Q$. The solid lines are a linear fit to the numerical data $t_1 = c_1 V/Q$; crosses represent $\beta_p = 1.8(c_0 = 5.59)$, squares represent $\beta_p = 1.1(c_0 = 13.3)$ and diamonds represent $\beta_p = 0.5(c_0 = 237)$.

**Fig. 12.** The advective cut-off time $t_2$ vs. the ratio of block volume to the central flux $Q/V$. The solid lines are a power law fit to the numerical data $t_2 = c_2 V/Q^{x_2}$; crosses represent $\beta_p = 1.8(c_2 = 1330, x_2 = 1)$, squares represent $\beta_p = 1.1(c_2 = 1330, x_2 = 1)$ and diamonds represent $\beta_p = 0.5(c_2 = 7.19, x_2 = 1.35)$. 
will be a spectrum of velocities encountered by the particles. This variation of velocities would therefore influence \( \beta_b \) with the slowest flowing velocity directly controlling the longest times to leave the system, \( t_2 \).

### 7.1. Validation

We validate our simulation method at the meter scale by predicting the experimental tracer tests performed by Levy and Berkowitz on homogeneous and heterogeneous sand packs [25]. For these tests we assume that the heterogeneity of these packs at the pore-scale can be modeled by the Berea network but allow for the fact that it may have a stretched throat-size distribution. As such we will use the same functional form of the core-scale transit distribution \( \psi_c(t) \) as we obtained for Berea but fit the value of \( \lambda \) in Eq. (12) as described below.

#### 7.1.1. Homogeneous sand pack

We first investigated the homogeneous system which was a sand of grain diameter 0.532 mm in a vessel with physical dimensions 86 cm \( \times \) 10 cm \( \times \) 45 cm. We then divided the domain computationally into 86 \( \times \) 10 \( \times \) 45 grid blocks with a uniform permeability of 1500 mD and a porosity of 0.38. The porosity was assumed to be a reasonable value for a well sorted sand and is the value used in the prediction work of Obi and Blunt [26]. We next ran our simulator for a flow rate of 36 ml/min. Since each grid block was 1 cm across we used \( \psi_c \) from Eq. (12) and adjusted \( k \) to obtain a best fit to the results. We found \( \lambda = 1 \). We then re-ran the experiments for 53 ml/min using the same \( \lambda \) and found that there was a very good prediction of the experimental data, as shown in Fig. 13.

#### 7.1.2. Heterogeneous porous media

We next predicted the transit time experiments of Ref. [25] on a heterogeneous porous medium. To generate the heterogeneity Levy and Berkowitz used the algorithm of Silliman and Wright [27] to produce a structure which was analogous to a random sedimentary system with three facies types. This was then used as a template to mix three different sands of grain diameters 1.105 mm, 0.532 mm and 0.231 mm in equal proportions into a glass case of dimensions 213 cm \( \times \) 10 cm \( \times \) 65 cm. To perform our simulations we generated a statistically equivalent system [24] with 213 \( \times \) 10 \( \times \) 65 grid blocks and a probability that a sand type occurred at a given location = 1/3, as shown in Fig. 14. Each sand was assumed to have the same constant permeability as used by Levy and Berkowitz: (1) 5200 mD, (2) 1500 mD, and (3) 144 mD and a constant porosity of 0.32. We show a picture of the system we use in Fig. 14.

We injected fluid into the left-hand face and produced from the opposite plane. We used the \( \lambda = 1 \) obtained previously in Eq. (12) to predict the transit distributions for flow rates of 11 ml/min and 74 ml/min. The quality of the prediction, shown in Fig 15, is as good as obtained using streamline based simulation solving an ADE with a dispersion coefficient chosen to match the homogeneous results [26] or using CTRW to describe the average response to the system [25].

<table>
<thead>
<tr>
<th>( \beta_p )</th>
<th>( \beta_{gb} )</th>
<th>( \omega_1 )</th>
<th>( \omega_2 )</th>
<th>( \varsigma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.8</td>
<td>1.9</td>
<td>5.59</td>
<td>1330</td>
<td>1.00</td>
</tr>
<tr>
<td>1.1</td>
<td>1.7</td>
<td>13.3</td>
<td>1330</td>
<td>1.00</td>
</tr>
<tr>
<td>0.5</td>
<td>1.5</td>
<td>237</td>
<td>7.19</td>
<td>1.35</td>
</tr>
</tbody>
</table>

### 8. Field-scale results

At the field-scale, we chose for our reservoir description the SPE10 model based on a North Sea aquifer. 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 [28]. We used a Cartesian grid.
In the first we completed an injector well and a producer containing 1,122,000 (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 injector well and a producer well at opposite corners of the model. We set the control on the injector to a flux of 800 m$^3$/day and the producer to a bottom-hole pressure of 27 × 10$^3$ 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. For transport, we represent the field scale as a cubic network of links joining neighboring nodes. The links join centers of adjoining blocks and the face flux Q is associated with the link, as shown in Fig. 8. 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; a pictorial representation of the plume profile can be seen in Fig. 16. 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 $\psi_{gb}(t)$, Eq. (14), for the transit time distribution.

While conceptually transport is node-to-node, the upsampling 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.

In this first implementation of the method we do make several assumptions. First, we consider only one generic pore, core and grid-block description. In reality we should use different sub-grid-models for sand and shale. Second, our grid block size used to compute $\psi_{gb}$ is smaller than the grid block size in the field-scale simulation. We assume that we can use a simple $Q/V$ scaling to account for the size discrepancy.

### 9. What affects field-scale transport: Small or large-scale heterogeneity?

Traditionally transport would be simulated directly on the field-scale model without any upscaling with some dispersion coefficient or tensor used to represent sub-grid-block heterogeneity. In the following sections we test to see if the proper incorporation of small-scale transport affects the large-scale results. We use, as a base case, the $\psi_{gb}$ corresponding, at the pore scale, to Berea sandstone with $\psi_{gb} = 1.8$.

#### 9.1. Upscaled $\psi_{gb}(t)$ vs. the traditional ADE approach

Fig. 17 shows the concentration, $C(t)$, arriving at the producer when we use Eq. (14) with $\psi_{gb} = 1.9$ (the base case) to model transport. We compare these results to solutions using the implementation of the ADE described in Appendix 1 with a dispersion coefficient $D = D_m$ and with $D = \alpha_l v + D_m$ where $\alpha_l = 3.5 \times 0.2 \times 10^{-4}$ m. For simplicity, we assumed that the transverse and longitudinal dispersivities were equal but this restriction may be easily relaxed. This is equivalent to a traditional approach to transport modeling with an infinitely-resolved discretization between nodes. The dispersivity $\alpha_l$ is found from the experimentally measured $D_l$ shown in Fig. 3 in the large Pe number limit ($Pe > 10^6$).

We find that at late times the concentration at the producer $C(t) - t^{-(1+\alpha_l)}$ with an exponent of $\alpha_l = 1.2 \pm 0.1$ for all three cases 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 boundary behavior with $\psi_{gb} = 1.2 \pm 0.1$ [29]. 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 200–1000 days, while it takes over 300,000–3,000,000 days for all the particles to traverse the system.

However, assuming the ADE at the grid-block scale with $D = D_m$ or $D = \alpha_l v + D_m$ under-predicts the breakthrough time by almost one order of magnitude, particularly for face-to-face transport. This is because neither of these methods account for the fact that particles will, occasionally, encounter stagnant regions at the sub-grid-block scale 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 where the plume moves at an average speed significantly smaller than $v$ [8]. A proper representation of the sub-grid-scale transport shifts the breakthrough curves to later times.

An analogy is to think of traffic in a city. We could calculate the average velocity $v$ by recording the instantaneous velocities of the cars which pass selected points. This is directly comparable to using Darcy’s Law to calculate an average velocity. However, to
travel a distance $l$, the average travel time will not be $l/v$; it is likely to be much larger since you would typically spend time stuck in traffic or waiting at traffic lights, which is not counted in a flux-weighted average: $t/(v)\neq l/v$.

9.2. Effect of increasing pore-scale heterogeneity on field scale transport

We ran another suite of tests, to demonstrate the effect of pore-scale heterogeneity on field-scale transport. At the pore-scale we assume that now $\beta_p = 1.1$ and $\mu_p = 0.5$. We use Eq. (14) with the appropriate $t_1$, $t_2$ and $\mu_p = 1.7$ or 1.5 for the field-scale simulations.

Fig. 16. The particle plume moving through the channels of the SPE10 reservoir.

Fig. 17. Breakthrough curves for field-scale transport. The late-time behavior is matched by an approximate power law $C(t) \sim t^{-\beta_m}$ with $\beta_m = 1.2 \pm 0.1$. The same late-time behavior is observed for two different boundary conditions with wells indicated by BC1 and face-to-face transport indicated by BC2. Results are shown using $\psi(t)$, Eq. (14), with $\beta_p = 1.9$ and an ADE with $D = D_m$ and $D = \chi D_m + D_m$. To reduce the noise in the tail of our distribution we generate these plots using a bin size which increases linearly with time. $\beta_m$ is then given by a best-fit slope through the points [30,31]. Note that using $\psi(t)$ to simulate transport shifts the breakthrough curves to later times.

Fig. 18. Breakthrough curves for field-scale transport showing the impact of pore-scale heterogeneity. The solid lines are a late-time power law fit to the transport distributions; crosses represent transport using $\psi(t)$ with $\beta_p = 1.9$ resulting in $\beta_m = 1.2 \pm 0.1$; squares represent $\beta_p = 1.7$ resulting in $\beta_m = 1.15 \pm 0.1$; while diamonds represent $\beta_p = 1.5$ resulting in $\beta_m = 1.1 \pm 0.1$. The pore scale $\beta_p$ decreases.
Fig. 19. Breakthrough curves for field-scale transport with ψg, and βg = 1.9 Eq. (14) compared to using ψ, Eqs. (12) and (13) with the three different βs and γs we obtain from simulation at the core-scale.

Fig. 18 shows the breakthrough curves for macroscopic face-to-face transport with differing amounts of pore-scale heterogeneity. Even though the reservoir description at the meter-scale, with over a million grid blocks, is the same, the macroscopic behavior is very different. We find that the breakthrough times vary by two orders of magnitude depending on the heterogeneity with slightly different late-time exponents, decreasing from an apparent βm of 1.2 to around 1.1 as the pore-scale βp decreases. Increasing the pore-scale heterogeneity forces the solute to sample stagnant regions of the reservoir more frequently. This slows down the overall transport and also leads to a very long tail in the breakthrough curve [8].

9.3. Effect of grid-scale heterogeneity on field-scale transport

We finally looked at the effect of ignoring meter-scale heterogeneity on field-scale transport. We do this by using ψ, (Eqs. (12) or (13) with the appropriate values of λ and γ) directly on the SPE10 model. This makes the assumption that there is no long-range heterogeneity at the grid scale and that an ensemble average network would be homogeneous.

We find that the macroscopic behavior at late times is similar to that using ψg, see Fig. 19. We see that the power law scaling of C(t) decreases from 1.2 to 1.1 as we increase pore-scale heterogeneity. There is a four-fold drop in breakthrough time for ψ, with λ = 1.5 when compared to ψg with βg = 1.9 making the results similar to using the ADE with D = Dmb or D = q,v + Dmb.

Ignoring meter-scale heterogeneity leads to a significant under-prediction of breakthrough time. The breakthrough time increases with increasing heterogeneity. Changing the pore-scale βp again leads to an almost 100-fold increase in breakthrough times.

Heterogeneity at all scales affects the macroscopic behavior. It is not correct to assume 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.

10. 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 or nodes 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 and grid block scales and how to use both in macro-scale simulation.

For advective-dominated transport the transit time distribution at the core scale (cm) 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 grid-block (meter) scale, for the cases we studied, transport remains advection-dominated. Transport is represented by a truncated power law distribution with a characteristic time t2, that is advective, an exponent βg that depends on the heterogeneity at the grid scale and an advective cut-off time t3 which depends on the slowest flowing velocity in our system. We validated our simulation approach at this scale by predicting experimental breakthrough curves in homogeneous and heterogeneous sand packs [25].

At the field scale, with a finely-resolved highly heterogeneous reservoir model, the overall transport behavior is anomalous with power law scaling of 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 or grid-scale heterogeneity delays the particle transport by an order of magnitude each, since advective trapping in slow-flowing regions becomes more common with significantly increased tailing of the breakthrough curves. It is erroneous to assume that transport is only controlled by large-scale geology; we are now able to perform rigorous pore-to-field simulation of effectively 10^12 grid cells and it is evident that such an assumption cannot be sustained.

11. Web-link

A copy of the code used to run these simulations can be found on the website below: http://www3.imperial.ac.uk/earthscience-andengineering/research/perm/porescalemodelling/software Then follow the link “Single Phase Code”.

Acknowledgements

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

Appendix 1. Solution of one-dimensional ADE with different branch dimensions

We consider a general system containing n nodes, labeled j, connected to a central node i by n branches labeled i − j. In each we assume there is a Darcy velocity qv, a dispersion coefficient Dq, a porosity ϕq, a cross-sectional area Aq, a length Lq and concentration at the node Cj(x, t). We define all variables as positive in the direction indicated by its index i − j. We can then write for each branch:

$$\phi_q \frac{\partial C_j}{\partial t} + q_v \frac{\partial C_j}{\partial x} = \phi_q D_q \frac{\partial^2 C_j}{\partial x^2}$$  
(A1)

For a particle tracking framework, assuming incompressible flow, we can write the initial conditions in the form [1]:

\[ \text{Initial Conditions:} \]

\[ C_j(x,t=0) = \begin{cases} 
1 & \text{if } x < L_j \\
0 & \text{if } x > L_j 
\end{cases} \]
\( C_j(x, 0) = \delta(x) \) \hspace{1cm} (A.2)
\( C_j(L_i, t) = C_j(-L_i, t) = 0 \) \hspace{1cm} (A.3)
\( \sum_{q_{ij} > 0} A_j q_j = \sum_{q_{ij} < 0} A_j q_j \) \hspace{1cm} (A.4)
\( C_j(0, t) = C_j(0, t) \) \hspace{1cm} (A.5)

Writing Eq. (A.1) and the above conditions in Laplace space we obtain
\[ \phi_j \partial \tilde{C}_j + q_j \frac{d \tilde{C}_j}{dx} - \phi_j D_q \frac{d^2 \tilde{C}_j}{dx^2} = \delta(x) \] \hspace{1cm} (A.6)
\( \tilde{C}_j(L_i, s) = \tilde{C}_j(-L_i, s) = 0 \) \hspace{1cm} (A.7)
\[ \sum_{q_{ij} > 0} A_j q_j = \sum_{q_{ij} < 0} A_j q_j \] \hspace{1cm} (A.8)
\( \tilde{C}_j(0, s) = \tilde{C}_j(0, t) \) \hspace{1cm} (A.9)

We can write a general solution for Eq. (A.6) in Laplace space as
\[ \tilde{C}_j(x, s) = e^{-\alpha s} \left[ a e^{-\alpha s} + b e^{-\alpha s} \right] \] \hspace{1cm} (A.10)
where \( \sigma_{ij} \) is given by
\[ \sigma_{ij} = \frac{\sqrt{q_j^2 + 4D_q \phi_j s}}{2D_q \phi_j} \] \hspace{1cm} (A.11)

Using (A.7) we can write:
\[ A_j = -B e^{-2\sigma_{ij} s} \] \hspace{1cm} (A.12)

We can then substitute Eq. (A.12) into (A.10) to get the solution for \( \tilde{C}_j \):
\[ \tilde{C}_j(x, s) = \pm \frac{2Be^{-\alpha s}}{2\alpha + 1} \sinh[\sigma_{ij}(L_i + x)] e^{-\alpha s} \] \hspace{1cm} (A.13)

Using condition (A.9) we can write \( B \) in terms of the coefficient of the zeroth branch which we write as \( B \). Let \( B(s) \) be given by
\[ B(s) = B(1 - e^{-2\sigma_{ij} s}) = B(1 - e^{-2\sigma_{ij} s}) \] \hspace{1cm} (A.14)

This can be used to rewrite Eq. (A.13) with respect to \( B(s) \):
\[ \tilde{C}_j(x, s) = \frac{B(s)e^{-\alpha s}}{\sinh[\sigma_{ij}(L_i + x)]} \sinh[\sigma_{ij} q_j] \] \hspace{1cm} (A.15)

We now invoke flux continuity at \( x = 0 \):
\[ \sum_{q_{ij}>0} \int_0^L A_j \phi_j \left( s \tilde{C}_j + \frac{q_j}{\phi_j} \frac{d \tilde{C}_j}{dx} + D_j \frac{d^2 \tilde{C}_j}{dx^2} \right) \cdot dx \]
\[ = \int_0^L A_j \phi_j(x) \cdot dx \] \hspace{1cm} (A.16)

and use this to obtain \( B(s) \):
\[ B(s) = \frac{1}{\sum_{q_{ij}>0} D_j A_j \sigma_{ij} \phi_j} \] \hspace{1cm} (A.17)

where \( k \) is equal to the direction where \( q_j > 0 \). The mass per unit time, \( \psi(s) \) first arriving at \( x = \pm L \) is given by
\[ \psi(s) = \pm A_j D_j \frac{\tilde{C}_j}{\phi_j} \left|_{x=\pm L} \right. + \frac{D_j B(s) A_j \phi_j e^{-\alpha s}}{\sinh(\sigma_{ij} L_j)} \] \hspace{1cm} (A.18)

where \( \rho_{en} = A_j L_j / D_j \phi_j \). The mass, \( F_j(s) \), exiting the system would therefore be
\[ F_j(s) = \frac{\psi(s)}{s} \] \hspace{1cm} (A.19)

The total mass leaving each branch can then be calculated using the final value theorem:
\[ p(i, j) = \frac{G A_i q_j}{1 - e^{-\sigma_{ij}}} \] \hspace{1cm} (A.20)
\[ p(i, j) = \frac{e^{-\sigma_{ij}}}{1 - e^{-\sigma_{ij}}} \] \hspace{1cm} (A.21)

where \( G \) is a normalization coefficient such that \( \sum_{i,j} p(i,j) = 1 \).

These are a generalization of the equations derived previously by [1] and are used to assign the probability of particles next hopping to a given nearest neighbor node, even when transport is not governed by an ADE.

**References**


