Anomalous transport in heterogeneous media demonstrated by streamline-based simulation

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[1] We use fine-grid streamline simulation to demonstrate that anomalous (non-Gaussian) transport arises from purely advective movement through heterogeneous systems. The simulation model represents a channeled sandstone North Sea oil field and contains over one million grid blocks. We find the average location and spreading of the plume and the breakthrough curves. These features are consistent with anomalous transport described by an exponent β that characterizes the long-time tail of the transit time distribution. β depends on the degree of heterogeneity and whether the tracer was injected or originally uniformly distributed across the domain. Incorporating dispersion to account for sub-grid-block heterogeneity does not affect the results. INDEX TERMS: 1832 Hydrology: Groundwater transport; 4808 Oceanography: Biological and Chemical: Chemical tracers; 5139 Physical Properties of Rocks: Transport properties. Citation: Di Donato, G., E.-O. Obi, and M. J. Blunt, Anomalous transport in heterogeneous media demonstrated by streamline-based simulation, Geophys. Res. Lett., 30(12), 1608, doi:10.1029/2003GL017196, 2003.

1. Introduction

[2] The traditional approach to modeling contaminant transport is by use of the advection-dispersion equation (ADE). Solutions to the ADE in a macroscopically homogeneous system give a plume that spreads by a Fickian dispersive process [Gelhar, 1993]: the average movement of the plume l scales with time as \( l(t) \sim t^{1/2} \). However, laboratory experiments [Silliman and Simpson, 1987; Farrell and Reinhardt, 1994; Werth et al., 1997; Hagerty and Gorelick, 1998; Hatano and Hatano, 1998] and field-scale tracer tests [Adams and Gelhar, 1992; Siddle et al., 1998; Becker and Shapiro, 2000; Hagerty et al., 2001] have indicated that in many circumstances the behavior is qualitatively dissimilar to that predicted using the ADE. This anomalous transport is characterized by one or more of the following features [Berkowitz and Scher, 1995, 1997, 1998, 2001]: (1) a maximum concentration that appears not to move, or to move very slowly; (2) a rapidly advancing front of contaminant at low concentration leading to early breakthrough times; and (3) long after breakthrough the concentration decreases as a power-law with time at production wells, resulting in very slow cleanup. In the column experiments listed above anomalous transport has been shown in some cases to be due to diffusion and sorption, while at the field scale its origin is not known definitively.

[3] Hagerty et al. [1995, 2000] used a multi-rate mass transfer model to match the results of field-scale tracer tests and laboratory experiments. In a more general mathematical framework, Berkowitz and Scher [1995, 1997, 1998, 2001] and Scher et al. [2002] have used continuous time random walk (CTRW) to explain and predict anomalous transport in laboratory experiments and field tests for both fractured and unfractured media. Their results strongly suggest that in heterogeneous media it is advective movement with particles experiencing a wide range of velocities that is the physical origin of anomalous transport. The CTRW formulation is based on \( \psi(s,t) \), the probability per unit time for movement between sites separated by a distance \( s \) in a time \( t \). If, at large times, \( \psi(s,t) \sim t^{1-\beta} \) for \( 1 > \beta > 0 \) then [Berkowitz et al., 2000]: (1) \( l(t) \sim t^{\beta/2} \); (2) \( \sigma(t) \sim t^{\beta} \) and (3) at late times the concentration at a production well, \( C(t) \sim t^{1-\beta} \). Tracer tests by Becker and Shapiro [2000] performed at different rates are also consistent with the assumption that it is advective-dominated transport that leads to anomalous behavior.

[4] We will confirm that anomalous transport can arise from purely advective movement through heterogeneous systems. We perform a simulation study using a finely-gridded model representing a sandstone North Sea oil reservoir. Tracer is transported along numerically computed streamlines. We associate \( \psi(s,t) \) with the time-of-flight distribution through each grid block and demonstrate power-law scaling at late times with an exponent \( \beta \) consistent with the computed \( l(t) \), \( \sigma(t) \), and \( C(t) \). \( \beta \) depends on both the degree of heterogeneity and on whether the tracer is injected or initially uniformly distributed in the domain. Including dispersion in the simulation to account for sub-grid-block heterogeneity does not affect the results.

2. Streamline-Based Transport Model

[5] The streamline method is described in detail by Crane and Blunt [1999] and Batycky et al. [1997]: it is ideally suited for advective-dominated displacements since it captures semi-analytically the tracer movement along streamlines and suffers from minimal numerical dispersion. The pressure field is computed numerically with known boundary conditions on the underlying Cartesian grid using standard numerical techniques [Krechel and Stueben, 1996]. Then from Darcy’s law the total velocity across each grid face is computed. From this streamlines are traced across the domain using the method of Pollock [1988]. A time-of-flight \( \tau(s) \) is defined as the time taken for a particle to move a distance \( s \) along a streamline:

\[
\tau(s) = \int_{0}^{s} \frac{df}{|v|} ds'
\]  

(1)
The concentration is transported in the direction of the streamlines \[ \frac{\partial C}{\partial t} + v \cdot \nabla C = 0 \] where \( C \) is the concentration and \( D \) is the dispersion tensor. Since the concentration is transported in the direction of the streamlines, using equation (1), equation (2) can be written (for constant porosity): \[ \frac{\partial C}{\partial t} = -v \cdot \nabla C \] We solve this equation using an operator splitting technique. First equation (3) with \( D = 0 \) is solved numerically along streamlines [Crane and Blunt, 1999]. Then the dispersive form of the equation is solved on the grid: \[ \frac{\partial C}{\partial t} = \nabla \cdot D \nabla C \] This results in a 19-point stencil in three dimensions. The concentrations are updated using a scheme that is implicit for the principal (diagonal) terms and explicit for the off-diagonal terms [Zheng and Wang, 1999; Kipp et al., 1998].

### 3. Results

We used a model based on a North Sea oil field with high permeability meandering sand channels surrounded by low permeability shale [Christie and Blunt, 2001]. The model was described on a Cartesian grid of dimensions \( 366 \times 670 \times 52 \) m; the number of grid cells used for the simulations was \( 1,122,000 \), given by \( 60 \times 220 \times 85 \) in the \( x, y \) and \( z \) directions respectively. The highly heterogeneous permeability field of this model (henceforth called the base case) had a standard deviation \( \sigma_{\text{lnkx}} = \sigma_{\text{lnky}} = 3.5 \) and \( \sigma_{\text{lnkz}} = 5.9 \) (Figure 1a shows a \( xy \) slice of the permeability field and the wells described below). This degree of heterogeneity is typical of deep sedimentary structures [Christie and Blunt, 2001]. We constructed two other permeability fields based on the previous one by varying the degree of heterogeneity: \( \sigma_{\text{lnkx}} = \sigma_{\text{lnky}} = 1.2 \) and \( \sigma_{\text{lnkz}} = 2.1 \) (less heterogeneous case) and \( \sigma_{\text{lnkx}} = \sigma_{\text{lnky}} = 4.6 \) and \( \sigma_{\text{lnkz}} = 7.7 \) (more heterogeneous case); the new permeability values of these two other fields were calculated by adjusting the permeability of each grid block using \( k_{\text{new}} = k_{\text{old}}(k_{\text{old}}/K)^{\alpha} \) where \( K \) is the geometric average permeability of the base case. We used \( \alpha = 0.3 \) for the more heterogeneous case and \( \alpha = -0.65 \) for the less heterogeneous case. The porosity \( \phi \) had a constant value of 0.25. There were ten injection wells (with a constant flow rate of \( 800 \text{ m}^3/\text{day} \) each) all along the edge \( y = 0 \), completed in the \( z \) direction and there was one extraction well at the center of the edge \( y = y_{\text{max}} \), completed in the \( z \) direction (with a constant pressure of \( 27,000 \text{ kPa} \)). The test designs performed in the simulations were: (1) water injection displacing a source of tracer initially set at a short distance from the injection well (uniformly along the cross section \( xy \) between the 10th and 11th blocks in the \( y \) direction); and (2) tracer injection followed by water injection after 0.1 day.

#### 3.1. Transit Times

We calculated the transit times, that is, the time-offlights through each grid block for each streamline and then the frequencies \( N(\tau) \) of the transit times encountered by the tracer. Streamlines are launched in proportion to the total flux across each grid block face containing an injection well. In total over 500,000 streamlines are launched. The results are insensitive to the number of streamlines used, as long as at least one streamline passes through each grid block. For tracer injection we compute \( N(\tau) \) by giving equal weight to each streamline. For tracer originally in the domain, the sampling is different-for each streamline \( i \) we weight \( N(\tau) \) by \( 1/W_i \) where \( W_i \) is the number of streamlines that pass through the same block initially containing tracer as streamline \( i \). This samples streamlines in proportion to original mass along a streamline. From CTRW, \( N(\tau) \) is proportional to \( \psi(s, \tau = \tau) \) if we ignore dispersion. Assuming that on average the distribution of streamline lengths \( s \) through a grid block does not affect the scaling, then for anomalous transport we predict \( N(\tau) \sim \tau^{-1-\beta} \). The cumulative distribution, \( K(\tau) = \frac{\int_0^\tau N(\tau') \, d\tau'}{\tau} = 1 - Ar^{-\beta} \) with some constant \( A \), and hence \( 1 - K(\tau) \sim \tau^{-\beta} \).

As shown in Figure 1b, for tracer test (1), at large values of \( \tau \), the \( 1-K(\tau) \) curves show approximate log-log slopes \( \beta \) that are 0.8 for the less heterogeneous case (\( \beta \) is identified over the range \( 1-6 \) days), 0.4 for the base case (\( \beta \) is identified over the range \( 10-300 \) days) and 0.35 for the more heterogeneous case (\( \beta \) is identified over the range \( 100-3000 \) days). When the tracer is injected, the \( 1-K(\tau) \) curve obtained by using the base case has a log-log slope \( \beta \) of

### Table 1. The \( \beta \) Values Estimated From Different Measurements

<table>
<thead>
<tr>
<th>Time of the flight</th>
<th>( k(t) )</th>
<th>( \sigma(t) )</th>
<th>( C(t) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test (1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Base case</td>
<td>0.4 ± 0.1</td>
<td>0.5 ± 0.2</td>
<td>0.65 ± 0.1</td>
</tr>
<tr>
<td>Less heterogeneous</td>
<td>0.8 ± 0.1</td>
<td>0.7 ± 0.2</td>
<td>0.85 ± 0.1</td>
</tr>
<tr>
<td>More heterogeneous</td>
<td>0.35 ± 0.1</td>
<td>0.4 ± 0.1</td>
<td>0.3 ± 0.1</td>
</tr>
<tr>
<td>Test (2)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Base case</td>
<td>1.2 ± 0.1</td>
<td>0.7 ± 0.2</td>
<td>0.5 ± 0.1</td>
</tr>
</tbody>
</table>

Notice that for test (1) the \( \beta \) values for a given simulation are broadly consistent with each other.
around 1.2 (see Table 1 for a listing of all computed $\beta$ values). Herrick et al. [2002] have also demonstrated that a power-law velocity distribution can be observed for flow in highly heterogeneous systems.

### 3.2. Average Tracer Concentration

[9] Considering advective transport only ($D = 0$), Figure 2 shows the average tracer concentration versus distance $y$ at different times. The results for test (1) see Figure 2a, clearly show anomalous behavior: the concentration peak hardly moves with a long forward advance of the tracer. For test (2), the concentration shown in Figure 2b resembles an approximately Gaussian profile, albeit with a large spread. Figure 3 shows the mean position $l(t)$ and the standard deviation $\sigma(t)$ of the mean concentration obtained in Figure 2, for all three permeability fields. For tracer test (1) both $l(t)$ and $\sigma(t)$ scale approximately as $t^\beta$ where $\beta < 1$ ($\beta$ is found from the average slope over the range 10-100 days; see also Table 1). In contrast with conventional dispersive transport where $l(t) \sim t$ and $\sigma(t) \sim t^{1/2}$, the ratio $l(t)/\sigma(t)$ is nearly constant with time and we obtain smaller and smaller values of $\beta$ as the degree of heterogeneity increases see Figure 3a. For tracer test (2), the scaling of the standard deviation $\sigma(t) \sim t^{1/2}$ is consistent with solutions to the ADE, but the mean concentration moves more slowly than linearly with time.

### 3.3. Breakthrough Curves

[10] The breakthrough curves for the cases considered in the previous section are shown in Figure 4. Notice the huge range of time scales-while breakthrough occurs in of order 10 days, significant amounts of tracer still remain in the system after 10,000 days. The spread of the breakthrough curve increases with the degree of heterogeneity. While the breakthrough time is governed by the permeability of the sand channels, the tail of the curve is controlled by slow flow through the low permeability shale. At late time each breakthrough curve in Figure 4 has an approximate log-log

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**Figure 2.** The average tracer concentration $C$ along the flow direction $y$ obtained for base case permeability field for: (a) test 1; and (b) test 2.

**Figure 3.** The mean position $l$ and the standard deviation $\sigma$ of the tracer plume.

**Figure 4.** The average produced concentration versus time (breakthrough curves) for the various cases discussed in the text. Notice the large range of times over which significant quantities of tracer are produced. At late times the concentration decreases as an approximate power-law with time and our estimated slopes are indicated on the figure.

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### 3.4. Dispersion

[11] To check that mixing of concentration between streamlines did not affect the results, we re-ran tracer test (1) with the base case permeability field including physically representative amounts of dispersion and diffusion. We set the molecular diffusion coefficient to $10^{-9}$ m$^2$/s and the longitudinal, horizontal transverse and vertical transverse dispersivities were $\Delta y/10 = 0.305$ m, $\Delta x/100 = 0.061$ m and $\Delta z/100 = 0.0061$ m respectively where $\Delta x$, $\Delta y$ and $\Delta z$ are the grid block sizes. The dispersivities account for sub-grid block heterogeneity and are typical of values measured in field tests [Gelhar, 1993]-dispersion due to larger-scale features is, of course, explicitly accounted for in the simulation. The breakthrough curve displayed in Figure 4 is very similar to the advection-only case.

### 4. Discussion and Conclusions

[12] We have demonstrated that anomalous transport arises from purely advective movement of tracer using a finely-gridded simulation model that contains large-scale high and low permeability features. Including a physical amount of molecular diffusion and sub-grid-block dispersion did not affect the results.

[13] We performed simulations using an upscaled permeability field with fewer grid blocks [Christie and Blunt, 2001]. The results were similar, but the late-time tails of the transit time distribution and the breakthrough curve were truncated. Coarse grid models tend to give a smoother response as details of the flow field are missed.

[14] The time dependence of the mean location of the plume, its spread and the breakthrough curves were all approximately characterized by an exponent $\beta$ derived from a CTRW formulation of transport that assumes a power-law transit time distribution. We showed that the distribution of times-of-flight through each grid block displayed a power-law tail at late time with an exponent $\beta$ broadly consistent with the measurements of the plume. $\beta$ decreased as the degree of heterogeneity increased, indicating more anoma-
lous behavior. However, $\beta$ is a single parameter approximation of the behavior—in the simulations we modeled the entire motion of the plume and the power-law scaling was only approximate.

[15] The boundary conditions for the tracer flow had a significant impact. If tracer is initially placed uniformly in a thin slice perpendicular to the overall flow direction (test 1) the transport is highly anomalous, since significant amounts of tracer can be placed in very slow flowing low permeability regions—this scenario is similar to that observed at the Columbus air force base [Adams and Gelhar, 1992]. In contrast, if tracer is injected (test 2), it preferentially enters high permeability regions and does not sample the low-flow areas of the domain. As a consequence, the motion of the plume is much less anomalous. While the behavior of test 2 was not entirely Gaussian (we saw slower than linear motion of the mean concentration and a power-law tail to the breakthrough curve), it was significantly less anomalous than test 1 due to different sampling of the streamlines.

[16] In future, we could use fine-grid streamline-based simulation to predict the anomalous behavior of contaminant plumes if a finely-resolved geological description of the aquifer were available.

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References


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