

Solute transport in porous media: Dispersion tensor of periodic networks

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The authors study solute transport in periodic networks of channels. They identify the parameter regime where a local physical mechanism that occurs at the intersections of channels is the dominant cause of dispersion and obtain the macroscopic transport equation that the concentration of solute satisfies. © 2007 American Institute of Physics. [DOI: 10.1063/1.2760180]

Transport of contaminants in soils,¹ nutrients in bones,² and movement of minerals in soils are examples of solute transport in porous media.³ Theoretical methods used to study solute transport in porous media include numerical experiments on networks, on media with fractal geometry and percolation methods,⁴ method of moments⁵ and homogenization techniques on periodic media,⁶ and method of moments on periodic networks.⁷ Notorious early works include Ref. 8. Further discussions can be found in Ref. 9.

Consider Fig. 1. The arrows in Fig. 1(a) indicate the direction of the flow. Figure 1(b) shows the solute concentration at time $t=0$. The darker the regions, the larger the concentration. Figure 1(c) shows the concentration at $t=t_1$, when solute reaches the intersection of the channels. Let $t_2 > t_1$. In the absence of diffusion, fluid from channel 2 with solute and fluid from channel 3 without solute would be convected next to each other along channel 1 during the time interval (t_1, t_2) and the concentration of solute at $t=t_2$ would look as in Fig. 1(d). However, if the channels are thin enough, as assumed here, diffusion homogenizes the concentration of solute in slices perpendicular to the channels and thus, the distribution of solute at $t=t_2$ is as illustrated in Fig. 1(e). In the interval (t_1, t_2) liquid with solute from channel 2 enters channel 1 and mixes with liquid without solute that enters channel 1 from channel 3. In this letter we identify the parameter regime where this effect is the dominant cause of dispersion and develop a method to compute the dispersion tensor when the void space of the porous media (i.e., the region occupied by the fluid) consists of a periodic network of thin channels.

Due to their computational efficiency and flexibility in modeling the *microgeometry* (shape, size, and location of the voids), methods that use periodic networks are very appealing. This class of methods are limited to Ref. 7. Moreover, the models in Ref. 7 use ad hoc rules that prevent them from accurately modeling the physical effect of Fig. 1. The strengths of our method include the following: (1) This method is exact to first order. It results from an asymptotic limit of the Navier-Stokes system for fluid flow and convection-diffusion equation for solute transport. (2) The asymptotic limit used results from the fundamental effect of Fig. 1. While this local effect has been identified and appears in standard texts in porous media and in Ref. 10, the combined effect of this phenomenon at all intersections has not been studied. This method is an ideal tool for those studies. (3) The computational cost of this method is relatively low.

(4) Extensions to three dimensions are immediate.

Consider a two-dimensional channel filled with a Newtonian incompressible fluid with viscosity μ subjected to pressures p_a and p_b at the channel ends and satisfying non-slip boundary conditions at the channel walls. Let $\hat{\mathbf{e}}$ be the unit vector parallel to the channel pointing from the end with pressure p_a to the other end. At low Reynolds numbers, the spatial average of the velocity of the steady (Poiseuille) flow is $\mathbf{v} = \delta^2(p_a - p_b)\hat{\mathbf{e}}/(12\mu\ell)$, where ℓ is the channel length and δ its width. Let D be the diffusion coefficient and v the spatial average of the norm of the fluid velocity. If $\delta^2/D \ll \ell/v \ll \ell^2/D$, it results from the works⁸ that the evolution of solute concentration is described by two rules: (1) Concentration of solute is homogeneous in slices perpendicular to the channel and (2) solute concentration is convected with the average fluid velocity within the channel.

We denote by Ω_p the void space of the porous medium. We assume the following: (1) Periodicity. There exist two vectors \mathbf{w} and \mathbf{q} such that $\Omega_p = \Omega_p + n\mathbf{w} + m\mathbf{q}$ for all integers n and m . (2) Ω_p is a collection of interconnected thin channels [see Fig. 2(a)] (3) Exactly three channels merge at each intersection. (4) Ω_p is connected. We associate a periodic graph with the medium in a natural way. As shown in Fig. 2(b), the edges are the channels and the nodes the intersection of channels. \mathcal{N} denotes the set of nodes and \mathcal{E} the set of edges. We identify the nodes with their location and thus, $\mathcal{N} \subset \mathbb{R}^2$. Given an edge e , its width (i.e., the width of the channel that corresponds to e) is denoted by δ_e and its length by ℓ_e .

The fluid within Ω_p is incompressible, Newtonian with density ρ , viscosity μ , and satisfies nonslip boundary conditions, i.e., fluid velocity vanishes at the channels walls.

We denote by p_a the pressure at the node \mathbf{a} . The medium is subjected to an applied pressure gradient $\mathbf{G}(t)$ periodic with period t_0 . Thus, we have

$$p_{\mathbf{a}+n\mathbf{w}+m\mathbf{q}} = p_a + \mathbf{G} \cdot (n\mathbf{w} + m\mathbf{q}), \quad (1)$$

for all integers n and m and nodes \mathbf{a} (\mathbf{w} and \mathbf{q} are the vectors that determine the periodicity of Ω_p and $\mathbf{r} \cdot \mathbf{s} = r_1s_1 + r_2s_2$). The

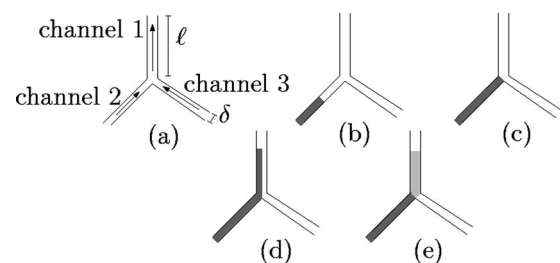


FIG. 1. Mechanism that mixes solute and solvent.

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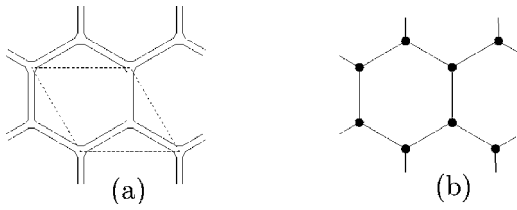


FIG. 2. Periodic network of channels and associated graph. The period cell is in dashed lines.

variations of \mathbf{G} in time are slow. Thus, the flow within each channel is Poiseuille. Mass conservation at each node \mathbf{a} (the rate at which fluid enters \mathbf{a} equals the rate at which it leaves \mathbf{a}) reduces to

$$\sum_{\{\mathbf{b} \in \mathcal{N}: \mathbf{b} \text{ is connected to } \mathbf{a} \text{ by an edge}\}} \frac{\delta_e^3}{12\mu\ell_e} (p_{\mathbf{b}} - p_{\mathbf{a}}) = 0. \quad (2)$$

Given a channel e , we denote by \mathbf{v}_e the average fluid velocity within e . We define $\mathbf{h}(e)$, the head of e , as the end point of e with smallest pressure. $\mathbf{k}(e)$, the tail of e , is the end point of e with largest pressure. Fluid within e flows from its tail $\mathbf{k}(e)$ to its head $\mathbf{h}(e)$. Since the flow is time dependent, an end point of an edge may be its head for some period of time and its tail for other times.

The pressures at the nodes are obtained from Eqs. (1) and (2). The velocities within the channels are $\mathbf{v}_e = \delta_e^2 (p_{\mathbf{k}(e)} - p_{\mathbf{h}(e)}) (\mathbf{h}(e) - \mathbf{k}(e)) / (12\mu\ell_e \|\mathbf{h}(e) - \mathbf{k}(e)\|)$, where we use the notation $\|\mathbf{r}\| = \sqrt{r_1^2 + r_2^2}$.

We assume $v_e = \|\mathbf{v}_e\| = O(v)$, $\ell_e = O(\ell)$, $\delta_e = O(\delta)$ for all edges e where the parameters v , ℓ , and δ satisfy $\delta^2/D \ll \ell/v \ll \ell^2/D$. Thus, solute transport within each channel follows rules 1 and 2 (previously described).

We parametrize each edge e by $\mathbf{x}_e(s) = \mathbf{k}(e) + s(\mathbf{h}(e) - \mathbf{k}(e)) / \|\mathbf{h}(e) - \mathbf{k}(e)\|$ and we denote by $u_e(s, t)$ the solute concentration in e at the point $\mathbf{x}_e(s)$ and time t . Since solute concentration in a channel is convected with the average fluid velocity within the channel, we have

$$\frac{\partial u_e}{\partial t} + v_e \frac{\partial u_e}{\partial s} = 0 \quad \text{for } 0 \leq s \leq \ell_e, \quad \text{and } t \geq 0. \quad (3)$$

Let e be an edge and $\mathbf{k}(e)$ its tail. Either $\mathbf{k}(e)$ is the head of two other edges or $\mathbf{k}(e)$ is the head of only one other edge. If $\mathbf{k}(e)$ is the head of two other edges, say, β_1 and β_2 , solute enters $\mathbf{k}(e)$ at the same rate that it leaves $\mathbf{k}(e)$ and thus, $\delta_e v_e u_e(0, t) = \delta_{\beta_1} v_{\beta_1} u_{\beta_1}(\ell_{\beta_1}, t) + \delta_{\beta_2} v_{\beta_2} u_{\beta_2}(\ell_{\beta_2}, t)$. This condition can be written as

$$u_e(0, t) = \frac{\sum_{\{\beta: \mathbf{h}(\beta) = \mathbf{k}(e)\}} \delta_{\beta} v_{\beta} u_{\beta}(\ell_{\beta}, t)}{\sum_{\{\beta: \mathbf{h}(\beta) = \mathbf{k}(e)\}} \delta_{\beta} v_{\beta}} \quad (4)$$

because mass conservation at $\mathbf{k}(e)$ is $\delta_e v_e = \delta_{\beta_1} v_{\beta_1} + \delta_{\beta_2} v_{\beta_2}$. Assume now that $\mathbf{k}(e)$ is the head of only one edge, say, β . Thus, $u_e(0, t) = u_{\beta}(\ell_{\beta}, t)$. This condition is, in fact, Eq. (4). Thus, Eq. (4) is valid for all edges e .

The system (3) and (4) uniquely determines the time evolution of the solute concentration within the channels once initial and boundary conditions are given.

We now describe the main result of this letter. We say that two edges are equivalent if one is the translation of the

other by a vector of the form $n\mathbf{w} + m\mathbf{q}$ where n and m are integers. Note that $\delta_{e_1} = \delta_{e_2}$, $\ell_{e_1} = \ell_{e_2}$, and $\mathbf{v}_{e_1} = \mathbf{v}_{e_2}$ if e_1 and e_2 are equivalent. In what follows we will take spatial averages of quantities. Thus, we need to be able to select exactly one edge per equivalence class. We denote by \mathcal{F} a set of edges that contains exactly one edge per equivalent class (\mathcal{F} could be the edges whose heads are in the period cell $Q = \{\mathbf{s}\mathbf{w} + r\mathbf{q}: 0 \leq s, r < 1\}$).

The area occupied by fluid within the period cell Q is $|\Omega_p \cap Q| = \sum_{e \in \mathcal{F}} \delta_e \ell_e$. The average fluid velocity is $\mathbf{V} = |\Omega_p \cap Q|^{-1} \sum_{e \in \mathcal{F}} \delta_e \ell_e \mathbf{v}_e$. Note that $\|\mathbf{V}\| = O(v)$. We assume that t_0 , the period of the applied pressure gradient \mathbf{G} , satisfies $t_0 \gg \ell/v$, i.e., the time required for solute concentration to be convected across a channel is much smaller than the period of the applied pressure gradient. *Macroscopically*, the solute concentration is convected with the average fluid velocity \mathbf{V} and dispersed with dispersion tensor

$$D_{ij}^{\text{eff}} = \langle D_{ij}^* \rangle = t_0^{-1} \int_0^{t_0} D_{ij}^*(t) dt, \quad (5)$$

$$D_{ij}^* = \frac{1}{2|\Omega_p \cap Q|} \left\{ \sum_{e \in \mathcal{F}} \delta_e \ell_e \left(\frac{\ell_e}{v_e} [\mathbf{v}_e - \mathbf{V}]_i [\mathbf{v}_e - \mathbf{V}]_j + [\mathbf{V} - \mathbf{v}_e]_i [\mathbf{f}_{\mathbf{k}(e)}]_j + [\mathbf{V} - \mathbf{v}_e]_j [\mathbf{f}_{\mathbf{k}(e)}]_i \right) \right\}. \quad (6)$$

$[\mathbf{y}]_i$ denotes the i th component of the vector \mathbf{y} and $(\mathbf{f}_{\mathbf{a}})_{\mathbf{a} \in \mathcal{N}}$ is a family of vectors periodic in space and time $(\mathbf{f}_{\mathbf{a}}(t) = \mathbf{f}_{\mathbf{a} + n\mathbf{w} + m\mathbf{q}}(t + p t_0))$ for all integers n , m and p) that, for each $\mathbf{a} \in \mathcal{N}$, satisfy

$$\sum_{\{e: \mathbf{h}(e) = \mathbf{a}\}} \delta_e v_e (\mathbf{f}_{\mathbf{k}(e)} - \mathbf{f}_{\mathbf{a}}) = \sum_{\{e: \mathbf{h}(e) = \mathbf{a}\}} \delta_e \ell_e (\mathbf{v}_e - \mathbf{V}). \quad (7)$$

More precisely, for each $\mathbf{a} \in \mathcal{N}$, let $u_{\mathbf{a}}(t)$ be the solute concentration that leaves the intersection \mathbf{a} at time t , i.e., $u_{\mathbf{a}}(t) = u_e(0, t)$ if $\mathbf{a} = \mathbf{k}(e)$ at time t . We obtained that $u_{\mathbf{a}}(t) \approx u(\mathbf{a}, t)$ where $u(\mathbf{x}, t)$ satisfies $\partial u / \partial t + \mathbf{V} \cdot \nabla u = \sum_{i,j} D_{ij}^{\text{eff}} \partial^2 u / \partial x_i \partial x_j$, where ∇u is the gradient of u with respect to \mathbf{x} and u is subjected to boundary and initial conditions that depend on the particular problem under consideration. \mathbf{D}^{eff} is referred to as the dispersion tensor.

We obtained our results by means of asymptotic expansions. Our work is different to that of Ref. 7. We obtain a different dispersion tensor. The reason is that the *ad hoc* rules used in Ref. 7 correspond formally to the parameter regime where the channels meet at pores with volume much larger than the channel volume and the solute concentration is homogeneous within each of these pores.

Note that if the applied pressure gradient \mathbf{G} is time independent, $\mathbf{D}^{\text{eff}} = \mathbf{D}^*$ [see Eqs. (5) and (6)]. Consider now the case $\mathbf{G}(t) = g(t)\mathbf{E}$ with \mathbf{E} constant and $g(t)$ real valued periodic. Let $\mathbf{D}_{\mathbf{E}}^{\text{eff}}$ be the dispersion tensor that corresponds to the applied pressure gradient \mathbf{E} . The dispersion tensor that corresponds to the applied pressure gradient $\mathbf{G}(t) = g(t)\mathbf{E}$ is $\mathbf{D}^{\text{eff}} = \langle |g| \rangle \mathbf{D}_{\mathbf{E}}^{\text{eff}}$.

Our next example is shown in Fig. 3. All the channels have the same length ℓ and form regular hexagons. The width of the channels are, as displayed in the figure, δ_1 , δ_2 , and δ_3 . We assume the applied pressure gradient to be $\mathbf{G}(t) = (0, g(t)/\ell)$, where g is a periodic function with period t_0 . Our results applied to this example imply

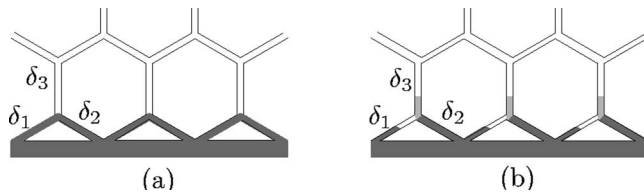


FIG. 3. Same microgeometry as in Fig. 2. There are three channels per period cell. In (a) $\delta_1 = \delta_2$. In (b) $\delta_1 < \delta_2$. The darker the region, the larger the solute concentration.

$$\mathbf{V}_2(t) = -\frac{3}{16\mu l} \frac{\delta_3^3(\delta_1^3 + \delta_2^3)}{(\delta_1^3 + \delta_2^3 + \delta_3^3)(\delta_1 + \delta_2 + \delta_3)} g(t), \quad (8)$$

$$\mathbf{D}_{22}^{\text{eff}} = \frac{9\langle |g| \rangle}{64\mu} \frac{\delta_3^3(\delta_1^3 + \delta_2^3)(\delta_1 + \delta_2)^2(\delta_1 - \delta_2)^2}{\delta_1 \delta_2 (\delta_1^3 + \delta_2^3 + \delta_3^3)(\delta_1 + \delta_2 + \delta_3)^3}. \quad (9)$$

To discuss the above formulas in a more concrete context, assume that the material occupies the region $x_2 > 0$. Also assume the material to be attached to a reservoir of solute located at $x_2 < 0$ and that initially there is no solute within the material (for $x_2 > 0$). Due to symmetry, the solute concentration u , in this example, depends only on x_2 . Thus, we only need \mathbf{V}_2 and $\mathbf{D}_{22}^{\text{eff}}$.

Note that $\mathbf{D}_{22}^{\text{eff}} = 0$ if $\delta_1 = \delta_2$. Thus, after each period, solute is convected a distance $\langle \mathbf{V} \rangle$ but it is not dispersed in our asymptotic limit (there is a smaller order dispersion that results from an effect known as Taylor dispersion inside each channel⁸). This is in accordance with the physical effect of Fig. 1(e). The mixing of solute with the host liquid occurs when solute from two different channels at different concentrations flow into the same intersection. In our example when $\delta_1 = \delta_2$, whenever solute from two channels flow into the same intersection the concentration in both channels is the same. This is illustrated in Fig. 3(a), where we show that solute reaches the upper ends of all the channels attached to the reservoir at the same time if $\delta_1 = \delta_2$.

In Fig. 3(b) we display an example where $\delta_1 < \delta_2$. As illustrated in that figure, the time required for solute from the reservoir to travel through the thinner channels is longer than the travel time of the thicker channels. Thus, the effect of Fig. 1(e) does occur and, as Eq. (9) implies, we have that $\mathbf{D}_{22}^{\text{eff}} \neq 0$. In the particular case that $\langle g \rangle = 0$, there is no convection after a complete period. Thus, there will be much more transport of solute if $\delta_1 \neq \delta_2$ (where $\mathbf{D}_{22}^{\text{eff}} \neq 0$) than if $\delta_1 = \delta_2$, where ($\mathbf{D}_{22}^{\text{eff}} = 0$).

¹M. L. Brusseau, *Rev. Geophys.* **32**, 285 (1994); A. M. M. Elfeki, G. J. M. Uffink, and F. B. J. Barends, *Groundwater Contaminant Transport. Impact of Heterogeneous Characterization: A New View on dispersion* (A. A. Balkema, Rotterdam, Netherlands, 1997).

²K. Piekarski and M. Munro, *Nature (London)* **269**, 80 (1977); M. L. Knothe Tate, U. Knothe, and P. Niederer, *Am. J. Med. Sci.* **316**, 189 (1998).

³J. Bear, *Dynamics of Fluids In Porous Media* (Dover, New York, 1972); B. Berkowitz, *Dispersion in Heterogeneous Geological Formations* (Kluwer, London, 2001); H. Brenner and D. A. Edwards, *Macrotransport Processes* (Butterworth-Heinemann, Stoneham, MA, 1993); M. Sahimi, *Flow and Transport in Porous Media and Fractured Rock* (Wiley, New York, 1995).

⁴P. M. Adler, *Porous Media. Geometry and Transports* (Butterworth-Heinemann, Stoneham, MA, 1992); B. Berkowitz and R. P. Ewing, *Surv. Geophys.* **19**, 23 (1998); B. Berkowitz, *Adv. Water Resour.* **25**, 861 (2002); V. I. Selyakov and V. V. Kadet, *Percolation Models for Transport in Porous Media* (Kluwer, Boston, MA, 1996).

⁵H. Brenner, *Philos. Trans. R. Soc. London, Ser. A* **297**, 81 (1980); H. Brenner and P. M. Adler, *Transport Processes in Porous Media* (Hemisphere/McGraw-Hill, New York, 1985).

⁶R. Mauri, *Phys. Fluids A* **3**, 743 (1991); C. C. Mei, *Transp. Porous Media* **9**, 261 (1992); J. Rubinstein and R. Mauri, *SIAM J. Appl. Math.* **46**, 1018 (1986).

⁷P. M. Adler and H. Brenner, *PCH, PhysicoChem. Hydrodyn.* **5**, 269 (1984); K. D. Dorfman and H. Brenner, *Phys. Rev. E* **65**, 021103 (2002).

⁸G. I. Taylor, *Proc. R. Soc. London, Ser. A* **223**, 446 (1953); R. Aris, *Proc. R. Soc. London, Ser. A* **235**, 67 (1956); P. G. Saffman, *J. Fluid Mech.* **6**, 321 (1959).

⁹G. Dagan, *Annu. Rev. Fluid Mech.* **19**, 183 (1987); G. Dagan, *Water Resour. Res.* **26**, 1281 (1990); J. Feyen, D. Jacques, A. Timmerman and J. Vanderborght, *J. R. Astron. Soc. Can.* **70**, 231 (1998); J. H. Cushman, L. S. Bennethum, and B. X. Hu, *Adv. Water Resour.* **25**, 1043 (2002).

¹⁰V. V. Mourzenko, F. Yousefian, B. Kolbah, J. F. Thovert, and P. M. Adler, *Water Resour. Res.* **38**, 1000 (2002).