Solute transport during cyclic flow in saturated porous media

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We consider materials with large pores interconnected by thin long channels saturated with an incompressible fluid. In the absence of fluid flow, solute transport in the porous network is diffusion controlled, however, solute transport can be enhanced when the porous network is subjected to a cyclic flow with zero time average velocity. We develop a mathematical model to analyze this physical phenomenon and obtain an effective macroscale diffusion coefficient for solute transport which dependends on cyclic flow conditions and the geometry of the porous network. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1791328]

We study solute transport in fluid filled porous networks. In the absence of fluid flow, solute transport is diffusion controlled. The diffusion time for distance X is of the order X^2/D, where D is the diffusion coefficient. The diffusion coefficient in electrolytes is small (typically in the order of $10^{-9}\mathrm{m}^2\ \mathrm{s}^{-1}$). Moreover, diffusion is reduced by interfacial phenomena and tortuosity in high specific surface porous networks (i.e., submicron pore size). In this study, we analyze a mechanism that enhances transport in porous networks subjected to zero time-average cyclic flow.

The material microstructure consists of large pores interconnected by long thin channels. Bones exhibit this type of porous structure where large pores are called "lacunae," channels "canaliculi," and the solutes transported include nutrients. The ideal lacunar-canalicular system we model is displayed in Fig. 1. The first channel is connected to a reservoir of solute with concentration c_r, while the initial concentration of solute is c_0 everywhere else in the network.

Mixing due to diffusion within a lacuna occurs in times of the order ℓ^2/D, where ℓ is the diameter of a lacuna (see Fig. 1), while the mixing time (due to diffusion) within a canaliculus is of the order $(L-\ell)^2/D$, where $L-\ell$ is the length of a canaliculus (see Fig. 1). We consider cyclic flows with periods much larger than ℓ^2/D and much smaller than $(L-\ell)^2/D$. Thus, we assume that mixing is instantaneous within lacunae and negligible within canaliculi (other mixing mechanisms within the channels, such as Taylor dispersion,[1] are neglected).

There is an inflow of volume V_F from the reservoir during the part of the period where the fluid velocity is positive. If $V_F < V_c$, where V_c is the volume of a channel, solute from the reservoir does not reach the first pore. Since there is no mixing within the channels and the time average velocity is zero, all the solute that enters the system goes back to the reservoir after a period. Therefore, there is no solute transport at the end of one cycle. However, if $V_F > V_c$, as soon as some solute from the reservoir reaches the first pore, there is instantaneous mixing in that pore and the fluid that flows from that pore into the second channel carries solute that was initially in the reservoir. After a complete period, solute that was initially in the reservoir will be left in pores and channels. Hence, there is a net transport of solute after each period.

Solute transport in porous media is a subject of intensive study. Examples include Refs. 2–4. In the context of bone, it was first noted in Ref. 5 that advection in the lacunar-canalicular system induced by loading and unloading increases the transport of nutrients (see also Ref. 6). This phenomena was studied experimentally in Ref. 7. The role of fast mixing within lacunae to enhance nutrient transport has been postulated and explored in Ref. 8. Our work is the first formal and detailed mathematical analysis of this transport phenomenon. We demonstrate the diffusion-like macroscale behavior and provide an explicit formula for the effective diffusion coefficient.

The lacunar-canalicular system we consider extends to infinite. The right wall of the reservoir is the origin of the coordinate system, $x=0$, the location of the ith canaliculus is the segment $[(i-1)L, iL-\ell]$ and the location of ith lacuna is $[iL-\ell, iL]$. The cross-sectional area of a canaliculus is a. We denote by $V_c=(L-\ell)a$ and V_ℓ the volume of each canaliculus and lacuna, respectively (Fig. 1). We assume rigid solid phase (i.e., a, V_c, and V_ℓ are constants). An incompressible fluid fills the lacunar-canalicular system. The solute concentration in the reservoir remains at the constant value c_r, while the concentration of nutrients in the lacunar-canalicular system starts at initial value c_0.

We denote by $c_i(t)$ the concentration of nutrients at time t in the ith lacuna. For x in canaliculi, we denote by $c(x,t)$ the concentration of nutrients at x and time t. Since diffusion and dispersion are negligible within canaliculi, the solute flows with the same velocity as the fluid $v=v(x,t)$ within canaliculi. Fluid incompressibility and mass conservation

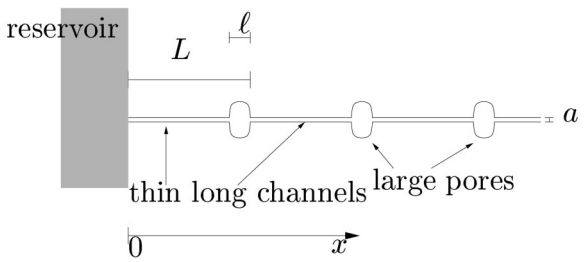

FIG. 1. Idealized one-dimensional lacunar-canalicular system.

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implies that v is independent of x, i.e., $v=v(t)$. Solute conservation within the channels reduces to

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = 0 \tag{1}$$

for all x in canaliculi.

Whenever the velocity is positive, there is flow of solute from the ith canaliculus into the ith lacuna at a rate $av(t)c(iL-\ell,t)$. Solute also flows out of that same lacuna into the $(i+1)$th canaliculus at a rate $av(t)c_i(t)$. Analogously, when the velocity is negative, there is flow of solute from the $(i+1)$th canaliculus into the ith lacuna at a rate $-av(t)c(iL,t)$ and flow out of that same lacuna into the ith canaliculus at a rate $-av(t)c_i(t)$. This implies

$$V_\ell \frac{\mathrm{d}c_i}{\mathrm{d}t} = \begin{cases} av(c(iL-\ell,t) - c_i(t)) & \text{when } v(t) > 0 \\ av(c_i(t) - c(iL,t)) & \text{when } v(t) < 0 \end{cases} \tag{2}$$

for all positive integer i.

Furthermore, whenever the velocity is positive, there is flow from each lacuna into the canaliculus located at its right and thus, the solute concentration in the left end of a canaliculus is equal to the solute concentration in the neighboring lacuna at the left of the canaliculus. Analogously, whenever the velocity is negative, the solute concentration in the right end of a canaliculus is equal to the solute concentration in the lacuna located at the right of end the canaliculus. Mathematically,

$$c((i-1)L,t) = c_{i-1}(t) \quad \text{if } v(t) > 0,$$

$$c((i+1)L-\ell,t) = c_{i+1}(t) \quad \text{if } v(t) < 0, \tag{3}$$

the first of the above equations being valid for all integer $i \geqslant 2$ and the second for all integer $i \geqslant 0$.

Similarly, whenever the velocity is positive, there is flow from the reservoir into the first canaliculus, i.e., the solute concentration at the left end of the first canaliculus is equal to the solute concentration in the reservoir c_r,

$$c(0,t) = c_r \quad \text{if } v(t) > 0. \tag{4}$$

The initial concentration in the network is c_0, thus

$$c_i(0) = c_0 \tag{5}$$

for all positive integer i.

We assume that the flow velocity in canaliculi v is a known periodic function with period t_0 and zero time average

$$\int_0^{t_0} v(t)dt = 0. \tag{6}$$

This restriction is inherent to closed systems such as bones, where the volume of the porous network returns to its original value at the end of every cycle.

To simplify our analysis we assume that there exist $0<t^\star<t_0$ such that $v(t)>0$ if $0<t<t^\star$ and $v(t)<0$ if $t^\star<t<t_0$. Thus, the volume of fluid that flows from the osteonal canal into the lacunar-canalicular system in the time interval $0<t<t^\star$ is

$$V_F = a\int_0^{t^\star} v(t)dt. \tag{7}$$

Let $\rho=\rho(z,t)$ be the solution

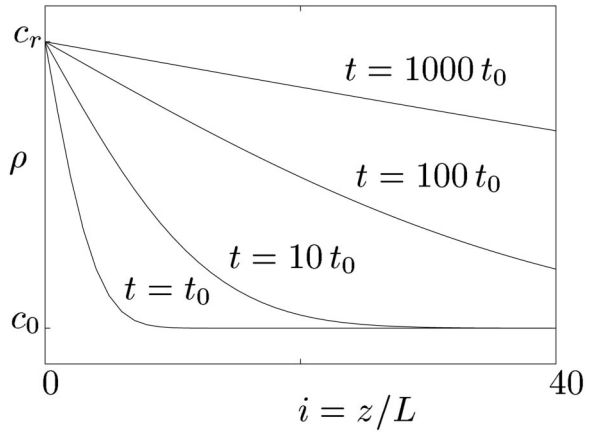

FIG. 2. Plot of concentration ρ vs normalized distance z/L for different fixed values of t. The selected parameter values are $\alpha=5$ and $\beta=0.99$ and the velocity profile $v(t)=(at_0)^{-1}(\pi V_F)\sin(2\pi t/t_0)$.

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial z^2} \text{ for } t>0 \text{ and } z>0, \tag{8}$$

where D is defined below in Eq. (16), subjected to the initial conditions

$$\rho(z,0) = c_0 \text{ for } z>0 \tag{9}$$

and boundary conditions

$$\rho(0,t) = c_r, \quad \lim_{z\to+\infty} \rho(z,t) = c_0 \text{ for } t \geqslant 0. \tag{10}$$

Extend the definition of ρ to $z<0$ as follows:

$$\rho(z,t) = c_r \text{ if } z \leqslant 0, \tag{11}$$

and let $z_i=z_i(t)$ be defined as

$$z_i(t) = iL - \frac{aL}{V_\ell + V_c}\int_0^t v(s)ds. \tag{12}$$

Note that the variable z is like a Lagrangian coordinate, which is related to the original space variable x by the formula

$$z = x - \frac{aL}{V_\ell + V_c}\int_0^t v(s)ds. \tag{13}$$

It can be shown that ρ gives the asymptotic approximation of the concentrations, more precisely

$$c_i(t) \simeq \rho(z_i(t),t) \text{ if } V_F \gg V_c. \tag{14}$$

This system of equations can be solved explicitly,

$$\rho(z,t) = c_r + (c_0 - c_r)\frac{2}{\sqrt{\pi}}\int_0^{z/(2\sqrt{Dt})} e^{-s^2}\,ds. \tag{15}$$

The effective diffusion coefficients is

$$D = D_{\text{eff}} = \left(\frac{V_\ell}{V_c + V_\ell}\right)^2\left(\frac{V_F}{V_c + V_\ell}\right)\left(\frac{L^2}{t_0}\right). \tag{16}$$

We define the parameters $\alpha=V_F/(V_c+V_\ell)$ and $\beta=V_\ell/(V_c+V_\ell)$. Figure 2 shows a plot of concentration $\rho(z,t)$ versus normalized distance z/L at different fixed values of t. Figure 3 shows the evolution of concentration in the fifteenth lacuna $\rho(z_{15}(t),t)$ versus normalized time t/t_0. The oscillations in concentration reflect the evolution in concentration

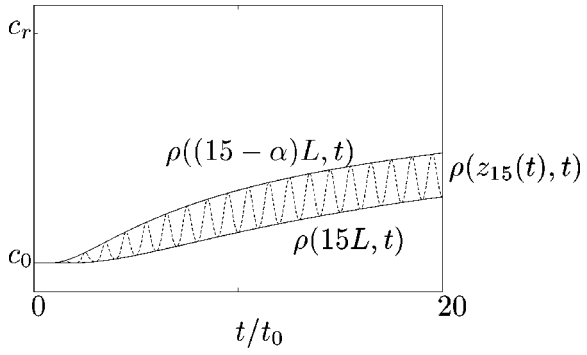

FIG. 3. Plot of concentration $\rho(z_{15}(t),t)$ (dashed line), $\rho(15L,t)$ (lower solid line), and $\rho((15-\alpha)L,t)$ (upper solid line) vs normalized time t/t_0. The parameters are the same as in Fig. 2.

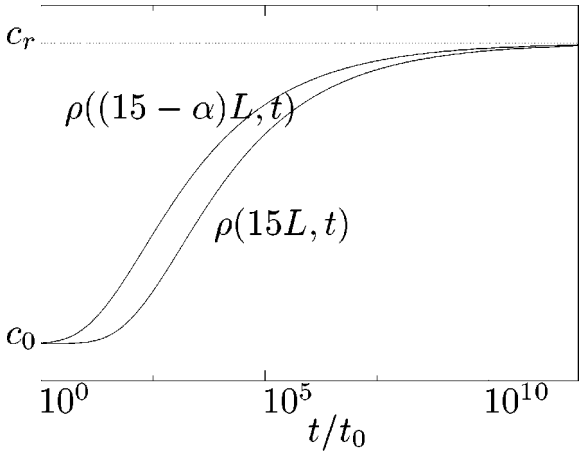

FIG. 4. Plot of concentration $\rho(15L,t)$ (lower line), and $\rho((15-\alpha)L,t)$ (upper line) vs normalized time t/t_0 in log scale. The parameters are the same as in Fig. 2.

in each cycle of the periodic velocity field v. Mathematically, these oscillations reflect the evaluation of ρ in $(z_i(t),t)$ in the approximation (14) and $z_i(t)$ are periodic functions with period t_0 (see Eq. (12)). We have also plotted the envelope of the concentration at the end of each cycle $\rho(15L,t)$ and the envelope of the concentration at flow reversal $\rho[(15-\alpha)L,t]$ versus normalized time t/t_0. Note that $\rho(iL,t)$ can be interpreted as the total concentration of nutrients $\rho(z_i(t),t)$ minus the oscillatory advective component. Figure 4 also shows $\rho(15L,t)$ and $\rho((15-\alpha)L,t)$ in a longer time scale to illustrate the convergence to c_r of the concentration in the fifteenth lacuna after a large number of cycles.

To conclude, we present a brief illustrative analysis for typical parameters in bones: lacunae (about 15 μm long and 5:1 to 10:1 aspect ratio), canaliculi (about 40 μm long, 0.2 μm diameter), and the excitation period ($t_0=1$ s). The following observations can be made. (1) Molecular diffusion in lacunae is faster than the natural excitation period, therefore the assumption of instantaneous mixing is adequate even in the absence of hydrodynamic mixing effects. (2) The volume of a lacuna is much greater than the volume of a canaliculus; then the effective diffusion coefficient (see Eq. (16)) becomes $D_{\text{eff}}=(L^2/t_0)(V_F/V_\ell)$. For the selected parameters, the ratio between $L^2/t_0=1.6\times10^{-9}\text{m}^2\ \text{s}^{-1}$ is in the order of molecular diffusion. Therefore, transport in cyclic flow with mixing will benefit the transfer of nutrients in bones if $V_F/V_\ell>1$. (3) The estimated Taylor dispersion (see Ref. 7) in canaliculi is in the order of $10^{-16}\text{m}^2\ \text{s}^{-1}$ and can be neglected.

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