FRACTIONAL MODEL FOR SOLUTE SPREADING IN RANDOMLY HETEROGENEOUS POROUS MEDIA

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Summary Experimental results [4], showed that solute spreading in saturated heterogeneous porous media does not always obey Fourier's law: the second moment of the concentration of a passive tracer dissolved in the saturating fluid may be proportional to a power of time, different from 1. A variety of fractional models are commonly used to account for the possibility, for the solute, to follow preferential paths or to be trapped by obstacles, depending on hypotheses concerning the small scale motion of dissolved particles. One can expect the internal self organization of the pores to influence the general trends of particle motion, at small and at large scale. Therefore we model diffusion, starting from hypotheses concerning the random structure of the heterogeneous porous medium. We consider a medium, which is a collection of tubes, randomly twisted around a general direction, and filled with motionless fluid. Solute spreading is assumed to obey Fick's law. Upon averaging over the tubes, we arrive at a modified version of Fourier's law for the evolution of the solute concentration. Properties of the impulse response of the thus obtained fractional equation are then discussed.

THE MEDIUM

Consider a three dimensional medium, made of a wide collection of tubes (indexed by ω) whose direction depends on the spatial coordinate x, which represents a general trend. As on Figure 1, let $\theta(\omega, x)$ be the angle between the direction x and the sample channel, indexed by ω, so that $\theta(., x)$ is a random variable. Suppose also that the tubes are saturated by motionless fluid. Solute is initially injected in a subset of the medium, which meets all the tubes (at $x = 0$ for instance). The concentration of solute $u(\omega, x, t)$ satisfies

$$\partial_t u(\omega, x, t) = \partial_x (D_0 cos^2\theta(\omega, x)\partial_x u(\omega, x, t)) \tag{1}$$

where D_0 is a coefficient, which also may depend on ω and x. Suppose that $\sqrt{D_0}cos(\omega, x) = \bar{\epsilon} + \tilde{\epsilon}$ is a stochastic process, for instance a Gaussian process with average $\bar{\epsilon}$, and correlation function $a^2 e^{-\nu|x-x'|}$. Moreover a^2 is supposed to be small, while ν is large.

FRACTIONAL DIFFUSION EQUATION FOR THE AVERAGE CONCENTRATION

Upon averaging (1) with respect to ω we obtain

$$\partial_t\langle u(x,t)\rangle - \bar{\epsilon}^2\partial^2_{x^2}\langle u(x,t)\rangle = 2\bar{\epsilon}\partial_x\langle\tilde{\epsilon}(\omega,x)\partial_x u(\omega,x,t)\rangle + \partial_x\langle\tilde{\epsilon}^2(\omega,x)\partial_x u(\omega,x,t)\rangle. \tag{2}$$

With $\frac{\delta v(\omega,x,t)}{\delta\tilde{\epsilon}(\omega,x')}$ denoting the functional derivative of v with respect to $\tilde{\epsilon}$ [1] , the Furutsu-Novikov formula [3] yields $\langle\tilde{\epsilon}^2\partial_x u\rangle = \langle\tilde{\epsilon}(\tilde{\epsilon}\partial_x u)\rangle = a^2\int_R\langle\frac{\delta(\tilde{\epsilon}\partial_x u)}{\delta\tilde{\epsilon}(x_1)}\rangle e^{-\nu|x-x_1|}dx_1$ and

$$\langle\tilde{\epsilon}^2\partial_x u\rangle = a^2\partial_x\langle u\rangle(x,t) + a^4\int_{R^2} e^{-\nu(|x-x_2|+|x-x_1|)}\langle\frac{\delta^2\partial_x u}{\delta\tilde{\epsilon}(x_1)\delta\tilde{\epsilon}(x_2)}\rangle dx_1 dx_2. \tag{3}$$

The functional derivative $f(\omega,x,x',t) = \frac{\delta u(\omega,x,t)}{\delta\tilde{\epsilon}(\omega,x')}$ satisfies $\partial_t f(x,x',t) - \partial_x((\bar{\epsilon}+\tilde{\epsilon}^2)\partial_x f(x,x',t)) = 2\bar{\epsilon}\partial_x(\delta(x - x')\partial_x u(\omega,x,t)) + 2\partial_x(\tilde{\epsilon}\partial_x u)$. Disregarding terms of the order of $a^2\langle\partial_x f\rangle$ in (2) and $a^4\langle\frac{\delta\partial_x f}{\delta\tilde{\epsilon}(x_2)}\rangle$ in (3) yields

$$\partial_t\langle f(x,x',t)\rangle - \bar{\epsilon}^2\partial^2_{x^2}\langle f(x,x',t)\rangle = 2\bar{\epsilon}\partial_x(\delta(x-x')\partial_x\langle u(x,t)\rangle \tag{4}$$

and

$$\partial_t\langle u(x,t)\rangle - \bar{\epsilon}^2\partial^2_{x^2}\langle u(x,t)\rangle = a^2\langle\partial^2_{x^2}u(x,t)\rangle + 2\bar{\epsilon}a^2\partial_x\int_R e^{-\nu|x-x'|}\langle\partial_x f(x,x',t)\rangle dx'. \tag{5}$$

Solving (4) for $\langle f(x,x',t)\rangle$, then setting $\eta = 2a^2/\nu$ and $D' = D - 3a^2$, we obtain that since ν is large $\langle u(x,t)\rangle$ solves the partial differential equation (6):

$$\partial_t\langle u(x,t)\rangle = D'\partial^2_{x^2}\langle u(x,t)\rangle + \eta\partial_t^{1/2}\partial^2_{x^2}\langle u(x,t)\rangle. \tag{6}$$

Here the fractional derivative $\partial_t^{1/2}$ is defined by $\partial_t^{1/2}v = \int_0^t \frac{v(\tau)}{\Gamma(1/2)\sqrt{(t-\tau)}}d\tau + \frac{v(0)}{\Gamma(1/2)\sqrt{t}}$, which is intermediate between the Riemann-Liouville derivative and the Caputo fractional derivative [2] of order $1/2$. The total amount of solute $\int_R\langle u(x,t)\rangle dx$ is conserved by (6), whose impulse response differs slightly from the heat equation's when η is small.

IMPULSE RESPONSE TO (6)

With $D' = 1$, the impulse response to (6) is $h(x,\eta,t) = \frac{1}{4\pi}\int_0^\infty e^{-\rho t}\rho^{-1/2}H(\rho,\eta,x)d\rho$, with $H(\rho,\eta,x) = \frac{1}{\sqrt{1-i\eta\rho^{1/2}}}e^{i\frac{\rho^{1/2}|x|}{\sqrt{1-i\eta\rho^{1/2}}}} + c.c.$. For $\eta = 0$ we recover the heat kernel $h(x,0,t) = \frac{1}{2\sqrt{\pi t}}e^{-\frac{x^2}{4t}}$. Setting $\eta \neq 0$ in (6) introduces slight but qualitative modifications of the impulse response, displayed on Figure 2. The behavior of h at $x = 0$ is sensible to $\eta\partial_t^{1/2}\partial_{x^2}^2\langle u(x,t)\rangle$ in (6), even when η is small. Indeed, for $\eta = 0$, the derivative of h with respect to x is zero at $x = 0$. For $\eta \neq 0$, oppositely, the left and right derivatives are non zero and opposite, so that the nose of h is sharper. Nevertheless, the effect is mainly visible at short and intermediate times. The value of η also influences the second moment of h, which is proportional to $t + 2\eta t^{1/2}/\sqrt{\pi}$, so, that non normal diffusive behaviors are visible at short and at intermediate times. At large times, the impulse response corresponding to $\eta \neq 0$ tend to be very similar to the homogeneous case.

CONCLUSION

In a heterogeneous medium, made of randomly twisted tubes where diffusion obeys Fick's law, the averaged concentration of a passive solute was shown to evolve according to a fractional partial differential equation. The fractional equation is a modified version of Fourier's law, including a non local term. Comparing with the bell-shaped Gaussian, the impulse response of the proposed variant has slightly heavier tails, and sharper nose at the point, where solute is initially injected. Nevertheless, the deviation from Fourier's law is less visible at large times.

References

[1] Donsker M.D., Lions J.L., Frechet Volterra variational equations, boundary value problems, and function space integrals, *Acta Mathematica*, **108**: 147–228, 1962.

[2] R.Gorenflo and F.Mainardi, Fractional calculus, integral and differential equations of fractional order, *Fractals and fractional calculus in continuum mechanics, Editors A.Carpinteri, F.Mainardi, CISM courses and lectures N 378, Springer Wien New-York* 223–276, 1997.

[3] Klyatskin V.I., *Izv.vuzov , Radiofisika* **20**,1977.

[4] Matheron G., de Marsily G., Is transport in porous media always diffusive? A counterexample, *Water Resource Research* **16** (5), 901–917, 1980.

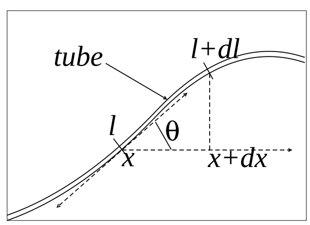

Figure 1. Part of a tube, inside which diffusion occurs. Displacement by dl along the tube increases the x coordinate by dx.

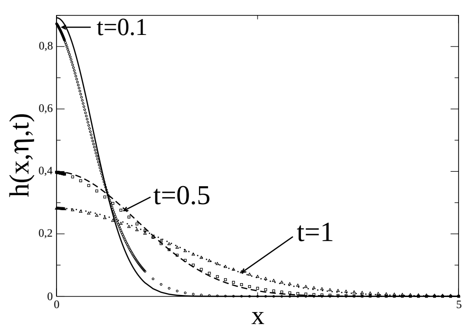

Figure 2. The impulse response of (6), compared with the purely diffusive case $\eta = 0$. Circles, squares and triangles represent the impulse response of (6) for $\eta = 0.1$ at times 0.1, 0.5 and 1. Full, dashed and dotted lines correspond to $\eta = 0$.