European Journal of Scientific Research
ISSN: 1450-216X / 1450-202X Vol. 95 No 3 January, 2013, pp.436-443

http://www.europeanjournalofscientificresearch.com

Diffusion Fractional Models for a Complex Porous Media in a Random Force Field for 3D Case

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Abstract

Fractional differential equation of particle transfer in porous and tubular media was obtained in the paper. It differs from the generally accepted ones by the dependence of the effective diffusion coefficient on the concentration. Together with 1D case problem also 3D problem of diffusion in normal random field was analyzed. For scales, lager then correlation lengths, fractional diffusion equation was derived which is valid for any time intervals. Diffusion equations in fractional derivatives in the limiting case of a zero correlation length of a random field of porosity or tube curvature were shown to be reduced to an ordinary diffusion equation with a renormalized diffusion coefficient. In case of a non-zero correlation length a general solution for the average square of the particle shift during random wandering was found. It was also found that in a certain time interval the coefficient of diffusion is time dependent, i.e. anomalous diffusion takes place.

Keywords: Diffusion Models; Porous Media; Diagram Techniques; Anomalous Diffusion; Fractional Equations

1. Introduction

It is known [1, 2], that a number of models for the transport of matter in a complex porous medium, saturated by motionless fluid were proposed. Complexity there was modeled by coefficients in the form of random processes. In addition [3] it was assumed the transport of matter to be ruled by one-dimensional (in space) partial differential equations. The random process also was assumed to be one-dimensional. This approach helped to see that the place where random coefficients appear in the small scale model influences the macroscopic equation which rules the evolution of the concentration, averaged with respect to those random fields. Other properties, e.g. the correlation function, have less importance. One-dimensional settings, such as the ones, considered up to this point, may correspond to realistic situations, such as for media, made of tubes randomly inter-twisted around a general direction [4, 5].

Now we perform a similar approach, in the dimension three. We start from a small scale model, designed for the spreading of solute in a fluid, with nearly spherical obstacles. Such a model may describe a saturated porous medium, whose solid matrix is composed up of the obstacles. Averaging with respect to the sample paths of a random process, meant to describe the complexity of the medium, allows us here again to bridge between small scales, where the medium appears as being disordered, and larger scales where disorder is less visible. This step will be achieved under strong hypotheses, concerning the random process itself: they concern the place, it enters the small scale equation, and the fact that it may be Gaussian, or not. This study only deals with rather easy situations, from this point of view. Once the structure of a random process has been set, some variants correspond to properties of the correlations. For a Gaussian process, only the two-points (or two-wave vectors) correlation has to be considered. The influence of the correlation function could be addressed for Gaussian (or nearly Gaussian) processes in the one-dimensional case and we learned that the point is not very important for the transport of matter over scales, larger than the correlation length, at least in the one-dimensional approach.

We address the question in a definitely three-dimensional setting [6-11], such as the one, described on the small scale by the three-dimensional version of equation [3]. This means that we assume that the logarithm of the porosity is a comfortable random process, within the frame-work of solute transport in a quiescent fluid, saturating the porous medium. In fact, this equation is also appropriate for solute spreading in a fluid, whose internal motions depend randomly on the location. We will average the concentration of solute with respect to some random process and obtain from this an equation, for the macroscopic scale. We will address the influence of the correlation function.

This way, we will arrive at an equation, whose Fourier-Laplace symbol is an integral, which depends on the correlation function of the random process, modeling the complexity of the medium. We will check against particular (but different) cases the influence on the correlation function, and see that it is apparently not crucial.

2. Diagram Technique for Porous Media in 3D Case

In [3] formerly we derived equation for diffusion process in three-dimensional random media. Let us present it again for convenience:

$$\frac{\partial}{\partial t}u\varepsilon - D_0\nabla\left(\varepsilon\nabla u\right) = 0 \quad . \tag{1}$$

Here $u(\mathbf{r},t)$ denotes the concentration of solute in point $\mathbf{r}$ at time t, while $\varepsilon(\mathbf{r})$ is the random porosity. The concentration is a functional of the porosity; hence it in turn is a random field. As in [3], we derive here an equation for the averaged concentration $\langle u \rangle$.

Let us as in {2, 3] put

$$\varepsilon(\boldsymbol{r}) = e^{\eta(\boldsymbol{r})}$$

in order to have at least a positively valued coefficient in the dispersive term.
Then (1) takes the form:

$$\frac{\partial u}{\partial t} - D_0\Delta u = D_0\nabla\eta\cdot\nabla u \quad , \tag{2}$$

which is the three-dimensional. Formally (2) is equivalent to the diffusion equation in a random force potential $\eta(\mathbf{r})$. The stationary variant ($\frac{\partial u}{\partial t}=0$) of (2) was addressed in [6, 7].

It is convenient for analysis (2) to use $(\mathbf{k},q)$ - representation, that is to use Fourier transform over space and Laplace transform over time. Then direct and backward Fourier transforms are used in such form:

$$\psi(\mathbf{r}) = \int_{-\infty}^{\infty}\psi(\mathbf{k})e^{i\mathbf{kr}}d\mathbf{k}$$

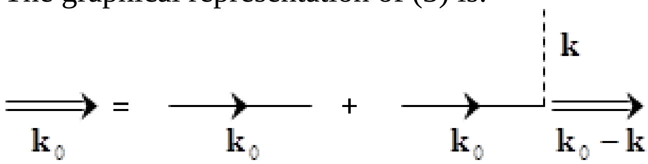
$$\psi(\mathbf{k}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\psi(\mathbf{r})e^{-i\mathbf{kr}}d\mathbf{r}$$

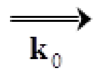
Therefore, we have:

$$u(\mathbf{k}_0,q) = \phi(\mathbf{k}_0)P_0(k_0,q) + P_0(k_0,q)\int_{-\infty}^{\infty}\tilde{\eta}(\mathbf{k})\mathbf{k}(\mathbf{k}_0-\mathbf{k})u(\mathbf{k}_0-\mathbf{k},q)d\mathbf{k}\ , \tag{3}$$

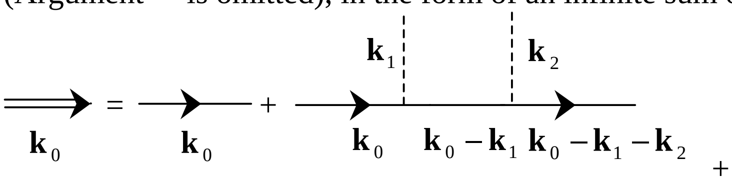
where P_0 is defined by $P_0(k_0, q) = \frac{1}{\left(q + D_0 k_0^2\right)}$. Moreover, we have set $\tilde{\eta}(\mathbf{k}) = -D_0 \eta(\mathbf{k})$, with , $k_0 = |\mathbf{k}|$ and $\phi(\mathbf{k}_0)$ is the Fourier image of the initial concentration $\phi(\mathbf{r}_0) = u(\mathbf{r}, \mathbf{0})$.

The graphical representation of (3) is:



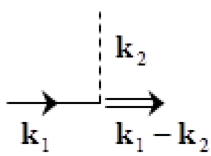
which gives the solution to (4.3) for $u(\mathbf{k}_0)$ represented by 

(Argument q is omitted), in the form of an infinite sum of diagrams



(4)

according to the rules, sated in [2, 3]:

- each single horizontal line  marked $\mathbf{k}$, corresponds to the value $P_0(k)$;
- each vertical line , marked by wave number $\mathbf{k}$, corresponds to multiplier $\tilde{\eta}(\mathbf{k})$;
- each three lines vertex of the form 

corresponds the scalar product

  $\mathbf{k}_2(\mathbf{k}_1 - \mathbf{k}_2)$
- each horizontal line, marked by $\mathbf{k}$, and leaving a three-lines vertex carries multiplier $\varphi(\mathbf{k})$
- each vertical line bearing wave vector $\mathbf{k}$ carries integration over R^3 with respect to $\mathbf{k}$.

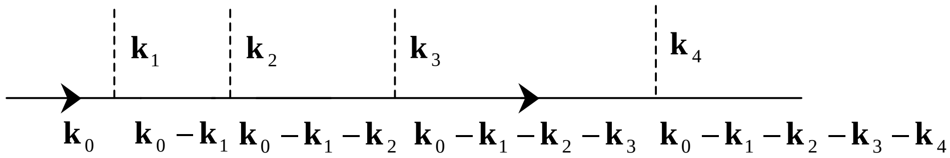
We are interested in the evolution of the concentration, on a large scale, so (4) ought to be averaged over realizations of random field $\tilde{\eta}(\mathbf{r})$ (or $\tilde{\eta}(\mathbf{k})$). We will assume, that $\tilde{\eta}(\mathbf{r})$ is a homogeneous and isotropic normal random field with zero mean and correlation function $\psi_{\tilde{\eta}}(\mathbf{r}_2 - \mathbf{r}_1) = \langle \tilde{\eta}(\mathbf{r}_2)\tilde{\eta}(\mathbf{r}_1) \rangle$. Then, in wave vector $\mathbf{k}$ - representation, we have

$$\langle \tilde{\eta}(\mathbf{k}_1)\tilde{\eta}(\mathbf{k}_2) \rangle = \psi_{\tilde{\eta}}(\mathbf{k}_1)\delta(\mathbf{k}_1 - \mathbf{k}_2), \text{ where } \psi(\mathbf{k}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \psi(\mathbf{r}) e^{-i\mathbf{kr}} d\mathbf{r} \quad (5)$$

Under these assumptions, the averaged equation (4) will only include diagrams with even numbers of vertices. Using fourth-order diagram for the case, let us examine in details the diagrams transformation for (4.4) after averaging. Because random field $\tilde{\eta}$ is normal and homogeneous, we have, according to (5):

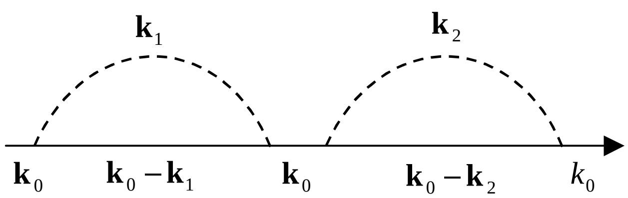
$$\begin{aligned}\langle \tilde{\eta}(\mathbf{k}_1)\tilde{\eta}(\mathbf{k}_2)\tilde{\eta}(\mathbf{k}_3)\tilde{\eta}(\mathbf{k}_4) \rangle = {} & \psi_{\tilde{\eta}}(\mathbf{k}_1)\psi_{\tilde{\eta}}(\mathbf{k}_3)\delta(\mathbf{k}_1 + \mathbf{k}_2)\delta(\mathbf{k}_3 + \mathbf{k}_4) + \\ & + \psi_{\tilde{\eta}}(\mathbf{k}_1)\psi_{\tilde{\eta}}(\mathbf{k}_2)\delta(\mathbf{k}_1 + \mathbf{k}_4)\delta(\mathbf{k}_2 + \mathbf{k}_3) + \\ & + \psi_{\tilde{\eta}}(\mathbf{k}_1)\psi_{\tilde{\eta}}(\mathbf{k}_4)\delta(\mathbf{k}_1 + \mathbf{k}_3)\delta(\mathbf{k}_2 + \mathbf{k}_4)\end{aligned} \quad (6)$$

Therefore, after averaging the diagram

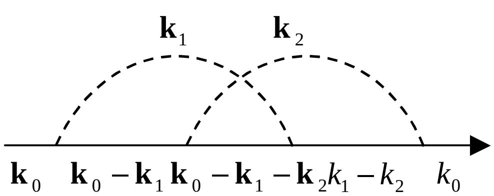


(7)

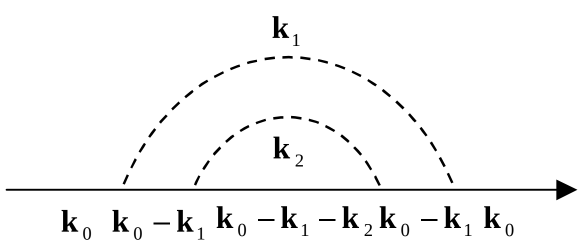
turns into the sum of A, B and C, defined as follows:



for A

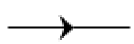
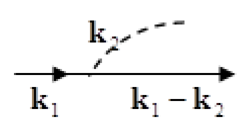


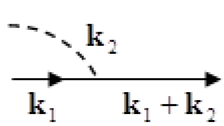
for B (8)



for C.

All this means that it necessary to connect by all possible means vertical lines pairs in initial diagram, so that to turn them into arcs with the same wave vector $\mathbf{k}$. After averaging incoming and leaving horizontal lines have the same vector $\mathbf{k}_0$. For our 3D case, the rules defining averaged diagrams (8) are such:

- each arc, marked $\mathbf{k}$ corresponds to multiplier $\psi_{\tilde{\eta}}(\mathbf{k})$;
- each horizontal line , marked $\mathbf{k}$, corresponds multiplier $P_0(\boldsymbol{k})$.
- for crossing from right to left over vertex 

for horizontal line, right from vertex there corresponds wave vector $(\mathbf{k}_1 - \mathbf{k}_2)$. Vertex itself corresponds factor $\mathbf{k}_2(\mathbf{k}_1 - \mathbf{k}_2)$;
- for crossing from left to right vertex 

, leaving horizontal line carries wave vector $(\mathbf{k}_1 + \mathbf{k}_2)$. Vertex itself corresponds factor $(-1)\mathbf{k}_2(\mathbf{k}_1 + \mathbf{k}_2)$.
- integration is held over all arc vectors.

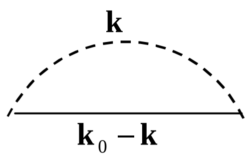
When all rules for diagrams are formulated for the three-dimensional, we can use the corresponding results. Summation results for all possible diagrams can be expressed via the sum of irreducible diagrams, that is the diagrams that split into sub diagrams separated by horizontal lines with wave vector $\mathbf{k}_0$, not being surrounded by any dashed bended line. If we denote by Σ^i the sum of all those irreducible diagrams, then we can derive in $(\mathbf{k},q)$ - representation the following equation, which is the three-dimensional

$$\left(P_0^{-1}-\Sigma^i\right)\left\langle u(\mathbf{k}_0,q)\right\rangle=\varphi(\mathbf{k}_0), \tag{9}$$

which brings the formal solution of our task.

3. Small Fluctuation. Fractional Equation

Herewe will examine the case when the amplitude of the fluctuations of random field η is small $(a_0^2<<1)$. Then, Σ^i is dominated by the first irreducible diagram with $\psi_{\tilde{\eta}}(\mathbf{k})$ in the first degree:

$\Sigma^i=$ 

$$-\int_{-\infty}^{\infty}\frac{\left(\mathbf{k}_0\cdot\mathbf{k}\right)\cdot\left(\mathbf{k}\cdot(\mathbf{k}_0-\mathbf{k})\right)}{q+D_0(\mathbf{k}_0-\mathbf{k})^2}\psi_{\tilde{\eta}}(\mathbf{k})d\mathbf{k} \tag{10}$$

If we assume that process η is isotropic, then $\hat{\psi}_{\tilde{\eta}}(\mathbf{k})$ in a function of the modulus k of $\mathbf{k}$. Setting θ for the angle between wave-vectors $\mathbf{k}_0$ and $\mathbf{k}$, and k_0 for the modulus of vector $\mathbf{k}_0$ while for $\mathbf{k}$ it is kk_0, also setting $q=D_0Qk_0{}^2$, the integral on the right-hand side of (10) is $2\pi k_0^5D_0^{-1}\int_0^{\infty}\int_0^{\pi}k^4\dfrac{\cos\theta-k}{Q+1+k^2-2k\cos\theta}\cos\theta\sin\theta d\theta\psi_{\tilde{\eta}}(k_0k)dk$. Upon integration with respect to angle θ, we obtain

$$-\Sigma^i=2\pi D^{-1}{}_0k_0^5\left[\int_0^{\infty}\left(\frac{k^2(k^2-Q-1)}{2}+\frac{k\left[k^4-(Q+1)^2\right]}{8}\cdot\ln\frac{Q+(k-1)^2}{Q+(k+1)^2}\right)\hat{\psi}_{\tilde{\eta}}(k_0k)dk\right] \tag{11}$$

The one-dimensional case could be worked out with more or less general assumptions, concerning the correlation function $\psi_{\tilde{\eta}}(\mathbf{r})$ (here in wave vector representation) of process η. There is some hope to arrive at similar conclusions in the three-dimensional case. Nevertheless, the task is more complex, and we only could obtain Σ^i from two different correlation functions, which are proportional to

$e^{-\frac{r}{l}}(1+\frac{r}{l})$ and $e^{-(\frac{r}{l})^2}$.

Here l is the correlation length of process η, and r denotes $|\mathbf{r}|$. Since we look at what happens when l tends to zero when k_0 and q are fixed, we set $L=lk_0$. In can be derived, that, with the above correlation functions, the leading terms in the expansion of $-\Sigma^i$ with respect to L are of the form

$$-\Sigma^i=D_0(-k_0^2\frac{a_0^2}{l}\nu_2+k_0^2a_0^2lq^{3/2}\nu_1)+... \tag{12}$$

with positively valued ν_1 and ν_2 when the Fourier transform of the correlation function $\psi_{\tilde{\eta}}(\mathbf{r})$ is $\hat{\psi}_{\tilde{\eta}}(\mathbf{k})=\dfrac{la_0^2D_0^2}{(1+k^2l^2)^3}$ or $\hat{\psi}_{\tilde{\eta}}(k)=lD_0^2a_0^2e^{-l^2k^2}$. Hence $\langle u\rangle$ satisfies

$$\frac{\partial\langle u\rangle}{\partial t}-D_0{}'\nabla^2\langle u\rangle+\chi\left(D_t^{3/2}\right)\nabla^2\langle u\rangle=0 \tag{13}$$

When a_0^2/l^2 is small, D_0' is just smaller than D_0 and χ is small ($D_0' = D_0(1-\nu_2 a_0^2 L l^2)$ and $\chi = a_0^2 l\ \nu_1 D_0$). Hence (13) rules the evolution on the macroscopic scale of the concentration of solute in a tree-dimensional porous medium whose porosity is the exponential of a Gaussian process.

4. Anomalous Diffusion

As we noticed before for usual media, stratum particle displacement media is proportional to t. This is not so for random media. It is known that for a special class of one-dimensional problems there exists finite time intervals, during transients, such that stratum particle displacement is not proportional to t. In this section, we will see that this also happens for (13).

Concentration function $\langle u \rangle$, being the solution to (13) under initial condition $\phi(\mathbf{r}) = \delta(\mathbf{r})$, can be interpreted as being the probability distribution density of finding in point $\mathbf{r}$ and at time t a particle that was in the origin for $t=0$. Let us denote it as being the density function $\rho(\mathbf{r},t)$.

In $(\mathbf{k},q)$ - representation the solution of (13) which corresponds to the initial condition $\phi(\mathbf{k}_0) = \frac{1}{(2\pi)^3}$ is as follows:

$$\rho(\mathbf{k}_0,q) = \frac{1}{(2\pi)^3}\cdot\frac{1}{q + D_0 k_0^2 F(q)}, \tag{14}$$

with $F(q) = 1 + \chi q^{3/2}$.

Backwards three-dimensional Fourier transform gives:

$$\rho(\mathbf{r},q) = \frac{1}{4\pi r D_0 F}\cdot\exp\left\{-r\sqrt{\frac{q}{D_0 F}}\right\},$$

from which the density function $\rho(r,q)$ over $r = |\mathbf{r}|$ is:

$$\rho(r,q) = \frac{r}{D_0 F}\cdot\exp\left\{-r\sqrt{\frac{q}{D_0 F}}\right\}. \tag{15}$$

With the help of (15) the mean displacement for $\overline{r^2}(q)$ as the function of Laplace parameter q is:

$$\overline{r^2}(q) = \int_0^\infty r^2 \rho(r,q)\,dr = 6D_0\frac{F(q)}{q^2} \tag{16}$$

By substituting the above expression for $F(q)$ into (16) and after backward Laplace transforms, we obtain that $\overline{r^2}$ is the following time function:

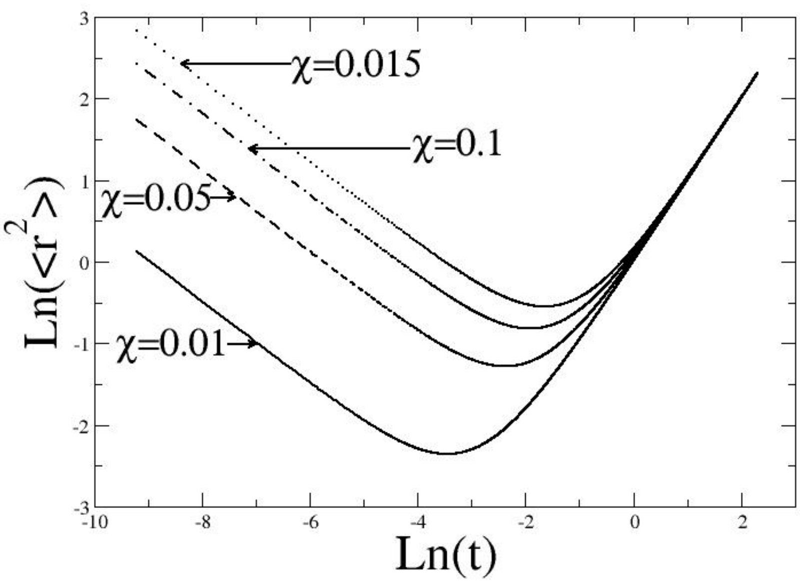
$$\overline{r^2} = 6D_0(t + \chi t^{-1/2}\pi^{-1/2}), \tag{17}$$

The above expression is valid for all time values. As it follows from (17) that if the correlation length (or equivalently χ) $\left(\tau = \frac{l^2}{D_0}\right)$ is zero, then we have the renormalization of diffusion coefficient. When l is different from zero, the figure 1 shows that during transients the mean square displacement is not proportional to t, and that it even does diverge in the limit $t \to 0+$. After some time, it finally becomes proportional to t.

Together with mean displacement coefficient, let us insert also the differential diffusion coefficient $D = \frac{1}{6}\frac{d\,\overline{r^2}}{dt}$. We obtain

$$\frac{D}{D_0} = 1 - \frac{\chi}{\pi^{1/2}} t^{-3/2} \tag{18}$$

Figure 1: The mean square displacement as a function of time, in logarithmic coordinates, for various values of χ with $D' = 0$



6. Summary and Concluding Remarks

Here we have presented a three-dimensional diffusion problem for random force field with normal stochasticity potential function.

1. For averaged concentration diffusion process diagrammatic technique was developed in analogy with the stationary case. Equation (9) was derived for $\langle u(\mathbf{k}_0, q)\rangle$. Assuming that heterogeneities correspond to small but disordered fluctuations led us to an expression in closed form for $\langle u(\mathbf{k}_0, q)\rangle$. From the latter we derived the integro-differential equation (16) for the evolution of the macroscopic concentration, over scales large compared with the length characterizing the randomness of the medium. This equation is valid for any times, and includes a fractional operator of order $3/2$, combined with the Laplacian.
2. Anomalous diffusion effect was found to take place during transients, but to disappear after some time.

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