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Disordered Structures Models for Heterogeneous Media

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Abstract

In this study we investigate the number of models for approach definition of disordered structures for heterogeneous media. The problem of definition equations is discussed. The survey of approaches is presented.

Keywords: Diffusion, Porous Media, Fractional Equations.

1. Introduction

Nowadays the interest to the study of disordered structures has drastically increased. Disordered structures include heterogeneous media with random (or periodical) positioning of different phases, amorphous and composite materials, alloyed semiconductors, liquid-metal solutions, water-bearing grounds etc. The investigation of disordered systems is stimulated by wide applications of such materials in different engineering areas ranging from microelectronics (when developing setups and devices with unusual physical properties) to agriculture (when it becomes necessary to take into account the distribution of fertilizers in various grounds). Here we face quite natural problems such as electron motion in a random electromagnetic field, diffusion and conductivity processes, water penetration and filtering, contaminant spreading and so on.

Fractal geometry, first introduced by V. Mandelbrot [1, 2], has been widely used for to describe disordered media. Indeed, fractal structure is characteristic of many physical phenomena. In addition, regular fractal objects (lines, surfaces, etc.) are characterized by invariance with respect to scale transformations [3, 4]. Regular fractal objects include, for example, a Koch curve [5], plotted in 1904. It is essential that the fractal dimension of objects may differ from the topological dimension. Thus, the fractal dimension of a broken curve (based on V. Mandelbrot definition) is equal to $d_f = -\lim\limits_{a\to 0}\frac{\ln N}{\ln a}$ where N in the curve length measured with an a-scale ruler. For a Koch curve, we have $d_f = \frac{\ln 4}{\ln 3} \approx 1.26$ while the topological dimension of any line is equal to a unit. The fact that the fractal dimension of a medium differs from the topological one results in a number of unusual physical consequences. Thus, if we consider the task of random wandering along a Koch curve (and, as a result, the problem of diffusion) then the mean squared displacement $\overline{x^2}$ of particles during the time t [6] is proportional to t^{1/d_f}, i.e. anomalous diffusion takes place.

In usual (non-fractal, homogenous) media $\overline{x^2} \sim t$ and thus, the diffusion coefficient that is defined as $\overline{x^2}/t$, is constant. For a general case, the critical index θ of anomalous diffusion is defined using the relation $\overline{x^2} = t^{\frac{2}{2+\theta}}$ [7]. For ordinary media $\theta = 0$. In the case of wandering along a Koch curve, we have $\theta = 2(d_f - 1) \sim 0.52$. In other cases, relations between the critical index and the fractional dimension of a medium are not as simple as that. The transfer of particles in regular fractal media turns out to be described by equations that include members with fractional [8] derivatives over time [9, 10]. These fractional derivatives formally describe the above-mentioned anomalous diffusion.

Along with purely fractal media, where random wandering of particles takes place along self-similar lines, there is a wide class of media where particle transfer processes are characterized by random media characteristics. E.g., in porous media a carrier that includes so-called grains of a matter chaotically distributed in space transports particles. As a result, the effective diffusion coefficient depends on the concentration of these grains. Here we face the problem of particle diffusion for a case when the diffusion coefficient (or, for some cases, the coefficient of conductance) is a random quantity [11, 12] with assigned stochastic properties. The present work investigates media whose parameters are random functions. Moreover, when we consider the process of particle transfer in those media, we face a number of problems.

2. Definition equations

Firstly, it is necessary to formulate properly the transfer equation taking into account the properties of the medium at hand. A model is necessary for that. A method, allowing dealing with the evolution of some physical quantity in a heterogeneous medium, consists in taking the partial differential equation, which holds in a homogeneous subset, then letting a coefficient, connected with a physical property, be a stochastic process. For each realization of the process, we thus have a “small scale” equation, which we hope to give a well-posed problem. Then, we average the solution with respect to the sample paths of the process, and we take the result for the macroscopic version of the studied quantity. The method was used in [13, 14] for the spreading of matter in heterogeneous porous media. This way of thinking can be considered as being a kind of ergodic hypothesis. In general, many coefficients depending on the location are present in a partial differential equation like the one, describing classical diffusion (of matter or heat) or for electromagnetic problems. The coefficient(s), we choose to replace by a sample stochastic process may or may not allow for a correct description of the medium at hand.

3. Small scale models

The small-scale diffusion equation given in [15] takes into account the dependency of the effective diffusion coefficient on the random concentration of grains, representing solid obstacles, more or less spherical, and constituting the solid matrix of a particular kind of porous media. It essentially differs from the equations given in [13, 14]. Different hypotheses for the structure of the medium correspond to different small-scale models [16-17]. The above evocated averaging method then yields different equations for the evolution of the average unknown, hence to different macroscopic models. As a result, the solutions of these equations behave differently.

There is another problem however. As the equation of impurity particle transfer includes some random parameters, the concentration of these particles, being the solution of the equation with random quantities (e.g. with random diffusion coefficients) is also a random function which itself depends on these parameters. As a rule, we are interested in averaged characteristics of the system, in particular, in the mean concentration. Averaging solutions to Cauchy problems based upon small-scale models may result in an endless chain of connected equations for mean values of functional concentration derivatives over random medium parameters [16]. The average also solves a fixed-point problem, whose solution is captured via an asymptotic expansion.

Several ways help solving such a closure problem. They mix physical and mathematical arguments, in general involving expansions at higher and higher orders, which we have to stop at some point. An endless chain of connected equations for mean values of functional concentration derivatives over random medium parameters [16]. In some situations, both points of view are equivalent, sometimes one of them is found to be more efficient.

In [16] the author indicates how to break this chain and get a closed system of equations. This regular procedure allows at least solving the problem of particle transport in random media with arbitrary accuracy. Another method allowing solving the problem of particle transport is the method of expansion of mean concentration in series over correlation functions of all orders. This procedure, developed in [11] and applied in [17] to porous media and, as a consequence, to other equations is also regular and allows to get the solution with required accuracy. Besides, it is shown in [17] that when summing up a certain class of diagrams, we can get the same equations and, as a result, the same solutions as those in the method of functional derivatives. Of course, there are other methods of getting a closed system of equations. Take, for example, the procedure described in [14]. However, this method is not regular and it is rather difficult to estimate the accuracy of the results obtained. Besides, the method in question is applicable only to a special class of random fields, namely to a telegraph random field [18] characterized by Poisson Law of polarity inversion. After we get a closed system of equations using this or that method, it is necessary to analyze it, which is not that simple, but realizable.

It is worth noting one more problem. The majority of publications (if not to say all) consider the physical aspect of the problem leaving apart the mathematical basis of the results obtained. The papers [19, 20, 21] proves the existence of the solution for a certain type class of equations.

The fact, that particle diffusion in random media (i.e. in media with random parameters) under quite reasonable assumptions is described by equations with fractional derivatives, turned out to be nontrivial. Moreover, here no initial geometrical assumptions on fractal dimensionality of paths along which the particles are randomly wandering are made. Only stochastic properties of the medium parameters e.g. the diffusion coefficient, are supposed to be assigned. Equation members with fractal derivatives over time lead to effects similar to those characteristic for transfer in a purely fractal medium. In particular, it concerns the effect of a slow or anomalous diffusion mentioned above. In connection with it, they sometimes speak about a random fractal medium. However, stochastic properties of a random medium can be only conditionally associated with its fractional dimensionality.

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Mathematical models for solute transport were initially based on the simplified assumptions of linear and instantaneous sorption in homogeneous media. However these models don't succeed in describing solute transport observed in. Save to Library. by Philippe Davy.Â Enhanced understanding of light non-aqueous phase liquid (LNAPL) infiltration into heterogeneous porous media is important for the effective design of remediation strategies. We used a 2-D experimental facility that allows for visual observation of LNAPL contours in order to study LNAPL redistribution in a layered porous medium. The heterogeneous autoregressive (HAR) models of high-frequency realized volatility are inspired by the Heterogeneous Market Hypothesis and incorporate daily, weekly and monthly realized volatilities in the volatility dynamics with a (1,5,22) time horizon structure. We build on the HAR models and propose a new framework, adaptive heterogeneous autoregressive (AHAR) models, whose time horizon structures are optimized by a genetic algorithm.Â Hui Qu, Ping Ji, "Adaptive Heterogeneous Autoregressive Models of Realized Volatility Based on a Genetic Algorithm", Abstract and Applied Analysis, vol. 2014, Article ID 943041, 8 pages, 2014. https://doi.org/10.1155/2014/943041. Show citation. Disordered media is the term used to denote media composed of a random agglomeration of at least two types of material. Examples include alloys, discontinuous deposits of metallic films, diluted magnetic materials, polymer gels, and general composite materials. This section will present percolation as a theoretical model, and describe experimental studies on evaporated films which, due to their two-dimensional nature, lend themselves to analysis. The study of other disordered materials such as alloys or composites is found in Chap. 5 on transport in heterogeneous media. 3.1.1 A model: percolat...Â Examples include: heterogeneous conductors, diffusion in disordered media, forest fires, etc. In Table I below, extracted from Zallen (1983), we give a partial list of its applications.