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Towards the modeling of impurity migration in a heterogeneous media

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One of the primary tasks of ensuring the safety of objects in contact with polluting objects (for example, radiation waste) is to assess the risks associated with the possible spread of impurities over long distances. Experiments that were carried out on a real natural scale, in which the migration of an impurity injected into a layer including a network of migration channels was studied under natural conditions, showed that in such heterogeneous media, the tracer concentration profiles are significantly asymmetric. In particular, they have an asymmetry strongly shifted towards the flow, in which the decrease in the impurity concentration does not correspond to the classical Fickian law of molecular diffusion and occurs not according to an exponential law, but rather according to a power law [1,2]. Such an anomalous nature of the dispersion of impurities (for example, radionuclides or other polluting components, such as heavy metal atoms) during natural filtration in highly heterogeneous layers is dangerous due to the possibility of their migration over longer distances than follows from estimates made based on of the classical diffusion model.

Models with fractional spatial derivatives used in theoretical works to describe such experiments are, as a rule, limited to the one-dimensional case and are not directly applicable to the calculation of natural processes in three-dimensional anisotropic media. To solve this problem, a concept for using multidimensional stochastic random walk models can be proposed, including modeling Lévy flights in the space of alpha-stable random processes [3].

Alpha-stable random processes are processes characterized by infinitely divisible scenarios (trajectories), which are, in a certain sense, an attractor for all other processes.

If, for example, we consider the well-known Kolmogorov equation [4] as a control equation in the one-dimensional case for different values of the control parameter, then for some certain values of it, it reduces to the usual diffusion equation. At the same time, there is such an interval of numerical values of the control parameter in which it turns into the diffusion equation with fractional derivatives (fractional diffusion equation). And, if the process characterized by the Gaussian distribution describes a random walk of a particle that does not make long (super-diffusive) movements, then under certain conditions we obtain distributions that describe so-called "Lévy flights", which are suitable for modeling the movement of impurities through a system of channels in a given medium (matrix).

In the context described above, for the problems of parameterization of experimental measurement data, this work directly proposes a phenomenological expression for the impurity concentration function, which depends on a small number of parameters and allows the description of the migration process in both classical diffusion and large-scale (super-diffusion) modes.

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