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Transport of dense pollutants: nonlinear random walk modeling and experimental validation

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Non-Fickian transport is widespread in radionuclides and/or chemical species migration, which is key in the context of nuclear waste disposal: the contaminant spread might grow nonlinearly in time, the resulting concentration profiles displaying a non-Gaussian behavior [1]. An important source of such anomalous features is the collective motion of pollutants due to reciprocal interactions. Migration of concentrated particles usually displays these nonlinear phenomena: indeed, the motion of a single contaminant parcel depends on the density of the fluid nearby, which in turn is affected by the number of such parcels at a given position. High density gradients are encountered when either the contaminant itself is strongly concentrated at the source, or the plume flows through regions that are rich in salt; this latter case might become a major concern for radioactive waste disposal near salt domes: even modest density differences with respect to the resident fluid might sensibly affect the contaminant dynamics [2-4].

We propose a model for the concentration-dependent dynamics of a dense contaminant plume through a porous material and we explore its qualitative behavior by resorting to Monte Carlo simulation. We start by considering a vertical column filled with fully saturated and uniformly packed sand. The injected contaminant can be conceptually represented as an ensemble of fluid parcels, whose force balance is then rewritten in nonlinear stochastic Langevin form. This equation can be directly integrated by particle tracking simulation. Nonlinearities arise from the fact that both advection and dispersion of the contaminant plume are concentration-dependent, so that microscopic particles trajectories are correlated via the density field: flow and transport are coupled. The strength of nonlinear terms is controlled by a parameter ϵ that is proportional to the molar concentration C^{mol} [mol/L] of the injected solution. When C^{mol} is weak, $\epsilon \to 0$ and standard Fickian transport with uncorrelated particles paths is recovered.

We have tested the proposed random walk model on experimental measurements of dense contaminant transport obtained with the BEETI experimental device, a dichromatic X-ray source coupled with a NaI detector [5] This setup allows quantitatively assessing the contaminant concentration $c_\ell(t)$ inside a vertical 80 cm column (as a function of time), at various sections ℓ. The injected contaminant is KI and the column is filled with homogeneously mixed Fontainebleau sand. As a salient feature, contaminant profiles are sensibly skewed (depending on the flow direction) and therefore non-Gaussian. Monte Carlo estimates of concentration profiles and temporal moments have been computed and a good agreement is found between simulation results and experimental data, for both downwards and upwards injection, at various flow regimes and molar concentrations.

The proposed random walk model is admittedly simple, since the full spectrum of interactions that actually take place between the velocity and density fields [2-4] has been condensed in a single nonlinear coupling at the scale of particles trajectories. Yet, despite its simplicity, it compares well to the set of dense contaminant transport measurements.

Finally, the random walk approach has been rephrased in terms of a more general nonlinear master equation [6], thus providing a link with the Continuous Time Random Walk (CTRW) formalism [1,7]. The CTRW framework can be used to deal with heterogenous and/or unsaturated porous media and this allows extending our model, so to make predictions about pollutants behavior in such complex materials.

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