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Approximations for transport in heterogeneous media by periodic random fields, ergodicity and related topics

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It is well known that for moderate variability of flow the stochastic model for advection dominated transport in saturated aquifers can be up-scaled to a "macrodispersion" process with constant coefficients. The relevance of the macrodispersion concept for the contamination in actual aquifers is, however, still a controversal issue. Most applications of the stochastic modelling are based on a ergodic hypothesis, by virtue of which, at large times or for large initial plumes, the solute transport in any given realization of the aquifer can be described by the same macrodispersion process. To check the existence, and to quantify the approach to the ergodic behavior, we study the fluctuations from realization to realization of the effective transport coefficients and of the cross-section averaged concentration at the plume center of mass. The groundwater flow was approximated by a widely used method in large scale simulations, based on a superposition of cosine modes with randomly chosen parameters (the Kraichnan routine). The transport in single realizations of the flow was investigated by two different techniques: the explicit computation of the effective diffusion coefficients based on the first order iteration of the Langevin equation, which describes the movement of solute particles, and simulations with the "global random walk" (GRW) algorithm, which provides accurate concentration fields for the same transport problem. In the case of point-like injection, both methods indicate that the average over the ensemble of flow realizations of the longitudinal effective coefficient tends to the macrodispersion coefficient in the large time limit. The GRW simulations also show the approach of the mean concentration to the corresponding Gaussian distribution. While these results can be obtained using a moderate number of periodic modes in the Kraichnan

routine (tens to hundreds), the investigation of the sample-to-sample fluctuations of the transport parameters requires thousands of modes. Both methods show a decreasing tendency for the fluctuations of the longitudinal coefficients, which, after 4000 times the advective time scale, become smaller than 10%, when 6400 modes were used in the Kraichnan routine. The same tendency was found, with GRW, for the concentration fluctuations, which at about 2000 times the advective time scale become smaller than 1%. Therefore, we can conclude that, for point injections, the coarse-grained process (defined through cross-section averaged concentration) becomes ergodic and the macrodispersion model predicts the contamination in actual aquifers after thousands heterogeneity scales. Our study also warns against the increase, in the case of extended plumes, of the sample-to-sample fluctuations for both effective coefficients and concentrations, which has serious implications in numerical simulations of large scale transport. Another useful remark is that the average over the ensemble of flow realizations of the effective coefficients given by the Langevin iteration yields a well known approximation, often used in investigations on the pre-asymptotic behavior of transport in aquifers. The comparison with GRW simulations shows that this approximation overestimates the pre-asymptotic time behavior of the effective coefficients by 20% to 40%.