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Solute transport in geological porous media: estimation of dispersion coefficients

Fulvia Baratelli[a,b,]*, Laura Cattaneo[a], Mauro Giudici[a], Chiara Vassena[a]

[a]*Università degli Studi di Milano, Dipartimento di Scienze della Terra "A. Desio", Sezione di Geofisica, via Cicognara 7, 20129 Milano, Italy*
[b]*Università degli Studi di Milano, Dipartimento di Fisica, via Celoria 16, 20133 Milano, Italy*

Abstract

The transport of contaminants in the subsurface is controlled by the heterogeneity of the hydraulic conductivity field. In order to emphasize some basic properties of transport phenomena in alluvial aquifers, a set of numerical experiments has been conducted on three blocks of sediments representing typical features of subsurface aquifer bodies.

Keywords: contaminant transport; model calibration; ground water; porous media; hydrology.

* Corresponding author. Tel.: +39-02-503-18481; fax: +39-02-503-18489.
E-mail address: Fulvia.Baratelli@unimi.it.

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1. Main text

The distribution of hydrofacies, i.e., geological materials with definite hydrodynamic characteristics, namely hydraulic conductivity (*K*) values, controls ground water flow and solute transport. In particular the presence of regions characterized by high *K* induce preferential flow paths (PFP) that influence the fate of contaminants in the subsurface and prevent the application of the classical Fickian approach.

These properties have been studied with numerical transport experiments on three blocks of alluvial sediments from the Ticino basin (Northern Italy), described by Zappa et al. (2006). The volume of each block is about 6 m^3 and a value of *K* is assigned to each cubic voxel (side-length equal to 2 cm) according to the corresponding hydrofacies. Flow modeling was conducted with a conservative finite difference scheme and convective transport with particle tracking (Vassena et al., 2007). The numerical experiments simulate the evolution of a tracer plume which is instantaneously injected through the incoming face and travels along a longitudinal average flow bounded by lateral no flow boundaries.

The interpretation of the results is conducted by fitting the outcomes of the numerical experiments with those obtained from the analytical solution of the 1D convective-dispersive equation, through the calibration of the Darcy's velocity (q) and the dispersion coefficient (D). Two sets of objective functions are considered: the χ^2 misfit of the cumulative breakthrough curve (BTC) and the sum of the relative errors for the zeroth, first and second order temporal moments of the BTC.

The results show some discrepancies between the fitted and the "experimental" cumulative BTC due to the presence of PFPs, whose effects could be taken into account if a dual porous medium (DPM) is considered. In particular the DPM domain is modeled as the superposition of two porous media, characterised by high and low conductivity. Most of the existing DPM models neglect the flow rate in the low *K* porous medium and include a possibly linear mixing between the two media: see, e.g., the reviews in Gerke and van Genuchten (1993) and Feehley et al. (2000). Here the flow in the low *K* porous medium is taken into account, but mixing is neglected.

The search for the optimal values of q and D is conducted with the Levenberg-Marquardt algorithm (Press et al., 1992), and is supported by the analysis of the uniqueness of the inverse problem, in order to assess the uncertainty on the identified values. This is crucial for the DPM approach, since five parameters have to be calibrated (the Darcy's velocities and the dispersion coefficients for both media and the fraction of solute mass traveling in the high *K* medium).

The tests show that the DPM model permits to improve the fit of the cumulative BTC, particularly for those blocks where PFP are more evident. Furthermore the DPM model reduces the differences between the temporal moments of the BTC computed from the analytical solution and from the numerical experiment data.

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