Upscaling retardation factors in 2-D porous media

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Abstract Even under the simple linear isotherm adsorption model, the parameters controlling adsorption under field conditions are frequently approximated by the values derived from batch experiments. First, the measurement scale and conditions are very different from those at the model scale. Second, the parameters are heterogeneous in space and, at most, there is some information about them at a few locations within an aquifer. For these two reasons, there is a need to consider how to treat the heterogeneity of the parameters that control adsorption, i.e. the retardation factor or distribution coefficient, and a need to establish upscaling rules to transfer the information about parameters at the measurement scale to those at the scale of model grid blocks. This paper presents some best upscaling rules for the distribution coefficient accounting for different heterogeneous structures for both the hydraulic conductivity and the distribution coefficient. Exhaustive numerical simulations are carried out by combining different heterogeneity patterns of the hydraulic conductivity and the distribution coefficient, the cross-correlation between them, overall degree of variability, and time dependence. It is demonstrated that under certain conditions, e.g. large variances and small correlation lengths of hydraulic conductivity $\ln K(\mathbf{x})$ and distribution coefficient $\ln K_d(\mathbf{x})$, the geometric mean is a good approximation for the upscaled retardation factor.

Keywords distribution coefficient; geometric mean; retardation factor; rules; upscaling

INTRODUCTION

Sorption processes occurring during radionuclide transport in the groundwater system can greatly modify the travel times of dissolved contaminants and, consequently, constitute an important factor regarding the long-term safety assessment of deep geological disposal of high activity and long-life radioactive waste. The conceptual model of sorption relies on the distribution coefficient, which defines the distribution of solute mass between the solid and liquid phases. Since hydrocarbons tend to sorb onto the solid grains by sorption processes, sorption causes solute retention which is of special importance in the context of the natural attenuation of contaminants from hydrocarbon releases; for instance, as a consequence of sorption, most spills of hydrocarbons from underground tanks go unnoticed as contaminant plumes can not travel much away from the release location.

Sorption is also especially important in the design of deep geological underground repositories for the disposal of radionuclide wastes, since proper modelling of the sorption processes can make the difference between acceptance and rejection of a given field site. In all cases, the numerical models used for the spatio-temporal prediction of solute migration use a discretization of the space with blocks much larger than the samples taken to the laboratory to determine distribution coefficients. At the same time, the distribution coefficient is not homogeneous in space. For these two reasons: the disparity of scales between measurements and modelling, and the spatial heterogeneity, it is necessary to derive some upscaling rules that will allow definition of equivalent distribution coefficients or retardation factors over areas compatible with the size of the numerical model blocks in a manner such that the behaviour of the model is, in some average terms, similar to that of the real, heterogeneous, and sparsely sampled aquifer.

This paper builds up these rules by examining some potential controlling factors for upscaling retardation factors by synthetic simulations. It combines different heterogeneity patterns of hydraulic conductivity and distribution coefficient, cross-correlation between them and the overall degree of variability. The effects of spatial variable porosity and local dispersion coefficient are also examined.

METHOD

We assume that the hydraulic conductivity (K) and the distribution coefficient (K_d) fields are log-normally distributed with the same exponential covariance function of the log values, which are modelled by joint multi-lognormal random functions. A 2-D isotropic aquifer is chosen to simulate the flow and transport of solutes. The unit-free size of domain is 200 × 200 which is discretized into 100 × 100 cells, each grid cell of size 2 × 2. Both random fields are correlated and are generated by GCOSIM3D (Gómez-Hernández & Journel, 1993). Three kinds of relationships between $\ln K(\mathbf{x})$ and $\ln K_d(\mathbf{x})$ are considered, i.e. negative-, positive-, and non-correlated.

The numerical simulations are designed with mean uniform flow conditions in a square field with prescribed heads on two opposite sides and impermeable boundaries at the other two faces. The five-point block-centred finite-difference method is employed to solve the steady-state flow problem. The imposed mean hydraulic gradient is 0.05 along the x-direction. The transport equation solver adopts a Random Walk Particle Tracking Scheme (Wen & Gómez-Hernández, 1996). For each realization of the random fields, 40 000 particles are released from the left boundary and tracked down until they exit the domain. The release source of particles covers the entire left boundary and, thus, the particles can largely sample the entire $\ln K(\mathbf{x})$ and $\ln K_d(\mathbf{x})$ fields when they move along with groundwater flow.

The main idea for calculating a block equivalent retardation factor R_V is to seek a single value, representative of the retardation factor field, $R(\mathbf{x})$, which is capable of reproducing the simulated mass flux breakthrough curve obtained for the heterogeneous media when applied to the homogeneous transport equation. Since it is impossible to find a single value to match the entire breakthrough curve, three equivalent values are separately calculated at different matching points, i.e. $R_V^{5\%}$, $R_V^{50\%}$, and $R_V^{95\%}$, which are, respectively, denoted to the early, median and late arrival time of particles. It should be emphasized that the selection of the most appropriate part of the breakthrough curve and its corresponding retardation factor is a very important step for the correct application of retardation factors in engineering environmental problems such as monitoring the extent and degree of groundwater contamination from a known source. The $R_V^{5\%}$ better reproduces the first part of the breakthrough curves and represents the fastest particles arriving at a control plane as needed for the design of a radioactive underground repository. The $R_V^{50\%}$ reproduces the median part of the breakthrough curve and reflects the portion of particles arriving at a control plane with high frequency. The $R_V^{95\%}$ reproduces the tail of the breakthrough curve and denotes the slowest particles arriving at a control plane as needed for mass removal calculations in remediation problems.

In some cases the block retardation factor is more influenced by low point values within the block domain, in other cases the high point values are more influential. The power-transform of the original variable, $R(\mathbf{x})$, allows focusing on either low or high values. Following the lines of power averaging formulae introduced for calculating the equivalent hydraulic conductivity (Journel *et al.*, 1986; Gómez-Hernández & Gorelick, 1989), we can obtain p norm distribution patterns of the block equivalent retardation factors using the following formula:

$$R_V = \left[\frac{1}{n} \sum_{i=1}^{n} R_i^p \right]^{1/p}$$

where n is the number of grid-cells or retardation factor measurements within the $R(\mathbf{x})$ random field, and $R_i(\mathbf{x})$ refers to the value of retardation factor assigned to the ith grid-cell. If $p > 1$, the equivalent retardation factor R_V is mostly influenced by larger values; if $p = 1$, the equivalent retardation factor R_V coincides with the arithmetic average and all $R_i(\mathbf{x})$ values receive equal weight; if $p = 0$, R_V corresponds to the geometric average; and if $p = -1$, R_V is equivalent to the harmonic average where R_V is mostly influenced by lower point values (Journel, 1999).

RESULTS

Effect of cross-correlation

The upscaled retardation factor is highly affected by the cross-correlation between log hydraulic conductivity and log distribution coefficient (denoted herein with the symbol ρ). For a strong negative correlation, e.g. $\rho = -0.75$, the block equivalent retardation factor for early times $R_V^{5\%}$ is smaller than the one corresponding to late time arrivals $R_V^{95\%}$, while, for a strong positive correlation, e.g. $\rho = 1$, the block equivalent retardation factor at early time is larger than those associated with late arrival times (Fig. 1). It is also noted that for a weak negative correlation, e.g. $\rho = -0.25$, the block retardation factor shares the same trend as for strong negative correlation coefficients.

The block R_V value based on the front of the breakthrough curve and its analogous value for the tail of the breakthrough curve, are remarkably different due to the time-dependence of retardation factors. This implies that an upscaling scheme should be adjusted to the specific engineering aim. For example, the p norm estimation for a goal of removing contaminants should be larger than the one required for monitoring the

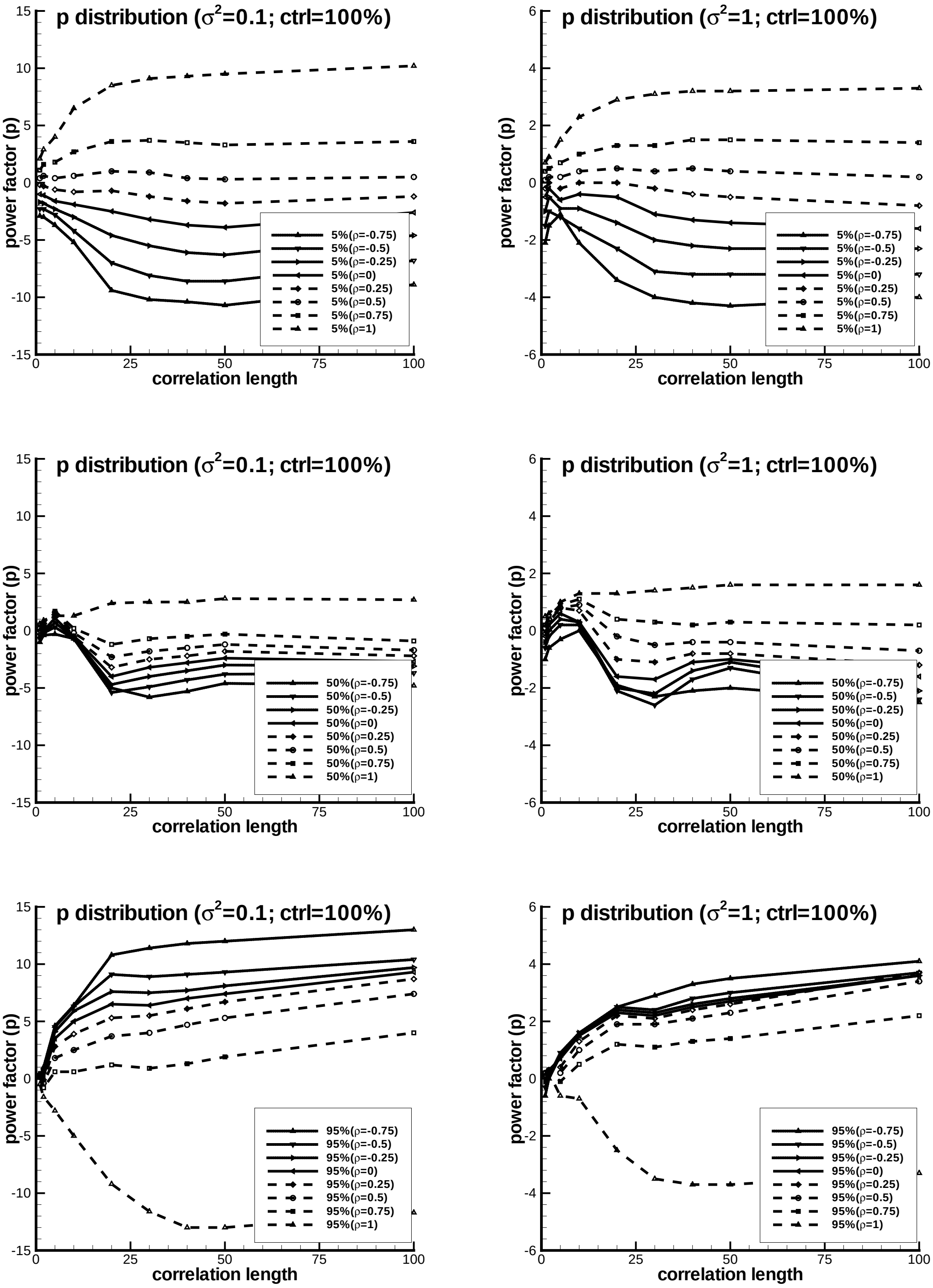

Fig. 1 Effect of cross-correlation and correlation length of both ln$K$(**x**) and lnK_d(**x**) on the upscaled retardation factor. The left column shows the p distribution of a smaller variance (σ^2 = 0.1) and the right column shows that of a larger variance (σ^2 = 1). The first row shows the p distribution of early arrival particles (5%), the second row shows that of median arrival particles (50%), and the third shows that of late arrival particles (95%). The cross-correlation coefficient ρ shown in each of the graphs ranges from –0.75 to 1. The correlation length of both ln$K$ and lnK_d(**x**) ranges from 1 grid-cell to 100 grid-cells as shown in the x axis.

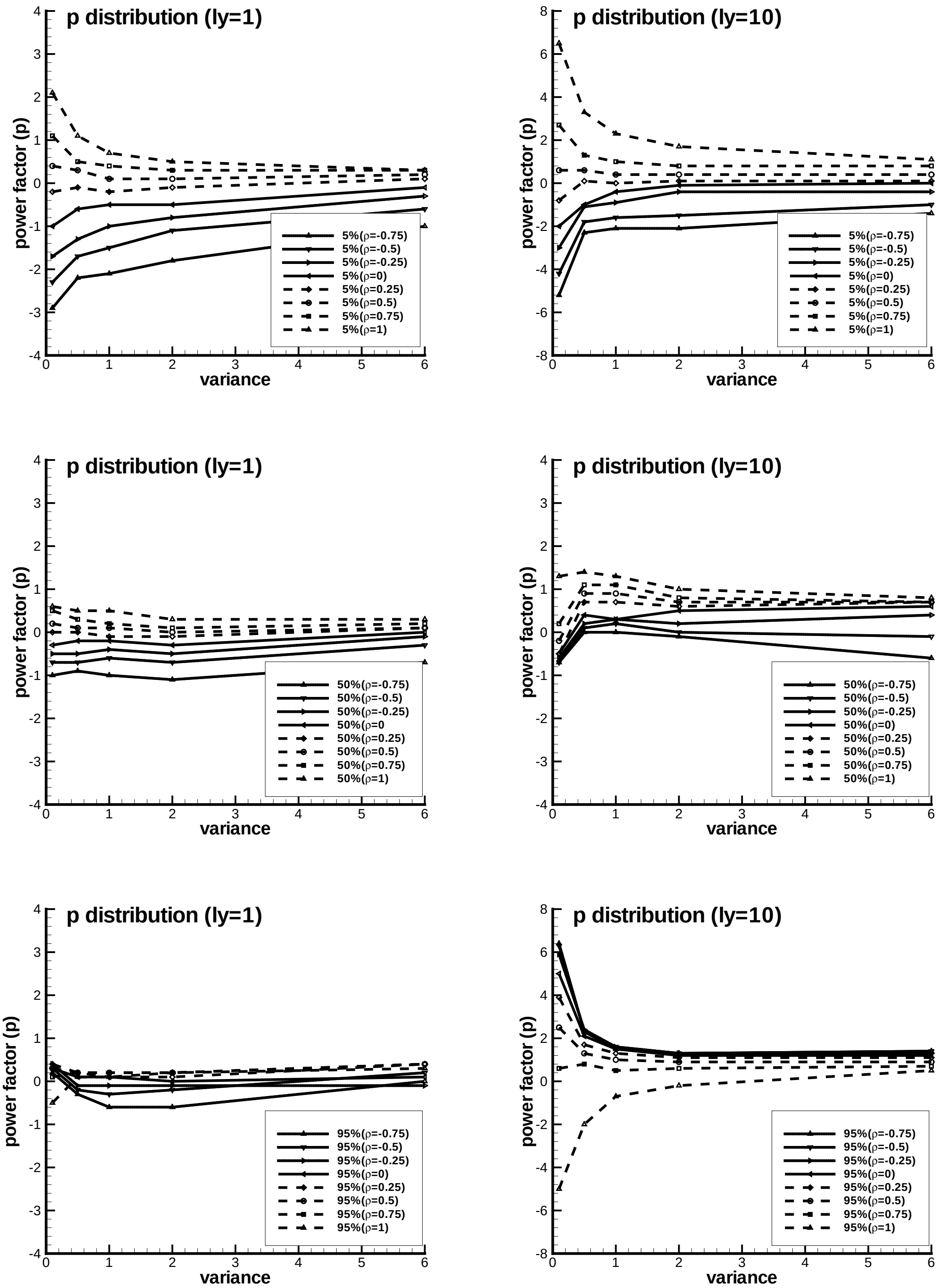

Fig. 2 Effect of variance of both ln$K$(**x**) and lnK_d(**x**) on the upscaled retardation factor. The left column shows the p distribution of a smaller correlation length (ly = 1 grid-cell) and the right one shows that of a larger correlation length (ly = 10 grid-cells). The first row shows the p distribution of early arrival particles (5%), the second row shows that of median arrival particles (50%), and the third shows that of late arrival particles (95%). The cross-correlation coefficient ρ shown in each of the pictures ranges from –0.75 to 1. The variance σ^2 ranges from 0.1 to 6 as shown in the x axis.

earliest arrival of contaminants if a negative correlation between hydraulic conductivity and distribution coefficient is observed at the field scale. Otherwise, if the correlation coefficient is positive, the former should be smaller than the latter.

Effect of correlation length

Figure 1 shows that the power factor p as a function of the correlation length, it is noted that R_V seems to approach to the geometric mean (p = 0), as the correlation length decreases. Thus, it is still proper to use the geometric mean as the upscaled retardation factor R_V as long as the size of the grid-block is relatively smaller than the correlation length. As a general rule, if the correlation coefficient between $\ln K(\mathbf{x})$ and $\ln R(\mathbf{x})$ is perfectly negative or positive, then R_V is, respectively, larger or smaller than the geometric mean, while for mild correlation coefficients R_V resides between both limits. There are some exceptions that may be caused by the fluctuation of the plume moments of a specific realization when we generate the hydraulic conductivity and distribution coefficient fields.

Effect of variance

As can be seen from Fig. 1, the degree of heterogeneity, i.e. the variance of both the hydraulic conductivity and the retardation factor fields, has a large influence on the block equivalent retardation factor.

Figure 2 illustrates that the block equivalent retardation factor converges to the geometric mean of the random fields as the variance increases. The pattern is more apparent as the correlation length increases. Yet, in this peculiar case, the influence has a direct relationship with the correlation coefficient between $\ln K(\mathbf{x})$ and $\ln K_d(\mathbf{x})$. For $R_V^{5\%}$, the geometric mean will overestimate the upscaled value R_V in the case of perfect negative correlation, but underestimate the upscaled value in the case of perfect positive correlation. For $R_V^{95\%}$, the effect is just the opposite; the geometric mean will underestimate the upscaled value in the case of perfect negative correlation but overestimate the upscaled value in the case of a perfect positive correlation.

CONCLUSIONS

We have conducted bidimensional reactive transport simulations in correlated $\ln K(\mathbf{x})$ and $\ln K_d(\mathbf{x})$ heterogeneous random fields to find a block equivalent retardation factor. It is shown that the upscaled retardation factor is a function of the correlation length and variance of the hydraulic conductivity and the distribution coefficient as well as cross-correlation between them. Cross-correlation plays an essential role in upscaling the retardation factor. For a negative correlation, the upscaled retardation factor at early time is smaller than that at late time; for a positive correlation, the block value at early time is larger than that at late time. The block retardation factor tends to converge to the geometric mean of a field as the variance increases, which is more apparent for larger correlation lengths. The geometric mean of the random field is a good approximation of the equivalent retardation factor under certain conditions, e.g. a short correlation length and relatively large variance. An upscaling scheme should be tailored to the specific engineering aim due to the time-dependence of retardation.

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