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Sensitivity analysis in the migration of radionuclides: differential Monte Carlo versus double randomization

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Abstract

We address in this paper the efficient estimation of sensitivity coefficients by Monte Carlo simulations. In the context of geological performance for the risk assessment of radioactive waste repositories, a recent non-analog Monte Carlo simulation [1] based on an integral equation for the transport of radionuclides in porous media is examined in the view of sensitivity analysis. Two methods are compared: Differential Monte Carlo which requires special care when the integral kernel of the integral equation vanishes; and Double Randomization technique which is used to evaluate an effective sensitivity coefficient. Numerical results illustrate the methods for radionuclide migration and focus on the fraction reaching the upper surface of the medium. © 2001 IMACS. Published by Elsevier Science B.V. All rights reserved.

Keywords: Radionuclide migration; Sensitivity analysis; Monte Carlo simulations; Contaminant transport; Hydrogeology; Porous media

1. Introduction

The uncertainty about parameters values is a subject of main concern for migration modelling in the context of the risk assessment of radioactive waste repositories in deep geological formations. Sensitivity analysis is essential for the validation of geological performance results. Combined with parameter calibration by an inverse problem it also yields a way of reducing uncertainties. In the context of Monte Carlo calculations, the straightforward perturbation approach (also called “brute force” approach) which consists of making two independent runs and then calculating the difference of the two results is very time consuming. An extremely low statistical error must indeed be achieved in the two independent runs carried out for the unperturbed and perturbed problems. Therefore, we need to implement more sophisticated methods for an accurate estimation. We study here the implementation of two methods for the evaluation of sensitivity coefficients by using a non analog Monte Carlo simulation. The first method addressed is Differential Monte Carlo which is a perturbation method based on correlated tracking [2,3].

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It is a very appealing method because it allows to estimate the sensitivity coefficients simultaneously with the concentrations by computing, during the simulation, an additional score. The second method (called here the method of sampled parameters) is based on a systematic random sampling of the value of the parameters distributed according given probability densities. The random sampling of the parameters is coupled with random walks for the transport calculations. It is not based on correlated tracking and could then be expected to yield less accurate results. One of the objectives in this paper is to investigate the capabilities of the Double Randomization method [4] in this situation. Both methods are compared. Each one is based on the same stochastic process for the construction of the particle trackings, but differs in the way these particle trackings are utilized to evaluate the sensitivity coefficients.

In the following, the sensitivity or importance coefficient S of a score J with respect to (w.r.t.) a parameter p is defined by

$$S = \frac{p}{J} \times \frac{\mathrm{d}J}{\mathrm{d}p} \tag{1}$$

This normalized quantity is only defined if J is not zero. The score J is any quantity like the activity at a point, the cumulative activity on a surface over a given period of time, etc., to be determined in the risk analysis.

2. Transport equations

We focus here on the migration of one radionuclide. The well-known advection–dispersion equation for the transport of a radionuclide in a saturated porous medium is the following partial differential equation

$$\left\{ \frac{\partial}{\partial t'}[\omega(\bar{r}')] + \bar{\nabla}_{\bar{r}'}[\bar{q}(\bar{r}')] - \bar{\nabla}_{\bar{r}'}[\bar{\bar{D}}(\bar{r}')\bar{\nabla}_{\bar{r}'}] + \lambda\omega(\bar{r}') \right\} A(\bar{r}', t') = S(\bar{r}', t') \tag{2}$$

where $\omega(\bar{r}') = \theta(\bar{r}')\, R(\bar{r}')$, with $\theta(\bar{r}')$ the porosity and $R(\bar{r}')$ the radionuclide retardation factor in the porous medium. In the advection term of Eq. (2), $\bar{q}$ is called Darcy's velocity. $\bar{\bar{D}}(\bar{r}')$ is the diffusion-dispersion tensor. The constant λ is the radioactive decay rate. Finally, $S(\bar{r}', t')$ is the independent source term. The advection–dispersion problem is a boundary value problem which can be solved by Monte Carlo methods [5]. A non-analog Monte Carlo simulation has been recently developed [1,6,7]. It is based on the construction of random walks from an integral equation obtained from Eq. (2). This integral equation is a Volterra equation of the second kind defined in a porous medium D bounded by an outer surface S

$$u_S(\bar{r})A(\bar{r}, t) = Q(\bar{r}, t) + \int_{t-T_0}^{t} \mathrm{d}t' \int_D \mathrm{d}\bar{r}'[K_D(\bar{r}', t'|\bar{r}, t) + K_S(\bar{r}', t'|\bar{r}, t)\delta_2(\bar{r}' - \bar{r}_S)]u_S(\bar{r}')A(\bar{r}', t'), \tag{3}$$

where $Q(\bar{r}, t)$ is a source term including the contributions of an independent source and the normal incoming radionuclide flux on the outer surface S. $u_S(\bar{r})$ is defined by: $u_S(\bar{r}) = 1$ if $\bar{r} \in D$ and 1/2 if $\bar{r} \in S$. The integral kernel appearing in Eq. (3) is the sum of two contributions. $K_D(\bar{r}', t'|\bar{r}, t)$ represents the contribution of particles inside the geological medium D and $K_S(\bar{r}', t'|\bar{r}, t)$ the contribution of particles on the boundary S. The expressions of these source term and integral kernels are given in previous publications [1] and reproduced in Appendix A. The random walks derived from this integral equation