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Using sparse polynomial chaos expansions for the global sensitivity analysis of groundwater lifetime expectancy in a multi-layered hydrogeological model

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ABSTRACT

The study makes use of polynomial chaos expansions to compute Sobol' indices within the frame of a global sensitivity analysis of hydro-dispersive parameters in a simplified vertical cross-section of a segment of the subsurface of the Paris Basin. Applying conservative ranges, the uncertainty in 78 input variables is propagated upon the mean lifetime expectancy of water molecules departing from a specific location within a highly confining layer situated in the middle of the model domain. Lifetime expectancy is a hydrogeological performance measure pertinent to safety analysis with respect to subsurface contaminants, such as radionuclides. The sensitivity analysis indicates that the variability in the mean lifetime expectancy can be sufficiently explained by the uncertainty in the petrofacies, *i.e.* the sets of porosity and hydraulic conductivity, of only a few layers of the model. The obtained results provide guidance regarding the uncertainty modeling in future investigations employing detailed numerical models of the subsurface of the Paris Basin. Moreover, the study demonstrates the high efficiency of sparse polynomial chaos expansions in computing Sobol' indices for high-dimensional models.

1. Introduction

With the improvement of computing power, numerical modeling has become a popular tool for understanding and predicting various kinds of subsurface processes addressed in the fields of geology and hydrogeology. However, the incomplete/imprecise knowledge of the underground system frequently compels the modeler to make a number of approximations and assumptions with regard to the geometry of geological structures, the presence of discontinuities and/or the spatial distribution of hydro-dispersive parameters in their models [1]. These uncertainties can possibly lead to large variabilities in the predictive modeling of subsurface processes and thus, it becomes of major importance to account for the aforementioned assumptions in the frame of uncertainty and sensitivity analyses. Uncertainty analysis (UA) aims at quantifying the variability of a given response of interest as a function of uncertain input factors, whereas sensitivity analysis (SA) has the purpose to identify the input factors responsible for this variability. Hence, SA determines the key variables to be described in further detail in order to reduce the uncertainty in the predictions of a model.

Methods of SA are typically classified into two categories: local SA and global SA methods. The former investigates effects of variations of the input factors in the vicinity of nominal values, whereas the latter aims at quantifying the output uncertainty due to variations in the input factors in their entire domain. Among several global SA methods proposed in the literature, of interest herein is SA with *Sobol' sensitivity indices*, which belongs to the broader class of variance-based methods [2]. These methods rely upon the decomposition of the response variance as a sum of contributions of each input factor or combinations thereof and do not assume any kind of linearity or monotonicity of the model. We note that the Fourier amplitude sensitivity test (FAST) [3,4] indices enter this class as well.

Various methods have been investigated for computing the Sobol' indices that were first defined in [5], see *e.g.* [6–10]. In these papers, Monte Carlo simulation is used as a tool to estimate these sensitivity indices. This has revealed extremely costly, although more efficient estimators have been recently proposed [11,12]. In

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the recent years, new approaches using surrogate models have been introduced in the field of global SA [13–16]. A popular method to compute the Sobol' indices, originally introduced by Sudret [17], is by post-processing the coefficients of a polynomial chaos expansion (PCE) meta-model of the response quantity of interest. PCE constitutes an efficient UA method in which the key concept is to expand the model response onto a basis made of orthogonal polynomials in the input variables. Once a PCE representation is available, the Sobol' indices can be calculated analytically with elementary operations at almost no additional computational cost. Sparse PCE make the approach even more efficient, as shown in [18].

In the frame of the stochastic modeling of subsurface flow and mass transport, PCE meta-models have proven to be comprehensive and robust tools for performing SA at low computational cost. As an example, applying a PCE-based global SA upon a fine-grid numerical model of flow and mass transport in a heterogeneous porous medium, Fajraoui et al. [19] and Younes et al. [20] established the transient effect of uncertain flow boundary conditions, hydraulic conductivities and dispersivities on solute concentrations at given observation points. Sochala and Le Maître [21] propagated uncertain soil parameters upon three different physical models of subsurface unsaturated flow. Their study proved the higher efficiency of PCE meta-models, in comparison to a classical Monte-Carlo method, for representing the variability of the output quantity at low computational cost. In the frame of radionuclide transport simulation in aquifers, Ciriello et al. [22] analyzed the statistical moments of the peak solute concentration measured at a specific location, as a function of the conductivity field, the dispersivity coefficients and the partition coefficients associated to the heterogeneous media. The comparison of the Sobol' indices obtained for various degrees of PCE meta-models showed that low-degree models can yield reliable indices while considerably reducing the computational burden. Formaggia et al. [23] used PCE-based sensitivity indices to investigate effects of uncertainty in hydrogeological variables on the evolution of a basin-scale sedimentation process. However, the various aforementioned contributions consider simplified models for the description of subsurface flow and mass transport. A detailed site characterization model was employed by Laloy et al. [24], but global SA was confined to flow processes.

In the scope of the deep geological storage of radioactive wastes, Andra (French National Radioactive Waste Management Agency) has conducted several studies to assess the potentiality of a clay-rich layer for establishing a mid to long-lived radioactive waste disposal in the subsurface of the Paris Basin. The thick impermeable layer from Callovo-Oxfordian (COX) age has been extensively studied [25–27] together with the two major limestone aquifers, in place of the Dogger and the Oxfordian sequences [28–30], encompassing the claystone formation. A recent study [31] used a high-resolution integrated Meuse/Haute-Marne hydrogeological model [32] to compute the average time for water molecules departing from a given area in the COX to reach the limits of the domain where the numerical model is defined. SA over hydro-dispersive parameters in 14 hydrogeological layers proved that the Dogger and Oxfordian limestone sequences have a large influence on the residence time of groundwater. Indeed, advection processes occurring in permeable layers strongly influence the water transit in the subsurface of the Paris Basin, in contrast to the slow-motion diffusive processes taking place in impermeable rocks.

However, the analysis of the effect of uncertainties related to other advective–dispersive parameters, such as boundary conditions, orientations and anisotropies of hydraulic conductivity tensors or magnitudes of dispersion parameters, represents a great effort that cannot be carried out with the integrated model at reasonable computational costs. Addressing the issue of performing UA with the use of high-resolution numerical models of geological reservoirs, Castellini and co-workers [33] established that numerical models built at the coarse scale, but covering a reasonable number of geological and geostatistical features, can be particularly informative in capturing the main subsurface processes at low computational costs.

The present study introduces a vertical two-dimensional multilayered hydrogeological model representing a simplification of the underground media of the Paris Basin in the vicinity of the site of Bure and does not integrate the complex geometry of the layers, neither does it include the numerous discontinuities nor heterogeneities observed in the field. It must be emphasized that this simplified model is not aimed at site characterization, but at evaluation of hydrogeological performance through SA for calibration purposes.

The main objective of the present work is to assess the effect of multiple advective–dispersive parameters on the mean lifetime expectancy (MLE) of water molecules departing from a target zone in the central layer. The MLE corresponds to the average time required for a given solute at a specific location to reach any outlet of the model domain and is a critical quantity in safety analysis dealing with subsurface contaminants such as radionuclides. This work represents a substantial complement to the study by Deman et al. [31] by encompassing a large scope of uncertain factors, which cannot be assessed using the integrated model due to the computational burden. Conservative uncertainty ranges are defined for the input factors analyzed in the frame of a SA relying on the estimation of PCE-based Sobol' indices. The sparse PCE approach was chosen because of its ability to tackle high-dimensional problems with great efficiency. The study provides recommendations for future investigations employing the high-resolution integrated Meuse/Haute-Marne hydrogeological numerical model of the Paris Basin; in particular, it identifies the sets of parameters that can be fixed to their nominal values without significantly affecting the MLE variability as well as the sets of parameters to be described in further detail.

The paper is organized as follows. The subsequent Section 2 provides a comprehensive description of the considered hydrogeological model, while Section 3 presents the concepts of SA with Sobol' indices and the computation of those indices using PCE. Section 4 includes the results of UA and SA of the model, along with interpretations accounting for the underlying physics. Finally, the conclusive Section 5 summarizes the study, highlighting the main findings of the above analyses, and provides recommendations for future investigations.

2. The numerical model

2.1. Geometry and finite element mesh

Originally inspired by the COUPLEX numerical model from Bourgeat et al. [34], the present model stands as a vertical two-dimensional (x–z) cross-section of $25{,}000 \times 1{,}040$ m representing a segment of the Paris Basin subsurface. The mesh is discretized into 5×5 m square elements with a total of 1,040,000 elements. In order to subdivide the domain into entities related to geological formations, the main features of the subsurface were extracted from the lithostratigraphic log of the deep EST433 borehole [30] in the vicinity of the experimental site of Bure (Haute-Marne, France). Therefore, the model consists of 15 hydrogeological layers characterized by tabular geometries, uniform thicknesses and homogeneous parameters. Fig. 1 summarizes the geometry of the model and gives an overview on the succession and thicknesses of layers.