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Probabilistic assessment of seawater intrusion under multiple sources of uncertainty

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ABSTRACT

Coastal aquifers are affected by seawater intrusion (SWI) on a worldwide scale. The Henry's problem has been often used as a benchmark to analyze this phenomenon. Here, we investigate the way an incomplete knowledge of the system properties impacts the assessment of global quantities (GQs) describing key characteristics of the saltwater wedge in the dispersive Henry's problem. We recast the problem in dimensionless form and consider four dimensionless quantities characterizing the SWI process, i.e., the gravity number, the permeability anisotropy ratio, and the transverse and longitudinal Péclet numbers. These quantities are affected by uncertainty due to the lack of exhaustive characterization of the subsurface. We rely on the Sobol indices to quantify the relative contribution of each of these uncertain terms to the total variance of each of the global descriptors considered. Such indices are evaluated upon representing the target GQs through a generalized Polynomial Chaos Expansion (gPCE) approximation. The latter also serves as a surrogate model of the global system behavior. It allows (a) computing and analyzing the joint and marginal probability density function (*pdf*) of each GQ in a Monte Carlo framework at an affordable computational cost, and (b) exploring the way the uncertainty associated with the prediction of these global descriptors can be reduced by conditioning of the joint *pdf* on available information. Corresponding analytical expressions of the marginal *pdfs* of the variables of interest are derived and analyzed.

1. Introduction

Saltwater intrusion (SWI) is a critical and widespread contamination problem in coastal aquifers. The complex interactions between fresh and salt water, with particular emphasis on management issues, has been the subject of active and intense research, including, e.g., a recent series of works highlighted in a special issue of Hydrogeology Journal (Special issue on: Saltwater and freshwater interactions in coastal aquifers, 2010, Vol 18, No 1).

Analytical or semi-analytical solutions of SWI problems have been mainly developed for homogeneous aquifers and consider saltwater and fresh water as immiscible fluids separated by a sharp interface (e.g. [9,6,7,32]). Within this context, Dagan and Zeitoun [13] illustrate a first attempt to analyze the effect of aquifer heterogeneity on SWI. These authors consider a vertical cross section of a confined aquifer with randomly layered permeability distribution and show that the variability of the position of the salt–fresh water interface (particularly the location of the toe) is markedly influenced by the permeability variance and integral scale. Al-Bitar and Ababou [2] adopt a vertically-integrated sharp interface approach and analyze the effects of variability of aquifer properties on the saltwater wedge through numerical simulations within horizontal two-dimensional randomly heterogeneous unconfined aquifer. Chang and Yeh [10] employ a spectral approach and determine the mean interface position and its associated variability due to heterogeneity of aquifer conductivity and to the spatial variability of recharge for an unconfined horizontal aquifer model.

A realistic approach dealing with SWI should explicitly account for the occurrence of a transition zone where variable density flow is coupled with a transport model. This coupling makes it difficult to obtain analytical solutions of SWI scenarios. Henry [21] presents a semi-analytical solution for steady-state variable density flow taking place along a two-dimensional vertical cross-section in a homogeneous isotropic coastal aquifer. Since this is the only analytical solution available, it has been widely used as a benchmark problem to SWI numerical approaches (e.g. [35,41]). Dentz et al. [14] present a methodology conducive to an analytical solution of the Henry's problem in dimensionless form. The Henry's problem has limited use in practical applications because it considers only diffusion while dispersion is not simulated. Abarca et al. [1] modified the Henry's problem upon introducing anisotropy in the

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conductivity tensor and a dispersion tensor to improve the representation of wide transition zones of the kind observed in several field sites. Held et al. [20] investigated the Henry's problem within a randomly heterogeneous aquifer. Making use of the homogenization theory, these authors found that the effective conductivity and dispersion coefficients are not affected by density effects, the effective dispersivity being close to its local counterpart. Otherwise, Kerrou and Renard [23] showed that macrodispersion coefficients differ from their local counterparts in two- and three-dimensional heterogeneous scenarios. The effect of density contrast on effective parameters has also been analyzed by Jiang et al. [22] by way of a stationary spectral approach. A discussion of current challenges in modeling density driven flows in the subsurface is offered by Werner et al. [41].

Here we consider the anisotropic dispersive Henry's problem introduced by Abarca et al. [1]. As key sources of model uncertainty we consider the following dimensionless parameters: (i) the gravity number, expressing the relative importance of buoyancy and viscous forces; (ii) the anisotropy ratio between aquifer vertical and horizontal permeabilities; (iii) the longitudinal and (iv) transverse Péclet numbers, quantifying the relative importance of the longitudinal and transverse dispersion on solute transport. These are critical in governing the general dynamics of density dependent flow and transport processes (see e.g. [1,14,25,29]). We then focus on a number of dimensionless global quantities (GQs) which are controlled by these parameters and are relevant to describe key features of the saltwater wedge and the width of the mixing zone. These global descriptors, as well as all system states such as pressure, concentration and velocity distributions within in the aquifer, are affected by uncertainty due to the lack of knowledge of the characteristic model parameters (e.g. [33]). Proper quantification of the uncertainty associated with the characterization of these GQs is of critical relevance for the management of coastal aquifers.

Propagation of model parameter uncertainty to a given quantity of interest can be quantified through a global sensitivity analysis (GSA). Here, we employ a variance-based GSA which allows assessing the relative impact of the model uncertain input parameters on the variability of model outputs [3]. We base our analysis on the Sobol indices [37], which are widely used sensitivity metrics and do not require any linearity assumptions in the underlying mathematical model of the system behavior.

Estimation of the Sobol indices is traditionally performed by Monte Carlo (MC) sampling in the uncertain parameter space. Therefore their computation can become highly demanding in terms of CPU time when the dimension of the parameters space and the degree of complexity of the problem increase. In this context, estimation of the Sobol indices is practically unfeasible in SWI problems because of the coupled nature of the flow and transport problems. We circumvent this problem upon relying on a generalized Polynomial Chaos Expansion (gPCE) approximation of the target GQs (e.g. [19,28]). This approach allows obtaining a surrogate model for a given quantity of interest and enables one to calculate the Sobol indices analytically via a straightforward post-processing analysis (e.g. [12,38]). Examples of application of this technique include the study of flow and transport in heterogeneous porous media (e.g. [26]). Formaggia et al. [17] and Porta et al. [31] demonstrate the reliability and computational efficiency of gPCE-based approaches in highly non-linear systems under the effect of mechanical and geochemical compaction processes.

The work is organized as follows. Section 2 presents the complete flow and transport mathematical model, the key dimensionless parameters governing the process and the global descriptors of interest. Section 3 is devoted to a brief description of the methodology we employ to perform GSA and to derive the gPCE surrogate model. Section 4 presents the setting analyzed and some details of the full and surrogate system models. In Section 5 we show the main results of our analysis in terms of the relative contribution of the uncertain parameters to the variance of each of the global quantities analyzed. We then study the joint and marginal probability density functions (*pdfs*) of these global quantities. We remark that these tasks are computationally unaffordable by making use of the complete system model, while they can be performed by means of the gPCE surrogate model. Moreover, our relying on the gPCE allows obtaining analytical expressions for the marginal *pdf* of the global quantities of interest.

2. Complete model and definition of the global quantities of interest

We consider the anisotropic dispersive Henry's problem introduced by Abarca et al. [1]. The setting is a modification of the original Henry's problem [21] and enables one to describe seawater intrusion in coastal aquifers in a way which renders vertical salinity distributions that mimic field evidences. Saltwater intrusion is modeled across a vertical cross-section of a homogeneous aquifer under isothermal conditions (see Fig. 1). Fluid flow is governed by the mass balance and Darcy equations, i.e.

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla\cdot(\rho\boldsymbol{q}) = 0; \quad \boldsymbol{q} = -\frac{\boldsymbol{k}}{\mu}\cdot(\nabla p + \rho g \nabla z) \tag{1}$$

where $\boldsymbol{q}$ [L T^{-1}] is specific discharge vector with components q_x and q_z respectively along x- and z-directions (see Fig. 1); $\boldsymbol{k}$ [L^2] is the homogeneous and anisotropic diagonal permeability tensor with components $k_{11} = k_x$ and $k_{22} = k_z$, respectively along directions x and z; ϕ [–] is the porosity of the medium; μ [M L^{-1} T^{-1}] and ρ [M L^{-3}] respectively are dynamic viscosity and density of the fluid; p [M L^{-1} T^{-2}] is pressure; and g [L T^{-2}] is the gravitational constant.

Solute transport is described by the advection–dispersion equation

$$\frac{\partial(\phi\rho C)}{\partial t} + \nabla\cdot(\rho C\boldsymbol{q}) - \nabla\cdot[\rho\boldsymbol{D}\cdot\nabla C] = 0 \tag{2}$$

Here C [–] is solute concentration and $\boldsymbol{D}$ [L^2 T^{-1}] is the dispersion tensor, whose entries are defined as

$$D_{xx} = \phi D_m + \left(\alpha_L\frac{q_x^2}{|\boldsymbol{q}|} + \alpha_T\frac{q_z^2}{|\boldsymbol{q}|}\right); \quad D_{zz} = \phi D_m + \left(\alpha_L\frac{q_z^2}{|\boldsymbol{q}|} + \alpha_T\frac{q_x^2}{|\boldsymbol{q}|}\right);$$
$$D_{xz} = D_{zx} = (\alpha_L - \alpha_T)\frac{q_x q_z}{|\boldsymbol{q}|} \tag{3}$$

where D_m is the molecular diffusion coefficient and α_L and α_T [L] respectively are the longitudinal and transverse dispersivity coefficients, which are considered as uniform in the system. Since molecular diffusion is commonly neglected in transport settings taking place in porous media under the conditions we consider (e.g. [16]), in the following we disregard the contribution of D_m in (3). Initial conditions corresponding to freshwater hydrostatic pressure distribution are set in the system. No-flow conditions are imposed at the bottom and top of the domain; constant freshwater influx, q_f, is prescribed along the inland boundary ($x = 0$), where $C = 0$; saltwater hydrostatic pressure distribution is imposed along the seaside boundary, $x = l$ (i.e., $p = \rho_s\ g\ (d - z)$, ρ_s being density of seawater) where the salt mass flux is set as

$$(\boldsymbol{q}C - \boldsymbol{D}\cdot\nabla C)\cdot\boldsymbol{n} = \begin{cases} q_x C & \text{if } q_x > 0 \\ q_x C_s & \text{if } q_x < 0 \end{cases} \quad x = l \tag{4}$$

$\boldsymbol{n}$ and C_s respectively being the normal vector pointing outward from the aquifer and the concentration of salt in seawater (salinity). According to (4) water entering and leaving the system has salt concentration C_s and C, respectively. Key features and limitations of this schematization are illustrated in Abarca et al. [1].