

Uncertainty analysis for seawater intrusion in fractured coastal aquifers: Effects of fracture location, aperture, density and hydrodynamic parameters

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1	Uncertainty analysis for seawater intrusion in fractured coastal aquifers:
2	Effects of fracture location, aperture, density and hydrodynamic
3	parameters
4 5	Behshad Koohbor ¹ , Marwan Fahs ^{1*} , Behzad Ataie-Ashtiani ^{2,3} , Benjamin Belfort ¹ , Craig T. Simmons ³ , Anis Younes ^{1,4,5}
6	
7 8	¹ Laboratoire d'Hydrologie et Geochemie de Strasbourg, University of Strasbourg/EOST/ENGEES, CNRS, 1 rue Blessig 67084 Strasbourg, France.
9 10	² Department of Civil Engineering, Sharif University of Technology, PO Box 11155-9313, Tehran, Iran.
11 12	³ National Centre for Groundwater Research & Training, College of Science & Engineering, Flinders University, GPO Box 2100, Adelaide, South Australia 5001, Australia.
13	⁴ IRD UMR LISAH, F-92761 Montpellier, France.
14 15	⁵ Laboratoire de Modélisation en Hydraulique et Environnement, Ecole Nationale d'Ingénieurs de Tunis, Tunisia
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21	Submitted to Journal of Hydrology: Special Issue "Improving model-data interaction in
22	Hydrogeology: Insights from different disciplines".
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25	
26	*Contact person: Marwan Fahs
27	E-mail: fahs@unistra.fr
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30 Abstract

31 In this study we use polynomial chaos expansion (PCE) to perform uncertainty analysis for 32 seawater intrusion (SWI) in fractured coastal aquifers (FCAs) which is simulated using the coupled discrete fracture network (DFN) and variable-density flow (VDF) models. The DFN-33 34 VDF model requires detailed discontinuous analysis of the fractures. In real field applications, 35 these characteristics are usually uncertain which may have a major effect on the predictive capability of the model. Thus, we perform global sensitivity analysis (GSA) to provide a 36 37 preliminary assessment on how these uncertainties can affect the model outputs. As our 38 conceptual model, we consider fractured configurations of the Henry Problem which is widely used to understand SWI processes. A finite element DFN-VDF model is developed in 39 the framework of COMSOL Multiphysics[®]. We examine the uncertainty of several SWI 40 41 metrics and salinity distribution due to the incomplete knowledge of fracture characteristics. 42 PCE is used as a surrogate model to reduce the computational burden. A new sparse PCE 43 technique is used to allow for high polynomial orders at low computational cost. The Sobol' 44 indices (SIs) are used as sensitivity measures to identify the key variables driving the model 45 outputs uncertainties. The proposed GSA methodology based on PCE and SIs is useful for 46 identifying the source of uncertainties on the model outputs with an affordable computational 47 cost and an acceptable accuracy. It shows that fracture hydraulic conductivity is the first 48 source of uncertainty on the salinity distribution. The imperfect knowledge of fracture location and density affects mainly the toe position and the total flux of saltwater entering the 49 50 aquifer. Marginal effects based on the PCE are used to understand the effects of fracture characteristics on SWI. The findings provide a technical support for monitoring, controlling 51 52 and preventing SWI in FCAs.

Keywords: Seawater intrusion, fractured coastal aquifers, uncertainty analysis, uncertain
 fracture characteristics, global sensitivity analysis, Sobol' indicies

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55 **1. Introduction**

56 Coastal aquifers (CAs) are currently in a critical situation throughout the world. These 57 aquifers are essential sources of freshwater for more than 40% of the world's population living in coastal areas [IOC/UNESCO, IMO, FAO, UNDP, 2011; Barragán and de Andrés, 58 2015]. The phenomenon of seawater intrusion (SWI), which encompasses the advancement of 59 60 saline water into fresh groundwater mainly caused by excessive groundwater extraction, is the 61 first source of contamination in CAs [Werner et al., 2013]. The European Environment 62 Agency [www.eea.europa.eu] declared SWI as a major threat for many CAs worldwide. This 63 phenomenon is exacerbated by the increasing demand for groundwater as a result of the 64 increase in population and anthropogenic activity. It is also amplified due to natural causes 65 such as climate change, Tsunami events and sea-level rise expected in the next century [e.g.,66 Ataie-Ashtiani et al., 2013; Ketabchi et al., 2016].

The impacts of local heterogeneities of CAs on the extent of SWI at the scale relevant for 67 management scenarios is well documented in the literature [e.g. Simmons et al., 2001; Kerrou 68 69 and Renard, 2010; Lu et al., 2013; Mehdizadeh et al., 2014; Pool et al., 2015; Stoeckl et al., 70 2015; Shi et al., 2018]. Fractured geology is the most challenging form of natural 71 heterogeneity. Fractures represent the preferential pathways that may enable faster SWI or 72 intensify freshwater discharge to the sea [Bear et al. 1999]. Fractured coastal aquifers (FCAs) 73 are found globally. Several examples can be found in France [Arfib and Charlier, 2016], 74 USA [Xu et al., 2018], Greece [Dokou and Karatzas, 2012], Italy [Fidelibus et al., 2011], 75 Ireland [Perriquet et al., 2014; Comte et al., 2018], UK [MacAllister et al., 2018] and in the 76 Mediterranean zone where more than 25% of CAs are typically karstic [Bakalowicz et al., 77 2008; Chen et al., 2017]. Despite the fact that FCAs are distributed throughout the world and 78 they often contain significant groundwater resources due to their high porosity, SWI in these 79 aquifers is rarely investigated and related processes are still largely unexplored and poorly

understood [Dokou and Karatzas, 2012; Sebben et al., 2015]. In the review paper of Werner
et al. [2013], the authors suggested SWI in FCAs as one of the potential remaining
challenging problems.

83 SWI can be tackled using either the sharp interface approximation or variable-density flow 84 (VDF) model [Werner et al., 2013; Llopis-Albert et al., 2016; Szymkiewicz et al., 2018]. VDF 85 model involves flow and mass transfer equations coupled by a mixture state equation 86 expressing the density in terms of salt concentration. This model is usually used in field 87 applications as it is more realistic than the sharp interface approximation and has the privilege 88 of considering the transition zone between the freshwater and saltwater, known as the mixing zone. Flow in fractured porous media can be described using three alternative approaches: i) 89 90 equivalent porous medium in which averaged estimations of the hydrogeological properties 91 over a representative elementary volume are used to represent the domain [Dietrich et al., 92 20051, ii) dual-porosity models where the domain is considered as the superposition of two 93 continuums representing, respectively, rocks and fractures [Fahs et al., 2014; Jerbi et al., 94 2017] and iii) discrete fracture model in which the fractures and matrix are handled explicitly 95 [Berre et al., 2018]. Discrete fracture model is the most accurate model because fractures are 96 considered without any simplification. It is usually used for domains with a relatively small 97 number of fractures [Hirthe and Graf, 2015; Ramasomanana et al., 2018] and has come into 98 practical use in recent years. However, discrete fracture models require enormous 99 computational time and memory due to the dense meshes resulting from the explicit discretization of the fractures. Discrete fracture network (DFN), in which the fractures are 100 101 embedded in (d-1) dimensional elements in (d) dimensional physical domain, is an alternative approximation that reduces the overhead computations of the discrete fracture model. 102

103 DFN model has been successfully coupled with VDF model to simulate SWI in FCAs. For 104 instance, *Grillo et al. [2010]*, based on a single fracture configuration of Henry Problem, 105 showed that DFN-VDF model is a valid alternative to the discrete fracture model for 106 simulating SWI. Dokou and Karatzas [2012] developed a hybrid model based on the combination of the DFN model (for main fractures and faults) and the equivalent porous 107 108 media model (for lower-order fractures) to investigate SWI in a FCA in Greece. By 109 confronting numerical simulations to chloride concentration observations, they showed that 110 the DFN model is necessary to accurately simulate SWI. Sebben et al. [2015] used the DFN-111 VDF model to present a preliminary deterministic study on the effect of fractured 112 heterogeneity on SWI, using different fractured configurations of Henry Problem. Mozafari et 113 al. [2018] developed a DFN-VDF model in the finite element frame-work of COMSOL Multiphysics®. Nevertheless, the DFN-VDF model requires the basic characteristics of 114 115 fractures as location, aperture, permeability, porosity, etc. These characteristics are subject to a large amount of uncertainties as they are often determined using model calibration 116 117 procedure based on relatively insufficient historical data provided by several measurement techniques as surface electrical resistivity tomography [Beaujean et al., 2014], borehole 118 119 concentrations and head measurements, multiperiod oscillatory hydraulic tests [Sayler et al., 2018], self-potential measurements [MacAllister et al., 2018], among others. These 120 121 uncertainties would reduce the predictive capability of the DFN-VDF model and impair the 122 reliability of SWI management based on these predictions. Thus, it is important to understand 123 how these uncertainties could propagate in the model and lead to uncertainty in outputs.

This work goes a step further in the understanding of SWI processes in FCAs. It aims to provide a preliminary investigation on the impacts of uncertainty associated to fractures characteristics on the extent of the steady-state saltwater wedge simulated using the DFN-VFD model. In particular, we investigate the effects of uncertainties on fracture network characteristics (location, aperture, density, permeability and dispersivity) on several SWI metrics, as the length of the saltwater toe, thickness of the mixing zone, area of the salted zone and salinity flux penetrating to the aquifer. As the underpinning conceptual model, we consider the fractured Henry Problem suggested in *Sebben et al.* [2015]. A finite element DFN-VDF numerical model is implemented using COMSOL Multiphysics® software. We include the Boussinesq approximation in the COMSOL model to reduce nonlinearity and improve computational efficiency.

135 In order to quantify the variability in model outputs resulting from the uncertain parameters, 136 we use the global sensitivity analysis (GSA). GSA is more appropriate than local sensitivity 137 analysis as it provides a robust and practical framework to explore the entire inputs space and 138 to assess the key variables driving the model outputs uncertainty [Saltelli, 2002; Sudret, 139 2008; De Rocquigny, 2012]. GSA is a powerful approach to fully understand the complex 140 physical processes and assess the applicability of models. It is also important for risk 141 assessment and decision-making. In hydrogeological applications, GSA has been used to 142 investigate saturated/unsaturated flow [Younes et al., 2013, 2018; Dai et al., 2017; Meng and 143 Li, 2017; Maina and Guadagnini, 2018; Miller et al., 2018], solute transport [Fajraoui et al., 2011, 2012; Ciriello et al., 2013; Younes et al., 2016], geological CO2 sequestration [Jia et 144 145 al., 2016], natural convection [Fajraoui et al., 2017] and double-diffusive convection [Shao 146 et al., 2017]. In SWI, GSA has been applied to study the effects of hydrodynamics parameters 147 in homogeneous CAs [Herckenrath et al., 2011; Rajabi and Ataie-Ashtiani, 2014; Rajabi et 148 al., 2015; Riva et al., 2015; Dell'Oca et al., 2017]. Rajabi et al. [2015] have shown that GSA 149 is the best-suited method for uncertainty analysis of SWI. Recently, Xu et al. [2018] used 150 GSA to investigate SWI in a karstic CA with conduit networks. To the best of our knowledge, 151 GSA has never been applied to SWI in heterogeneous and/or FCAs. Different alternatives can be used to perform GSA [looss and Lemaître, 2015]. Among these alternatives, in this paper, 152 we use the variance-based technique with the Sobol' indices (SIs) as sensitivity metrics 153 154 [Sobol', 2001]. These indices are widely used because they do not assume any simplification

155 regarding the physical model and provide the sensitivity of individual contribution from each 156 parameter uncertainty as well as the mixed contributions [Sarkar and Witteveen, 2016]. SIs are usually evaluated through Monte Carlo methods which require a large number of 157 158 simulations to cover the parameters space and, as a consequence, might be impractical in high CPU consuming problems (as is the case for SWI in FCAs) [Sudret, 2008; Herckenrath et al., 159 160 2011]. To meet the numerical challenges of Monte Carlo methods, we use the polynomial 161 chaos expansions (PCE) which proceeds by expressing each model output as a linear 162 combination of orthogonal multivariate polynomials, for a specified probability measure 163 [Crestaux et al., 2009; Konakli and Sudret, 2016; Fajraoui et al., 2017]. In particular, we implement the sparse PCE technique developed by Shao et al. [2017] to allow high 164 165 polynomial orders (i.e. high accuracy) with an optimized number of deterministic samples. 166 With this technique, the number of terms in the PCE decomposition is reduced by excluding 167 insignificant terms. The polynomial order is updated progressively until reaching a prescribed 168 accuracy. During the procedure, Kashyap information criterion is used to measure the 169 relevance of PCE terms [Shao et al., 2017]. The sparsity of the PCE allows accurate surrogate 170 model even if the optimal number of samples necessary for a total order expansion is not 171 achieved. Once the PCE is constructed for each model output, the SIs can be directly 172 calculated, with no extra computational cost, by a post-processing treatment of the PCE 173 coefficients.

The paper is organized as follows: Section 2 is for material and methods in which we present two fractured scenarios of the Henry Problem investigated in this study, the DFN-VDF model developed with COMSOL and the SWI metrics used as model outputs. Section 3 is devoted to the GSA method. In section 4, we validate the developed COMSOL model and the Boussinesq approximation by comparison against exact solutions and an in-house research

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179 code. Section 5 discusses the GSA results; it includes PCE construction, validation of PCE180 and uncertainties propagation. A conclusion is given in section 6.

181 **2. Material and methods**

182 2.1. Conceptual model: Fractured Henry Problem

183 The conceptual model is based on the fractured Henry Problem, suggested by Sebben et al. 184 [2015]. A detailed review of the Henry Problem and its applications can be found in Fahs et al. [2018]. This problem deals with SWI in a confined CA of depth H and length ℓ . Sea 185 186 boundary condition (constant concentration and depth-dependent pressure head) is imposed at the left side and constant freshwater flux $(q_d [L^2 T^{-1}])$ with zero concentration is assumed at 187 188 the right side. Two fracture configurations are investigated in our analysis. The first 189 configuration deals with a single horizontal fracture (SHF) extending on the whole domain and located at a distance (d^F) from the aquifer top surface (Fig. 1a). This configuration is 190 191 specifically considered to investigate the effect of uncertainty related to fracture location on the extent of saltwater wedge. In the second configuration, we assume a network of 192 orthogonal fractures (NOF) (Fig. 1b), as in Sebben et al. [2015]. Square sugar-cube model 193 with elementary size δ^F (distance between 2 consecutive fractures) is considered as fracture 194 195 network. This configuration is considered since it allows for performing uncertainty analysis 196 of the SWI metrics with respect to the fracture density. Furthermore, vertical fractures are 197 important to investigate buoyancy effects.

198 2.2. DFN-VDF mathematical model:

Under steady-state conditions and based on Boussinesq approximation, the VDF model in theporous matrix is given by [*Guevara Morel et al., 2015*]:

$$\nabla \cdot \mathbf{q} = 0 \tag{1}$$

$$\mathbf{q} = -K^{M} \left(\nabla h + \frac{\rho - \rho_{0}}{\rho_{0}} \nabla z \right)$$
⁽²⁾

$$\mathbf{q}\nabla c - \nabla \cdot \left(\boldsymbol{\varepsilon}^{M} D_{m} \mathbf{I} + \mathbf{D}\right) \nabla c = 0 \tag{3}$$

$$\mathbf{D} = \left(\alpha_L^M - \alpha_T^M\right) \frac{\mathbf{q} \times \mathbf{q}}{|\mathbf{q}|} + \alpha_T^M |\mathbf{q}| \mathbf{I}$$
⁽⁴⁾

$$\rho = \rho_0 + \Delta \rho c \tag{5}$$

where q is the Darcy's velocity $[LT^{-1}]$; ρ_0 the freshwater density $[ML^{-3}]$; g the gravitational 201 acceleration $[LT^{-2}]$; K^{M} is the freshwater hydraulic conductivity of the porous matrix 202 $[LT^{-1}]$; h the equivalent freshwater head [L]; ρ $[ML^{-3}]$ the density of mixture fluid and z 203 is the elevation [L]; c is the relative solute concentration [-]; D_m the molecular diffusion 204 coefficient $[L^2T^{-1}]$; ε^{M} is the porosity [-] of the porous matrix; **I** the identity matrix and **L** 205 is the dispersion tensor; $\alpha_L^M[L]$ and $\alpha_T^M[L]$ are the longitudinal and transverse dispersion 206 207 coefficient of the porous matrix, respectively.

208 With the DFN approach, the mathematical model for fractures can be obtained by assuming 1D flow and mass transport equations along the fractures direction. The resulting equations 209 are similar to the ones in the porous matrix, but with ε^{F} , K^{F} and α_{L}^{F} as porosity, hydraulic 210 conductivity and longitudinal dispersivity in the fractures, respectively. Transverse 211 dispersivity in the fracture (α_T^F) is neglected, as in Sebben et al. [2015]. The 1D flow and 212 mass transport equations in fracture involve the thickness of the fracture (e^{F}) as parameter. 213 2.3. DFN-VDF finite element model: COMSOL Multiphysics®:

The DFN-VDF simulations are performed using a finite element model developed with 215 216 COMSOL Multiphysics® software package. COMSOL is a comprehensive simulation

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217 software environment for various applications. The use of COMSOL in applications related to 218 hydrogeology is increasingly frequent as this software is a user-friendly tool that facilitates all the modeling steps (preprocessing, meshing, solving and post-processing) and allows an easy 219 220 coupling of different physical processes [Ren et al., 2017; Fischer et al., 2018]. Our 221 COMSOL model is created by coupling the "Subsurface Flow" and "Transport of Diluted 222 Species" modules and by assuming concentration-dependent fluid density. The Subsurface 223 Flow module is an extension of COMSOL modeling environment to applications related to 224 fluid flow in saturated and variably saturated porous media. In this module, we use the 225 "Darcy's Flow" interface. The fractures are included via the DFN model by adding the "Fracture Flow" feature to the "Darcy's law" interface. The "Transport of Diluted Species" 226 227 module is used to solve the advection-dispersion equation. The Boussinesq approximation is 228 implemented by considering constant density in the fluid properties and setting a buoyancy 229 volume force depending on the salt concentration. The numerical scheme suggested by 230 default in COMSOL is used to solve the system of equations. The flow and transport models 231 are solved sequentially via the segregated solver. Accurate solutions of the flow model can be 232 obtained using finite volume or finite difference methods [Deng and Wang, 2017]. However, 233 in COMSOL, quadratic basis finite element functions are used for the discretization of the pressure in the flow model while the concentration in the transport model is discretized using 234 235 the linear basis functions. The consistent stabilization technique is used to avoid unphysical 236 oscillations related to the discretization of the advection term. This technique is often called 237 upwinding. It adds diffusion in the streamline direction. Triangular meshes suggested by the 238 COMSOL meshing tool are used in the simulations. With the DFN model, the COMSOL 239 meshing tool generates 2D triangular cells to represent the matrix and 1D cells to represent 240 the fractures. The fracture cells are positioned along the sides of the matrix triangular cells. With the finite-element modeling framework, the common degrees of freedom at the triangle 241

nodes in the matrix and at the 1D segments in the fractures are used to model the volumetric and mass fluxes between the matrix and the fractures. First runs have shown that, with the steady-state mode, COMSOL is bound to run into convergence difficulties. To avoid this problem, we used the transient mode. This problem is related to the initial guesses, required for the nonlinear solver, that are often hard to obtain. Hence, the steady-state solutions are obtained by letting the system evolve under transient conditions until steady-state.

248 2.4. Metrics Design:

The main purpose of this study is to perform GSA in regards to certain metrics characterizing the steady state salt-wedge and saltwater flux associated with SWI. The model inputs will be discussed later in the results section since they are dependent on the fracture configuration. As model outputs, we consider the following SWI metrics:

- The spatial distribution of the salt concentration: It is obtained in a pattern of a
 100×50 regular 2D square grid (5,000 nodes).
- Length of the saltwater toe (L_{toe}) : The distance from sea boundary to the 0.5 isochlor on the bottom surface of the aquifer (Fig. 2).
- 257 Thickness of the saltwater wedge (L_s) : The distance between the 0.1 and 0.9 258 isochlors on the aquifer bottom surface (Fig. 2).
- 259 Average horizontal width of the mixing zone (\overline{W}_{mz}) : The average horizontal 260 distance between the 0.1 and 0.9 isochlors from the bottom to the top of the 261 aquifer (Fig. 2).
- 262 The height of the inflection point (Z_I) : The freshwater-seawater inflection point 263 located on the seaward boundary (Fig. 2). Below this point, the seawater flows 264 toward the land, and above it the freshwater is discharged to the sea.

11

265 - The dimensionless mass of salt persisting in the aquifer
$$\left(M_s = \frac{1}{\ell \cdot H} \int_{0}^{\ell} \int_{0}^{H} c \cdot dx dz\right)$$
:

The double integral is calculated with the grid used for the spatial distribution of salt concentration. Only nodes with concentration above 0.01 are considered.

- Total dimensionless flux of saltwater entering the aquifer (Q_S^{total}) : defined as the flux of saltwater entering the domain by advection, diffusion and dispersion normalized by the freshwater flux imposed at the inland boundary (q_d) .

271 **3.** Global sensitivity analysis

272 GSA is a useful and a widespread tool that aims to quantify and evaluate the output 273 uncertainties resulting from the uncertainties in the model inputs, which could be considered 274 singly (for one parameter) or coupled together (several parameters). In this study, the 275 variability of the model responses is quantified throughout a variance based technique using 276 SIs as sensitivity metrics. On the one hand, variance-based sensitivity measures are of interest 277 as they typically specify the relationship between model outputs and input parameters. And on 278 the other hand, the major advantage of using SIs is that they do not require any assumptions of monotonicity or linearity in the physical model. The main stages of this technique are 279 280 developed here. More details can be found in Sudret [2008], Fajraoui et al. [2017] and Le 281 Gratiet et al. [2017]

Let us consider a mathematical model, $Y = M(\mathbf{X})$, delivering the outputs of a physical system that presumably depends on M-uncertain input parameters $\mathbf{X} = \{X_1, X_2, ..., X_M\}$. For further developments, $f_{Xi}(x_i)$ and $f_x = \prod_{i=1}^{M} f_{Xi}(x_i)$ refer to their marginal probability density function (PDF) and the corresponding joint PDF of a given set.

286 3.1 Sobol' indices

287 The Sobol' decomposition of M(X) reads [Sudret, 2008; Fajraoui et al., 2017]:

$$\mathbf{M}(\mathbf{X}) = \mathbf{M}_0 + \sum_{i=1}^{M} \mathbf{M}_i(X_i) + \sum_{1 \le i < j \le M} \mathbf{M}_{ij}(X_i, X_j) + \dots + \mathbf{M}_{1, 2, \dots, M}(X_1, \dots, X_M),$$
(6)

where \mathbf{M}_0 is the expected value of $\mathbf{M}(\mathbf{X})$ and the integral of each summand M_{*i*₁,*i*₂,...,*i*_{*i*} $(X_{i_1}, X_{i_2}, ..., X_{i_s})$ over any of its independent variables is zero, that is:}

$$\int_{\Gamma_{X_{i_k}}} \mathbf{M}_{i_1, i_2, \dots, i_s} \left(X_{i_1}, X_{i_2}, \dots, X_{i_s} \right) f_{X_{i_k}} (x_{i_k}) = 0 \text{ for } 1 \le k \le s ,$$
(7)

where $f_{X_{i_k}}(x_{i_k})$ and $\Gamma_{X_{i_k}}$ represent the marginal PDF and support of X_{i_k} , respectively.

291 The orthogonality M_i leads a unique Sobol' decomposition:

$$\mathbf{E}[\mathbf{M}_{u}(X_{u})\mathbf{M}_{v}(X_{v})]=0, \tag{8}$$

Where, E[.] is the mathematical expectation operator, $u = \{i_1, i_2, ..., i_M\} \subseteq \{1, 2, ..., M\}$ represents the index sets and X_u are the subvectors involving the components for which the indices belong to u. As a result of uniqueness and orthogonality of Y, its total variance D is decomposed as below:

$$D = \operatorname{Var}[\mathcal{M}(X)] = \sum_{u \neq 0} D_u = \sum_{u \neq 0} \operatorname{Var}[\mathcal{M}_u(X_u)], \qquad (9)$$

296 where D_u is the partial variance expressed as below:

$$D_{u} = Var[\mathcal{M}_{u}(X_{u})] = E[\mathcal{M}_{u}^{2}(X_{u})]$$
⁽¹⁰⁾

297 Consequently, the SIs are naturally defined as:

$$S_u = \frac{D_u}{D} \tag{11}$$

The influence on *Y*, of each parameter (considered singly), is given by the first order Sobol' indices (S_i) defined by:

$$S_i = \frac{D_i}{D} \tag{12}$$

The total SI that includes the effect of an input parameter with the contribution from other parameters, is defined as follows *[Homma and Saltelli, 1996]*:

$$S_{i}^{T} = \sum_{\vartheta} \frac{D_{u}}{D}, \qquad \vartheta_{i} = \left\{ u \supset i \right\}$$
⁽¹³⁾

The SIs can be calculated by performing Monte-Carlo simulations. This can be done using the estimates of the mean value, total and partial variance of a large number of samples, as explained in Sudret [2008]. The drawback of Monte-Carlo simulations lies in the computational cost especially when time-consuming models are investigated. To circumvent this problem, *Sudret* [2008] introduced the PCE for the computation of SIs.

307 *3.2 Polynomials chaos expansion (PCE)*

308 Each model output is expanded into a set of orthonormal multivariate polynomials of309 maximum degree M:

$$Y = M(X) \approx \sum_{\alpha \in A} y_{\alpha} \Phi_{\alpha}(X), \qquad (14)$$

where A is a multi-index $\alpha = \{\alpha_1, \alpha_2, ..., \alpha_M\}$ and $\{y_{\alpha}, \alpha \in A\}$ are the polynomial coefficients. $\Phi_{\alpha}(X)$ are the base functions of vector space of polynomial functions. These functions should be orthogonal in the vector space with the joint PDF f_X of X as a dot product.

The polynomial coefficients $\{y_{\alpha}\}$ are evaluated using the regression method (least-square technique) that proceeds by minimizing an objective function representing the difference between the meta-model and physical model (see Fajraoui et al. [2017]). Based on the PCE, the mean value (μ) and total variance (D) of any model output can be calculated as follows:

$$\mu = y_0 \tag{15}$$

$$D = \sum_{\alpha \in A \setminus 0} y_{\alpha}^{2}$$
(16)

317 Then the SIs of any order can be computed using the coefficients, D and μ in a 318 straightforward manner as followed:

$$S_{i} = \sum_{\alpha \in A_{i} \setminus 0} y^{2}_{\alpha} / D, \qquad A_{i} = \left\{ \alpha \in A : \alpha_{i} > 0, \alpha_{j \neq i} = 0 \right\},$$

$$(17)$$

319 and

$$S_i^T = \sum_{\alpha \in A_i^T \setminus 0} y_{\alpha}^2 / D, \qquad A_i^T = \left\{ \alpha \in A : \alpha_i > 0 \right\}$$
(18)

As suggested by *Deman et al.* [2016], we also evaluate the marginal effect (ME) to understand the relation between the important variables and the model outputs. ME is given by:

$$E[\mathcal{M}(X) \mid X_i = x_i] = \mathcal{M}_0 + \sum_{\alpha \in A_i} y_\alpha \Phi_\alpha(x_i)$$
(19)

323 *3.3 Sparse polynomial chaos expansion*

324 To minimize the number of physical model evaluations and therefore reduce the 325 computational cost, the estimation of the Sobol' indices could be done with a sparse PCE 326 instead of a full PCE approach. In other words, instead of using the expression Eq. (14), we 327 can only use some relevant coefficients of the PCE. The key idea consists in discarding the 328 irrelevant terms in the estimated truncated PCE and for this purpose, several approaches have been developed. Blatman and Sudret [2010] utilized an iterative forward-backward approach 329 330 based on nonintrusive regression or a truncation strategy based on hyperbolic index sets coupled with an adaptive algorithm involving a least angle regression (LAR). Meng and Li 331 332 [2017] modified the LAR algorithm with a least absolute shrinkage and selection operator 333 (LASSO-LAR). An adaptive procedure using projections on a minimized number of bivariate basis functions has been provided by Hu and Youn [2011], whereas Fajraoui et al. [2012] 334 worked with a fixed experimental design and retained only significant coefficients that could 335

336 contribute to the model variance. The approach developed in Shao et al. [2017], which has 337 been implemented in this work, consists in progressively increasing the degree of an initial PCE until a satisfactory representation of the model responses is obtained. The computation 338 339 of the Kashyap information criterion (KIC) based on a Bayesian model averaging is used to 340 determine the best sparse PCE for a input/output sample. Evaluating KIC is an efficient (from 341 a computational point of view) and feasible alternative to directly computing the Bayesian 342 model evidence, being known that this later evaluates the likelihood of the observed data 343 integrated over each model's parameter space. Hence, it is a key term to obtain the posterior 344 probability in the Bayesian framework. For more details on the Bayesian sparse PCE, for 345 constructing the algorithm and computing the KIC, readers can refer to Shao et al. [2017].

4. Validations: COMSOL model and Boussinesq approximation

347 Although COMSOL has great potential for modelling density-driven flow problems, it has 348 rarely been used for SWI. Thus, the main purpose of this section is to validate our developed 349 COMSOL model. In addition, as explained previously, Boussinesq approximation was 350 implemented in our COMSOL model to improve its computational efficiency. This is a 351 popular approximation for the VDF model as it allows for reducing the computational costs 352 and renders convergence more likely to be achieved. It assumes that variations in density only 353 give rise to buoyancy forces and have no impact on the flow field. Boussinesg approximation 354 ignores density-concentration dependence except in the buoyancy term. This approximation is 355 common for SWI in non-fractured CAs [Guevara Morel et al., 2015]. Its validity for SWI in 356 FCAs is not discussed in the literature. Thus, another goal of this section is to investigate the 357 validity of this approximation for such a case.

For this purpose, we first use the new semi-analytical solutions of the Henry Problem (homogeneous aquifer) developed by *Fahs et al.* [2016]. We compare these solutions against

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two COMSOL models: i) SWI-COMSOL model based on the standard COMSOL approach 360 361 and ii) SWI-COMSOL-Bq based on the Boussinesq approximation. We investigate two test cases presented in Fahs et al. [2016] which deal with constant and velocity-dependent 362 363 dispersion tensor, respectively. The corresponding physical parameters are summarized in Table 1. It is noteworthy that, for the validation cases, similar to the semi-analytical solution, 364 365 the sea boundary is assumed at the right side of the domain. The main isochlors (0.1, 0.5 and 366 0.9) obtained with COMSOL models as well as the semi-analytical ones are plotted in Fig. 3. 367 The corresponding SWI metrics are given in Table 2. The COMSOL simulations have been 368 performed using a mesh consisting of about 18,000 elements. As is obvious from Fig. 3, 369 excellent agreement is obtained between the COMSOL and the semi-analytical results. This 370 highlights the accuracy of the developed COMSOL models and the related post-treatment procedure applied to obtain the SWI metrics. It also confirms the validity of the Boussinesq 371 372 approximation for SWI in homogenous CAs.

373 For FCAs, analytical or semi-analytical solutions do not exist. We compare the developed 374 COMSOL models (SWI-COMSOL and SWI-COMSOL-Bq) against an in-house research 375 code (TRACES) based on advanced space and time discretization techniques [Younes et al., 376 2009]. This code has been validated by comparison against several configurations of semi-377 analytical solutions in *Fahs et al.* [2018]. It has proven to be a robust tool for the simulation 378 of SWI in both homogeneous and heterogeneous domains. DFN approach, which is based on 379 average properties over the fracture width, is not available in TRACES. Thus, the fractures 380 are modeled by considering heterogeneity of material without reduction of the dimensionality; 381 i.e. fracture is a specific layer of the 2D domain with different assigned properties. We 382 considered two validation cases which are based on a single horizontal and vertical fractures, respectively. The horizontal fracture is located at the aquifer middle-depth ($d^F = 0.5m$) 383 384 while the vertical fracture is located near the seaside at x=1.8m. The physical parameters are 385 given in Table 1. The mesh used in the COMSOL simulations involves about 50,000 386 elements. In the in-house code we use a mesh with about 70,000 elements. The obtained main isochlors are given in Fig. 4 and the corresponding SWI metrics are summarized in Table 2. 387 388 Fig. 4a shows that, in the case of single horizontal fracture, the high conductivity in the 389 fracture increases the freshwater discharge to the sea and pushes the saltwater wedge toward 390 the sea, especially around the fracture. In the case of vertical fracture (Fig. 4b), the high 391 permeability in the fracture enhances the upward flow and push up the saltwater around the 392 fracture Fig. 4 and Table 2 show excellent agreement between COMSOL and TRACES. They 393 confirm the validity of the Boussinesq approximation in the presence of fractures and 394 highlight the accuracy of the developed COMSOL model. It should be noted also that the 395 comparison between the COMSOL model (in which the fracture is considered as a line) and 396 TRACES (in which the fracture is a 2D layer) confirms the results of Grillo et al. [2010] 397 about the validity of the technique based on (n-1) dimensional fractures (i.e. average 398 properties over the fracture) for the simulation of SWI in FCAs.

399 5. Global sensitivity Analysis: results and discussion

The methodology used to perform GSA is described in the flowchart presented in Fig. 5. In this section we present the assumptions and numerical details related to the PCE construction. We also validate the PCE meta-model by comparison against physical COMSOL model and we present the results of the GSA based on the SI's, for both salinity distribution and SWI metrics.

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407 *5.1 The single horizontal fracture configuration (SHF)*

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408 Several studies showed that, under steady-state condition, the isotropic Henry Problem is 409 governed by six dimensionless quantities which are the gravity number, longitudinal and 410 transverse Peclet numbers, ratio of the fresh water density to the difference between 411 freshwater and saltwater densities, Froude number and the concentration of salt in seawater 412 [Riva et al., 2015; Fahs et al., 2018]. Uncertainty analysis related to these parameters is 413 performed in Riva et al. [2015]. The main goal of our work is to investigate the effect of 414 uncertainties related to the presence of fractures. Thus, for the SHF configuration, we assume that the hydraulic conductivity (K^{F}), aperture (e^{F}), depth (d^{F}) and longitudinal dispersivity 415 (α_L^M) of the fracture are uncertain. For the matrix domain, we only include the longitudinal 416 dispersivity (α_I^M) in our analysis as this parameter is important for the exchange between 417 fracture and matrix domain. The dispersivity ratio (transverse to longitudinal) is set to be 0.1. 418 419 Other parameters are kept constant. Table 3 summarizes the values of the deterministic 420 parameters as well as the range of variability of the uncertain parameters. The values used in 421 this table are similar to Sebben et al. [2015].

We should mention that network connectivity (i.e. how fractures are interconnected) has a clear and large impact on the extent of SWI. However, in the cases investigated in this work, all the fractures are fully connected (abutting and crossing fractures). Thus the effect of network connectivity is not considered. Disconnected cases are not considered because it is not obvious to find well defined parameters (required for GSA) to describe the connectivity. Also, disconnected fractures can lead to discontinuous model outputs for which the PCE surrogate model could not approximate the true system with an acceptable degree of accuracy.

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- PCE construction: Numerical details, orders and accuracy

432 The uncertain parameters are assumed to be uniformly distributed over their ranges of 433 variability. The PCEs are evaluated using an experimental design consisting of 100 samples. 434 To obtain a deterministic experimental design that covers the parameter space, we use the 435 Quasi-Monte-Carlo sampling technique. A preliminary mesh sensitivity analysis is performed 436 to ensure mesh-independent solutions for all the simulated samples. These simulations were 437 important in order to verify that the GSA results are not affected by numerical artifacts related 438 to the finite element discretization. The mesh sensitivity analysis is performed using the most challenging numerical case that deals with the highest value of K^F and lowest values of α_L^M 439 , α_{I}^{F} and e^{F} . In such a case the advection and buoyancy processes are very important and the 440 corresponding numerical solution could be highly sensitive to the mesh size as it might suffer 441 442 from unphysical oscillations or numerical diffusion. A mesh-independent solution is achieved 443 for this case using a grid consisting of about 50,000 elements. This mesh is used for the 100 444 simulations required for computing the PCE expansions.

445 For each SWI metric (or model output), the corresponding PCE surrogate model is calculated 446 using the technique described in section 3. For the salt concentration distribution (multivariate 447 output), component-wise PCE is constructed on each node of the regular 2D square grid 448 defined for the control points (involving 5,000 control points). The MATLAB code developed 449 by Shao et al. [2017] is used to compute the sparse PCE. To give more confidence to the 450 sparse PCE, we also compute total order PCE using the UQLAB software [Marelli and 451 Sudret, 2014]. As five input variables are considered and 100 samples are available, only 452 third-order polynomial could be reached via the total order PCE expansion. The 453 corresponding optimal number of samples is 56. With the sparse technique, implemented in 454 this work, higher orders can be reached even if the optimal number of samples required for 455 full PCE is not achieved. Sixth order PCE is reached for the salt concentration distribution 456 and all SWI metrics except the width of the mixing zone for which the polynomial order is

457 limited to five. The accuracy of the resulting sparse PCE surrogate model is checked by 458 comparison against the physical COMSOL model. In Fig. 6, we compare the values obtained with the sparse PCE with those of DFN-VDF physical model implemented with COMSOL 459 460 for parameter inputs corresponding to the experimental design (i.e. used for the PCE 461 construction) and also for new samples. Some examples of the results, precisely the length of saltwater toe (L_{toe}) and the mass of salt persisting in the aquifer (Ms), are plotted in Fig. 6. 462 463 We can observe an excellent match which confirms that the PCE surrogate model reproduces 464 the physical model outputs well.

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- Uncertainty propagation and Marginal Effects (ME)

Based on the PCE, we calculate the first and total SIs which are used for uncertainty propagation. We also calculate the ME (univariate effect) to obtain a global idea about the impact of the input parameters on the model output. The ME of a certain parameter represents the variability of the model output to this parameter when other parameters are kept constant, at their average values.

471 The GSA results for the spatial distribution of the salt concentration are illustrated in Fig. 7. 472 Fig. 7a shows the distribution of the mean concentration based on the PCE expansion. At each 473 node of the mesh used for the control points, the mean value of the salt concentration is 474 calculated as the arithmetic average of the concentrations corresponding to the 100 samples 475 used in the experimental design which are evaluated via the PCE surrogate model. This figure 476 shows that the mean concentration distribution reflects the systematic behavior of SWI. The 477 isochlors are more penetrated at the bottom aquifer due to the saltwater density. This confirms 478 that the PCE surrogate model mimics the full model's response. We also calculate the 479 concentration variance to evaluate how far the concentrations are spread out form their 480 average values (Fig. 7b). As expected, the variance is significant in the saltwater wedge. The

481 largest values are located near the aquifer bottom surface where the SWI is usually induced by 482 mixing processes that can be highly sensitive to the model inputs (fracture characteristics and matrix dispersivity). The variance is negligible near the sea-side as the boundary conditions 483 484 are almost deterministic and the sole acting random parameter is the longitudinal dispersivity 485 that can affect the dispersive entering flux. The sensitivity of the concertation distribution to 486 the uncertain parameters is assessed with the maps of the total SI (Figs 7 c-g). The total SI of α_{L}^{M} (Fig. 7c) shows that the uncertainty related to this parameter affects the concentration 487 488 distribution at the top aquifer, outside the saltwater wedge. In this zone, the salt transport 489 processes are dominated by the longitudinal dispersion flux as the velocity is toward the sea 490 and it is almost horizontal and parallel to the salt concentration gradient. The zones of largest total SI for K^{F} and e^{F} are located within the saltwater wedge toward the low isochlors (Fig. 491 492 7d and 7e). In this region, the mass transfer is mainly related to the advection process which is 493 related to the velocity field. This later is highly depending on the fracture permeability and aperture. The zone of influence of d^F is also located within the saltwater wedge, but toward 494 495 the aquifer bottom surface and at the vicinity of the high isochlors (Fig. 7f). The influence of α_{L}^{F} is limited to the vicinity of the sea boundary where α_{L}^{F} can impact the saltwater flux to 496 497 the aquifer (Fig. 7g). In the fracture, advection is dominating and dispersion is negligible. It is 498 worthwhile noting that the total SIs count in the overall contribution of a parameter including 499 nonlinearities and interactions. Thus, SIs allow for ranking the parameters according to their importance. It appears on Figs. 7 that d^F , K^F and e^F are the most influential parameters 500 501 because their total SI are more pronounced in the region where the salt concentration variance is maximum. From the scales of Figs. 7 (d-f), it is clear that K^F and e^F are more influential 502 than d^{F} . Figs. 7c shows that the salinity distribution is weakly sensitive to the longitudinal 503 504 dispersivity of the matrix as in its zone of influence the variance is negligible.

Inspection of the sensitivity of SWI metrics to uncertain parameters is given in Fig. 8. This figure represents the bar-plots of the total and first-order SIs of the SWI metrics. As mentioned previously for a further understanding of the uncertainty on SWI metrics related to the imperfect knowledge of input parameters, we also investigate the MEs of the most relevant parameters. These MEs are plotted in Fig. 9. The large variability of the SWI metrics (see vertical scales in Figs. 9a-j) confirms that the MEs are in agreement with the SIs.

Fig. 8a shows that the uncertainty on L_{toe} is mainly due to the effects of d^F and K^F . With a 511 total SI of 0.54, d^F is considered as the most influential parameter. The ME of d^F and K^F on 512 L_{toe} are given in Fig. 9a and 9b, respectively. Fig. 9a shows that L_{toe} decreases with d^{F} 513 which is coherent with the results of Sebben et al. [2015]. Fig. 9b shows that L_{toe} increases 514 with K^{F} . The physical interpretation of this variation is that the increase of K^{F} heightens the 515 potential of the fracture to constitute a preferential freshwater flow path. This slow down the 516 517 freshwater flow in the matrix which in turn facilitates SWI and leads to the increase of the penetration length of the saltwater wedge. Fig. 8b indicates that the variability of $L_{\rm S}$ is mainly 518 impacted by α_L^M . This makes sense as L_S measures the salinity dispersion along the aquifer 519 bottom surface which is mainly controlled by α_L^M . L_S is even expected to increase with α_L^M , 520 which is confirmed from the ME in Fig. 9c. We can also notice in Fig. 8b the slight sensitivity 521 of L_{S} to d^{F} . The corresponding ME (Fig. 9d) shows that this sensitivity is relatively 522 important for deep fractures ($d^F > 0.6$). 523

The SIs for \overline{W}_{mz} are given in Fig. 8c. The width of the mixing zone is mainly controlled by the dispersive flux. This is why, α_L^M is the main parameter affecting \overline{W}_{mz} . As expected, increasing variation of \overline{W}_{mz} against α_L^M can be observed in Fig. 9e. For Z_I (Fig. 8d), with a

total SI of 0.58, d^F is the most important parameter. Fig. 9f shows that Z_I decreases with d^F , 527 which is in agreement with the results of Sebben et al. [2015]. Variability of Z_I could be also 528 affected by the uncertainty of K^{F} . The corresponding ME in Fig. 9g shows that Z_{I} increases 529 with K^{F} . Fig. 8e depicts the SIs for the mass of salt persisting in the aquifer (M_{s}) . It indicates 530 that M_S is primarily sensitive to d^F (SI=0.62). It is also sensitive to K^F . ME (Fig. 9h) shows 531 that M_s decreases with d^F , which is also consistent with the results Sebben et al. [2015]. 532 $M_{\rm S}$ increases with $K^{\rm F}$ (Fig. 9i). This behavior is related to fact that the increase of $K^{\rm F}$ 533 534 enhances the inland extent of the saltwater wedge, as explained in the previous section. Finally, the SIs for Q_S^{total} shows that this output is mainly affected by d^F (Fig. 8f). As show 535 in Fig. 9j (Q_{S}^{total}) increases with d^{F} . In general, the SIs show that the uncertainty associated 536 with α_{L}^{F} has no effect on the SWI metrics, which is logical, as salt transport in the fracture is 537 dominated by the advection processes. 538

539 5.2 The network of orthogonal fractures configuration (NOF)

In this configuration, our goal is to investigate the effect of uncertainty related to the fractures 540 density on the model outputs. Thus, we keep the same uncertain parameters as for the SHF 541 configuration but we replace (d^F) by (δ^F) . The latter is considered here as the parameter 542 representing the fracture density. The values of the deterministic parameters and the range of 543 variability of the uncertain inputs are given in Table 3. The lowest value of δ^F corresponds to 544 545 a network with 13 horizontal and 26 vertical fractures. These values are used to obtain the 546 results in affordable CPU time, as denser fractured configurations would require a large 547 number of simulations to construct the PCE and the COMSOL model in this case becomes 548 very CPU time consuming. We should mention that, for this configuration, we reduce the 549

hydraulic conductivity of the fractures. If the same values would have been used as in SHF configuration, freshwater flow would have been so intensive that no SWI would occur.

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- PCE construction: Numerical details, orders and accuracy

552 The NOF configuration is more sensitive to the fractures characteristics than SHF configuration. The number of samples is progressively increased until obtaining accurate 553 554 PCEs. The corresponding experimental design involves 200 samples. The mesh sensitivity analysis for the most challenging cases (the smallest value of δ^F) reveals that mesh-555 556 independent solution can be obtained using a grid of 70,000 elements. As for the SHF 557 configuration, sparse and total PCE are calculated. With 200 samples, order 4 total PCE can 558 be obtained. The optimal number of samples is 126. With the sparse technique, sixth order polynomial is reached for L_{toe} , M_S , Z_I and Q_S^{total} . For L_S and \overline{W}_{mz} orders 4 and 8 are 559 achieved, respectively. Fig.10 shows some comparisons between the sparse PCE surrogate 560 561 and COMSOL models and highlights the accuracy of the PCE expansions. A good matching 562 is observed both for the input parameters of the experimental design and for new samples. It is relevant to emphasize that this level of accuracy is acceptable to obtain good GSA results 563 with the SIs evaluated using the surrogate model. 564

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- Uncertainty propagation and marginal effects

The distribution of the mean concentration based on the PCE expansion is given in Fig. 11a. The mean PCE isochlors emulate the ones obtained using the physical model (Fig. 12). They present some discontinuous points where saltwater is pushed toward the sea due to high permeability in the fractures. The spatial map of the concentration variance is plotted in Fig. 11b. Compared to the SHF configuration, the zone of significant variance is contracted and concentrated toward the bottom surface of the aquifer near the low mean isochlors. The map of the total SIs of α_{L}^{M} (Fig. 11.c) is quite similar to the one in the SHF configuration but it 573 echoes the presence and influence of fracture network. Fig.11c shows that the zone of influence of α_L^M falls where the concentration variance is negligible. Thus, α_L^M is not an 574 important parameter for salinity distribution. Sensitivity to K^{F} and e^{F} are both important 575 (Fig. 11d and e). The zone of influence of K^{F} is discontinuous and mainly located toward 576 577 the sea boundary in at the bottom of the aquifer. Important values can be observed landward 578 (see Fig. 11. d) but these values do not express high sensitivity as the concentration variance is negligible in this zone. The sensitivity to the fractures density (δ^F) is given in Fig. 11f. 579 This figure shows that uncertainty associated δ^F can mainly affect the salinity distribution 580 within the mixing zone toward the bottom surface. It confirms that δ^{F} is an influential 581 parameter. Finally, and in contrast to the SHF configuration, α_L^F appears to be an important 582 583 parameter in the NOF configuration (Fig. 11g). It affects mainly salinity distribution around 584 the low isochlors.

The bar-plots in Fig. 13 depict the total and first-order SIs for the SWI metrics to the 585 uncertain parameters and Fig. 14 gives the MEs of these parameters. In general Fig. 14 586 confirms the results of the SIs as large variations of SWI metrics can be observed with respect 587 to the uncertain parameters. Fig. 13a demonstrates that L_{toe} is mainly controlled by K^{F} and 588 δ^{F} . The corresponding total SIs are $S_{K^{F}}^{T} = 0.52$ and $S_{\delta^{F}}^{T} = 0.32$, respectively. Fig. 14a shows 589 an increasing variation of L_{toe} against K^{F} . As for the SHF configuration, this is related to the 590 fact that the increase of K^{F} concentrates the freshwater flow in the fractures and entails a 591 592 weaker freshwater flow in the matrix. As consequence, the saltwater wedge expands landward and L_{toe} increases. This behavior can be understood also using the equivalent porous media 593 model which is based on a bulk hydraulic conductivity. As given in Sebben et al. [2015], the 594 bulk equivalent conductivity (K^{eq}) for a network of orthogonal fractures is given by: 595

$$K^{eq} = \left[\left(K^{M} + \frac{K^{F} e^{F}}{\delta^{F}} \right)^{-1} + \frac{e^{F}}{K^{F} \delta^{F}} \right]^{-1}$$
(20)

Eq. (20) shows that K^{eq} increases with the increase of K^{F} . The equivalent gravity number, which compares the buoyancy forces to the inland freshwater flux, is given by *[Fahs et al.* 2018]:

$$Ng^{eq} = \frac{K^{eq}.H.(\rho_{1} - \rho_{0})}{\rho_{0}q_{d}}$$
(21)

The increase of K^{eq} leads to the increase of Ng^{eq} . This latter can be interpreted, at constant densities and hydraulic conductivity, as a decrease in the inland freshwater that opposes SWI. This enhances the extend of SWI and leads to the increase of L_{toe} .

Fig. 14b shows that L_{toe} decreases with δ^F . In fact, the increase of δ^F corresponds to the 602 603 reduction of the fracture density. This enhances the freshwater flow in the porous matrix and 604 pushes the saltwater wedge toward the sea. The equivalent bulk hydraulic conductivity model 605 can be also useful in explaining this variation, by reasoning in the same way as for the variation of L_{toe} against K^{F} . As it is clear from Eq. (20), the increase of δ^{F} (for the average 606 value of K^{M} , K^{F} and e^{F}) corresponds to a decrease in K^{eq} and the related equivalent gravity 607 number. This can be interpreted as an increase of the freshwater flux that lowers the extent of 608 SWI and decreases L_{toe} . 609

The bar-plots in Figs. 13b and 13c indicate that, as for the SHF configuration,
$$\alpha_{L}^{M}$$
 is the most
important parameter affecting L_{S} and \overline{W}_{mz} . The corresponding SIs are calculated to be 0.68
and 0.34, respectively. Figs. 14c and 14d display increasing variation of L_{S} and \overline{W}_{mz} against
 α_{L}^{M} . This makes sense as L_{S} and \overline{W}_{mz} are mainly related to the mixing processes which are
controlled by α_{L}^{M} . Fig. 13d shows that, with $S_{K^{F}}^{T} = 0.50$ and $S_{\delta^{F}}^{T} = 0.27$, K^{F} and δ^{F} are the

615 most important parameters affecting Z_I . MEs in Figs. 14e and 14f indicate that Z_I increases 616 with K^F and decreases with δ^F . The reason behind these variations is the enhancement (resp. 617 reduction) in the saltwater wedge extent associated with the variation of K^F (resp. δ^F), 618 explained previously. These results related to the variation of Z_I against δ^F are found to be in 619 agreement with those in *Sebben et al.* [2015].

The dimensionless mass of salt persisting in the aquifer (M_s) appears to be sensitive to all 620 uncertain parameters, except α_L^F (Fig. 13e). The total SIs with respect α_L^M , K^F , e^F , δ^F are 621 calculated to be 0.34, 0.41, 0.22 and 0.27, respectively. The MEs show that M_s decreases 622 with δ^F and increases with K^F and α_L^M (Figs. 14g-i). The variation against δ^F and K^F is 623 related to the behavior of the saltwater wedge when these parameters change (see above). The 624 increase of α_{L}^{M} pushes the saltwater wedge landward [Fahs et al., 2018] and increases the 625 area of the salted zone as well as the mass of salt persisting in the aquifer. The total flux of 626 saltwater entering the aquifer (Q_s^{total}) is mainly affected by α_L^M , K^F (Fig. 13f). The total SIs 627 of these parameters are calculated to be 0.43 and 0.42, respectively. The MEs (Figs. 14j and 628 14k) show that Q_s^{total} increases with α_i^{M} and decreases with K^F . Indeed, Q_s^{total} is advective 629 and dispersive saltwater flux at the sea boundary. The dispersive flux is proportional to α_L^M . 630 This explains why Q_{S}^{total} increases with α_{L}^{M} . The increase of K^{F} corresponds to the decrease 631 of the gravity number (see above). A lower gravity number indicates less significant effect of 632 633 the buoyancy forces for which the saltwater velocity decreases and reduces the advective saltwater flux. Finally, it is worth noting that, for the NOF configuration, the SIs for α_{L}^{F} are 634 more important than for the SHF configuration. α_L^F appears to be an important parameter, 635 especially for L_{toe} and L_s . In general, physical consistency of the results for both SHF and 636

NOF configuration provides insight on the validity of our analysis based on the PCE as ameta-model.

639 5. Conclusion

640 In this work, the DFN model is coupled with the VDF model to simulate SWI in FCAs. The 641 DFN-VDF model requires the discontinuous description of the fracture characteristics which 642 are usually uncertain. Thus, it is essential, for several practical and theoretical purposes, to 643 understand/quantify how the uncertainties associated with the imperfect knowledge of the 644 fracture characteristics can propagate through the model and introduce uncertainties into the model outputs. Despite the high performance of computer codes for SWI models, run-time of 645 these codes is still high because of the high nonlinearity, dense grids required for fractures 646 647 and large space and time scales associated with studied domains. Thus the traditional 648 techniques for uncertainty analysis (i.e. Monte-Carlo simulations) cannot be easily applied in this context, as they require a large number of simulations to achieve reliable results. To meet 649 the computational challenges of traditional techniques, we develop in this work a GSA based 650 651 on the non-intrusive PCE. In particular, we apply an efficient sparse technique to construct the 652 PCE with a reduced number of model evaluations, based on Kashyap information criterion. In the literature, GSA has been recently applied to SWI but previous studies are limited to 653 654 homogeneous domain. Two configurations of the fractured Henry Problem, dealing with a 655 single horizontal fracture (SHF) and a network of orthogonal fractures (NOF), are considered 656 as conceptual models. The simulations required to construct the PCE are performed using a 657 finite element model developed in the framework of COMSOL software. Boussinesq approximation is implemented to improve the computational efficiency of the COMSOL 658 659 model. From technical point of view, this work shows several novelties that are important for 660 the simulation of SWI. It shows the ability of COMSOL to accurately simulate SWI in simple 661 and fractured aquifers. It also proves that the dimension reduction of fractures in the frame of 662 the DFN model is a valid approach to simulate SWI in FCAs and confirms the validity of the 663 Boussinesq approximation in such a case. Regarding uncertainty analysis, this study presents 664 an efficient (low cost) methodology to understand uncertainty propagation into SWI models. 665 This methodology is generic and can be efficiently applied to real field investigations. In hydrogeological applications, GSA is often applied to investigate uncertainty propagation 666 667 associated with hydrogeological parameters. This work shows that GSA is generic and can be 668 a valuable tool for different kinds of uncertainties. The GSA results showed that, for the SHF 669 configuration, the uncertainty associated with the fracture hydraulic conductivity and depth is 670 the first sources of uncertainty on the salinity distribution. The spatial distributions of the SIs 671 are given as maps. This represents an important feature of this study as these maps are not 672 only important for uncertainty analysis but also provide relevant locations for measurement required for aquifer characterization. Fracture hydraulic conductivity and depth are also 673 important parameters for the toe position (L_{toe}), thickness of the freshwater discharge zone 674 (Z_l) , the mass of salt persisting in the aquifer (M_s) and the flux of saltwater entering the 675 aquifer (Q_s^{total}) . The thickness of the saltwater wedge and the width of the mixing zone are 676 677 mainly controlled by the dispersion coefficient in the matrix. The uncertainty related to the fracture aperture has a slight impact on the SWI metrics. Its major effect is observed on L_{toe} . 678 679 Uncertainty associated with the fracture dispersion coefficient does not affect in any way the 680 SWI metrics. For the NOF configuration, the imperfect knowledge of fracture hydraulic 681 conductivity and density are the first source of uncertainty of the salinity distribution. 682 However, it is observed that all the uncertain parameters become important for the salinity 683 distribution, in this case. In contrast to the SHF configuration, in which the dispersion in the fracture is not important, in the NOF configuration the salinity distribution at the aquifer top 684 surface is influenced by this fracture dispersivity. L_{toe} and Z_I are mainly controlled by the 685

fractures density and hydraulic conductivity. As for the SHF configuration, the width of the mixing zone is mainly affected by uncertainty associated with the dispersion coefficient in the matrix. L_s is also majorly affected by the dispersion coefficient in the matrix, but the other uncertain parameters are also influencing it. All the uncertain parameters have distributed effects on M_s and Q_s^{total} .

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Fig. 1. Conceptual model of the fractured Henry Problem: (a) Single horizontal fracture configuration (SHF) and (b) Network of orthogonal fractures configuration (NOF).



Fig. 2. Schematic representation of the SWI metrics.



Fig. 3. Isochlors obtained using the semi-analytical solution (SA) and COMSOL model (with and without Boussinesq approximation) for the homogenous test cases: (a) diffusive case and (b) dispersive case.



Fig. 4. Isochlors obtained using TRACES (in-house code) and COMSOL model (with and without Boussinesq approximation) for the fractured test cases: a) single horizontal fracture and b) single vertical fracture.



Fig. 5. A flowchart describing the methodology and approaches used to perform the global sensitivity analysis: The first block (in purple) describes the physical processes and the corresponding mathematical models used in this study; The second block (in olive-green) presents the finite element model used to simulate the physical processes (COMSOL with and without Boussinesq approximation); The third block (in orange) describes the approach used to perform global sensitivity analysis (polynomial chaos expansion as meta-model and Sobol's indices as sensitivity metrics).



a) The length of the saltwater toe (L_{toe}).



b) The dimensionless mass of salt persisting in the aquifer (M_s) .

Fig. 6. Comparison between the PCE surrogate model and physical (COMSOL) model for the SHF configuration: On the left side, 100 samples used for the experimental design and on the right side, 20 simulations which do not coincide with the experimental design (R^2 is the coefficient of determination).



Fig. 7. GSA results for the spatial distribution of the salt concentration (SHF configuration): (a) mean salt concentration (b) variance of the salt concentration, (c) total SI of α_L^M , (d) total SI of K^F , (e) total SI of e^F , (f) total SI index of d^F and (g) total SI index of α_L^F .



Fig. 8. Total (blue) and first order (red) SIs for the SHF configuration: (a) L_{toe} , (b) L_{S} , (c) \overline{W}_{mz} , (d) Z_{I} , (e) M_{S} and (f) Q_{S}^{total} .



Fig. 9. The marginal effects of uncertain parameters on SWI metrics for the SHF configuration.



a) The length of the saltwater toe (L_{toe})



b) The dimensionless mass of salt persisting in the aquifer (M_s) .

Fig. 10. Comparison between the PCE surrogate and physical (COMSOL) models for the NOF configuration: On the left side, 200 samples used for the experimental design and on the right side, 20 simulations which do not coincide with the experimental design.



Fig. 11. GSA results for the spatial distribution of the salt concentration (NOF configuration):

(a) mean salt concentration (b) variance of the salt concentration, (c) total SI of α_L^M , (d) total SI of K^F , (e) total SI of e^F , (f) total SI index of δ^F and (g) total SI index of α_L^F



Fig. 12. Isochlors distribution for the NOF configuration ($\alpha_L^M = \alpha_L^F = 0.05m$; $K^F = 0.07m / s$; $e^F = 0.1mm$; $\delta^F = 0.2m$, others parameters are the same as Table 3).



Fig. 13. Total (blue) and first order (red) SIs for the NOF configuration: (a) L_{toe} , (b) L_S , (c) \overline{W}_{mz} , (d) Z_I , (e) M_S and (f) Q_S^{total} .



Fig. 14. The marginal effects of uncertain parameters on SWI metrics for the NOF

configuration.

Parameters	Homoge	enous cases	Fractured cases			
$\rho_1 [kg/m^3]$	1	,025	1,025			
$\rho_0 [kg/m^3]$	1,000		1,000			
$q_d [m^2/s]$	² /s] 6.6×10 ⁻⁵		6.6×10 ⁻⁶			
H[m]		1	1			
ℓ [m]		3	2			
K^{M} [m/s]	1.00	01×10 ⁻²	2.5×10^{-4} Horizontal Fracture 1.0×10^{-3} Vertical Fracture			
$K^F [m/s]$		-	7.72×10^{-1}			
$\boldsymbol{\varepsilon}^{\scriptscriptstyle M}$ [-]	().35	0.2			
\mathcal{E}^{F} [-]		-	1.0			
$e^F[m]$		-	0.001			
$d^F[m]$		-	0.5			
$D \left[m^2/s\right]$	18.86×10 ⁻⁶	Diffusive case	18.86×10 ⁻⁷ Horizontal Fracture			
$D_m [m/3]$	9.43×10 ⁻⁸	Dispersive case	1.0×10 ⁻⁶ Vertical Fracture			
α^{M} [m]	0	Diffusive case	0			
$\alpha_L [m]$	0.1	Dispersive case	0			
α^{M} [m]	0	Diffusive case	0			
$\alpha_T [m]$	0.01	Dispersive case	0			
$\alpha_{\scriptscriptstyle L}^{\scriptscriptstyle F}[m]$	$\alpha_L^F[m]$ -		0			
$\alpha_T^F[m]$		-	0			

Table 1. Physical parameters used for the validation of homogeneous and fractured cases

Table 2. SWI metrics for the validation cases: Semi-analytical solution (S-Anl), SWI-COMSOL (Co-st) and SWI-COMSOL-Bq (CO-Bq). The width of the mixing zone for the homogenous case is calculated vertically as in *Fahs et al. [2016]*.

Metrics	Homogenous Diffusive			Homogenous Dispersive			Fractured (Horizontal)		
	S Anl	CO St	CO-	S Anl	CO-St	CO-	TRACES	CO-St	CO-
	S-AIII	0-51	Bq	S-AIII		Bq			Bq
L _{toe}	0.624	0.626	0.625	1.256	1.253	1.251	0.460	0.461	0.460
L_{s}	0.751	0.754	0.752	0.368	0.392	0.391	0.768	0.777	0.776
\overline{W}_{mz}	0.757	0.763	0.760	0.295	0.295	0.294	0.451	0.455	0.455
Z_I	0.419	0.430	0.429	0.527	0.521	0.519	0.492	0.478	0.478
M_{s}	0.109	0.109	0.109	0.150	0.151	0.150	0.113	0.114	0.114
Q_S^{total}	1.068	0.970	0.976	1.061	1.037	1.049	0.625	0.618	0.622

Parameters	Configuration SHF	Configuration NOF			
$\rho_1 [kg/m^3]$	1,025	1,025			
$\rho_0 [kg/m^3]$	1,000	1,000			
$q_d [m^2/s]$	6.6×10^{-6}	6.6×10 ⁻⁶			
H[m]	1	1			
ℓ [m]	2	2			
K^M [m/s]	2.49×10^{-5}	2.49×10 ⁻⁵			
K^F [m/s]	$[1.17 \times 10^{-1} - 7.65 \times 10^{-1}]$	$[1.86 \times 10^{-2} - 1.17 \times 10^{-1}]$			
$\boldsymbol{arepsilon}^{M}$ [-]	0.2	0.2			
$oldsymbol{\mathcal{E}}^{F}$ [-]	1.0	1.0			
e^F [m]	$[3.8 \times 10^{-4} - 9.7 \times 10^{-4}]$	$[3.8 \times 10^{-4} - 9.7 \times 10^{-4}]$			
$d^{F}[m]$	[0.1 - 0.9]	-			
$\delta^{\scriptscriptstyle F}[m]$	-	[0.08 - 0.25]			
$D_m[m^2/s]$	10 ⁻⁹	10 ⁻⁹			
$\alpha_{\scriptscriptstyle L}^{\scriptscriptstyle M}[m]$	[0.05 - 0.3]	[0.05 - 0.3]			
$\alpha_{T}^{M}[m]$	$0.1 imes lpha_L^M$	$0.1 imes lpha_L^M$			
$\alpha_{\scriptscriptstyle L}^{\scriptscriptstyle F}[m]$	[0.05 - 0.3]	[0.05 - 0.3]			
$\alpha_T^F[m]$	0	0			

Table 3. Values and ranges of variability of the parameters used for the GSA.



Order		Or	der s	spars	e PCI	Ξ	
lotal PCE	C _{salt}	L _{toe}	Z_I	M_{s}	$Q_{\scriptscriptstyle S}^{\scriptscriptstyle total}$	L_{s}	\overline{W}_{mz}
3	6	6			5		
4	6	6 4			8		