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Uncertainty analyses of seawater intrusion : numerical and stochastic approaches

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Abstract We consider immiscible saltwater-freshwater flow in heterogeneous coastal aquifers subject to seawater intrusion (sharp interface approach). We focus on the numerical modelling of the saltwater wedge, taking into account the variability and uncertainty due to highly heterogeneous random permeabilities. In this work, we focus on plane flow problems, with vertically integrated permeabilities, without hydrologic sink/source terms. We use a continuation method to obtain solutions for highly variable aquifers. The long term goal is to analyse the resulting uncertainty of the salt wedge penetration inland by various methods, such as spatial sampling; Monte-Carlo simulation; analytical perturbation methods. In this paper, we present statistical results (moments) obtained by spatial sampling of large single replicate numerical simulations based on the statistical homogeneity of the salt wedge in the seashore direction. The variables of interest are the random interface elevation ($Z_{\text{salt}}(x,y)$), and the penetration length of the salt wedge toe ($X_{\text{salt}}(x,y)$).

Key words Seawater intrusion; saltwater; coastal aquifers; porous media; random media; uncertainty; hydrogeology; numerical modelling; perturbation methods; upscaling.

INTRODUCTION

Seawater intrusion is a well known problem occurring in coastal aquifers. This phenomenon can take the form of a seawater wedge extending inland below freshwater. Here we focus on the effects of permeability heterogeneity on the extent of the seawater wedge in a phreatic coastal aquifer. Seawater intrusion is analysed using 2D plane flow Dupuit-Boussinesq approximation, combined to a sharp interface approach (Ghyben-Herzberg). Aquifer heterogeneity is represented *via* a 2D random field permeability (vertically integrated). The simulations are conducted for mildly to highly heterogeneous random fields, with natural log-permeability standard deviation ($\sigma_{\ln k}$) ranging from 1.0 to 4.0. This paper focuses on the need for numerical accuracy in the case of highly heterogeneous aquifers. An optimized continuation method for modelling flow in highly heterogeneous domains is introduced and implemented in a Graphical User Interface (GUI) environment. While the domain geometry is simple, the main computational challenge is to solve the seawater intrusion problem on large numerical grids, with both nonlinear and highly variable coefficients. The numerical results are then analysed in terms of spatial statistics, such as the standard deviation of the seawater interface elevation versus distance from the seashore ($\sigma_{Z_{\text{SALT}}(x)}$).

PROBLEM FORMULATION AND NUMERICAL MODEL

Seawater intrusion is modeled in the framework of the sharp interface approach, while still retaining the essential feature of aquifer variability in the 2D plane. Our approach

assumes that seawater and freshwater are immiscible fluids, and relies on pressure equilibrium relations (Ghyben-Herzberg) to close the resulting system of equations. In this 2D framework, all variables and parameters are spatially distributed in (x,y) .

Applying the hydrostatic assumptions and the pressure continuity condition at the interface, and modifying the Badon-Ghyben-Herzberg configuration to account for a finite outflow face of height ΔZ located undersea, we obtain:

$$\rho_F g (H - Z_{SALT}) = \rho_S g (Z_{SEA} - Z_{SALT} - \Delta Z) + \rho_F g \Delta Z \quad (1)$$

where H is the total freshwater hydraulic head (m), Z_{SALT} is the salt/freshwater interface level (m), g is the gravitational acceleration (m s^{-2}), ρ_F is the freshwater density (kg m^{-3}), ρ_S is the saltwater density (kg m^{-3}), and ΔZ is the vertical depth of the freshwater outflow face at the shoreline (m). The Ghyben-Herzberg closure relation (above) is inserted in the vertically-averaged Boussinesq equations for freshwater, leading to a nonlinear system of equations, namely : steady-state mass conservation for freshwater (2); vertically integrated Darcy's law (3); & freshwater transmissivity (4) :

$$\frac{\partial \Theta}{\partial t} = -\text{div}(\mathbf{Q}) \quad (2)$$

$$\mathbf{Q} = -T(H, Z_{SALT}, Z_{INF}, x, y) \mathbf{grad}(H) \quad (3)$$

$$T = \begin{cases} K(x,y) \times (H - Z_{INF}(x,y)) & \text{if } Z_{SALT} < Z_{INF} \\ K(x,y) \times (H - Z_{SALT}(x,y)) & \text{if } Z_{SALT} \geq Z_{INF} \end{cases} \quad (4)$$

where $K(x,y)$ is hydraulic conductivity (m s^{-1}), Z_{INF} is the impervious substratum level (m), Z_{SALT} is the salt/Freshwater interface level (m), Q is the Darcy specific discharge rate ($\text{m}^2 \text{s}^{-1}$), Θ is the water content ($\text{m}^3 \text{m}^{-3}$), and T the transmissivity ($\text{m}^2 \text{s}^{-1}$). Here we focus on steady state problems. For more details, see Ababou & Al-Bitar (2005).

Numerical simulations of seawater intrusion are carried out using the BigFlow code BF 2000 (Ababou & Trégarot, 2002). The model is based on a single generalized flux-divergence equation (conservative, mixed form) for either 3D or 2D plane flow. Space-time discretization is based on implicit finite volumes, leading to sparse nonlinear systems. These are solved using two interspersed loops: the outer loop implements fixed point (modified Picard) iterations; the inner loop solves the linearized system by preconditioned Conjugate Gradients (DSCG). The 2D plane flow option was specialized for sharp interface seawater intrusion problems (BF-SWIM2D).

CONTROL OF NUMERICAL ACCURACY AND ROBUSTNESS

Continuation method for highly heterogeneous media

Some special considerations were given to the non-linear aspects of the SWIM problem. Indeed, Seawater Intrusion Modeling is “doubly non-linear” because of the non-linearity of the Dupuit Boussinesq equation (head-dependent transmissivity) and because of the nonlinearity due to the interception of the salt interface by the aquifer's substratum. This non-linearity is even stronger when the domain is highly heterogeneous ($K(x,y)$). For these cases, we used a special iterative “re-start method”,

also known as “continuation” or “homotopy” method. The continuation parameter is chosen to be $\sigma_{\ln K}$, the standard deviation of $\ln K$.

The method is implemented iteratively as follows. Step 1: we generate an aquifer with mildly heterogeneous log-permeability ($\ln K(x,y)$) characterized by its mean, standard deviation, and covariance function, using the turning band method (Tompson *et al.*, 1989). Step 2: we simulate seawater intrusion with the SWIM2D module for this first $\ln K$ field. Step 3: we increase the heterogeneity of $\ln K$ by incrementing $\sigma_{\ln(K)}$ while maintaining the other parameters constant. Step 4: we simulate seawater intrusion using the $\ln K$ field from step 3. Steps 3 and 4 are then iterated.

Since the numerical difficulty increases as $\sigma_{\ln K}$ increases, we use a logarithmic function to control the $\sigma_{\ln K}$ increment:

$$\frac{\sigma_i}{\sigma_N} = \frac{\ln(i+1)}{\ln(N+1)} \quad (5)$$

where σ_i is the standard deviation of the i^{th} $\ln K$ field, N is the number of increments, σ_N is the standard deviation of the objective (final) standard deviation. Other incremental functions have been tested; the logarithmic increment proved to be the most efficient.

Fig. 1(a) shows the values of $\sigma_{\ln K}$ for 10 continuation steps (final value $\sigma_{\ln K} = 4.0$). The results are analysed in Fig. 1(b), in terms of error norm vs iteration number. The root-mean-square norm of δH is used, where δH is the head variation over two successive iterations. This δH is to be compared to the total head variation of 1 meter along the mean flow path. The 2D random seawater intrusion problem was solved on a 1000x1000 node grid. The total CPU time for the 10 continuation steps was on the order of one day on a PC Intel Pentium-4 processor, in double precision.

Inside each continuation step, there are two interlooped solvers: (1) the inner loop is the iterative DSCG solver (stopping criterion $\delta H < \varepsilon = 10^{-9}$ (m), and $\text{ITER} \leq 1000$); (2) the outer loop is the fixed point (Picard) iteration solver (stopping criterion $\delta H < \varepsilon = 10^{-6}$ and $\text{ITER} \leq 20$). In Fig. 1(b), the average number of iterations within each continuation step is 18596. However the actual number of iterations per step increases with successive steps. The problem is more difficult as $\sigma_{\ln K}$ increases.

The continuation algorithm, as well as file management and graphic tasks, have been implemented as an option in the GUI application (BF-Py) under development for the BigFlow code. The BF-Py application has been implemented under Python^{®1} and using the wxPython[®] library.

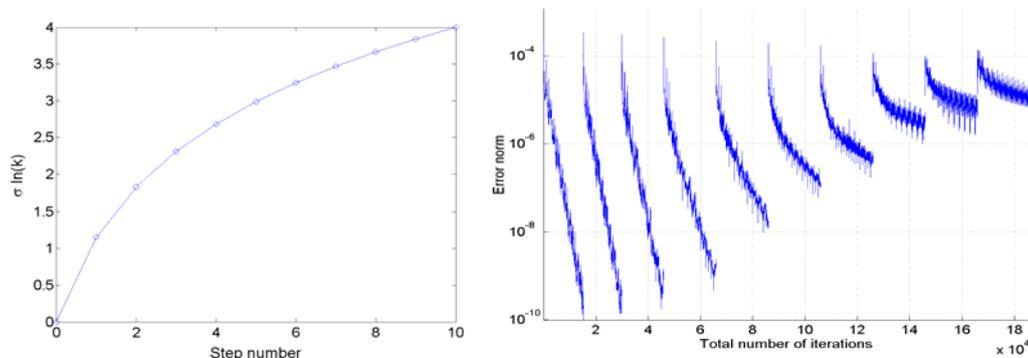


Fig. 1 a Evolution of $\sigma_{\ln K}$ in the homotopy method with $N = 10$ and $\sigma_N = 4.0$ (left)
Fig. 1 b Error norm for ten continuation steps (tens of thousands of iterations).

¹ Python is a freeware, Object Oriented Programming Language, available at <http://www.python.org>; wxPython is a freeware, GUI library, for the Python programming language, based on wxWindows.

Numerical accuracy for high contrast simulations

One issue in simulating highly heterogeneous flows is to ensure numerical accuracy. For this purpose, double precision computations need to be implemented, rather than single precision. To inspect the solver's robustness under double precision computations, a simple configuration with high contrast field properties was used, as shown in Fig. 2(a). The computational domain consists of a square domain with constant permeabilities in which a bar shape with a different permeability is inserted perpendicularly to the flow direction and over the entire width. Fixed heads are applied in the direction of flow, and no flux Neumann conditions perpendicular to the flow.

This heterogeneous "bar shape" configuration has a $\ln K$ contrast that can be expressed in terms of a geometric mean and a standard deviation (Ababou, 1988):

$$K_G = (K_1)^{\alpha_1} (K_2)^{\alpha_2} \quad \sigma_{\ln K} = \sqrt{\left[\left(\ln \left\{ \frac{(K_1)^{\alpha_1}}{K_G} \right\} \right)^2 + \left(\ln \left\{ \frac{(K_2)^{\alpha_2}}{K_G} \right\} \right)^2 \right]} \quad (6)$$

where α_i is the area fraction of the domain associated with permeability K_i ($\alpha_1 + \alpha_2 = 1$).

We conducted seawater intrusion simulations for several values of the permeability contrast (K_1/K_2 or $\sigma_{\ln K}$) and we analysed mass balance (*not shown here for lack of space*). Mass balance remains quite good even for extremely high contrasts: the relative error on the net computed flux is 0.5 % for $K_1/K_2 = 10^8$ or $\sigma_{\ln K} = 5.58$.

Fig. 2(b) shows the analytical solution and the numerical hydraulic head transect $H(x)$ in the middle of the domain, for $K_1/K_2 = 10^{+8}$; the local relative error is less than 10^{-7} .

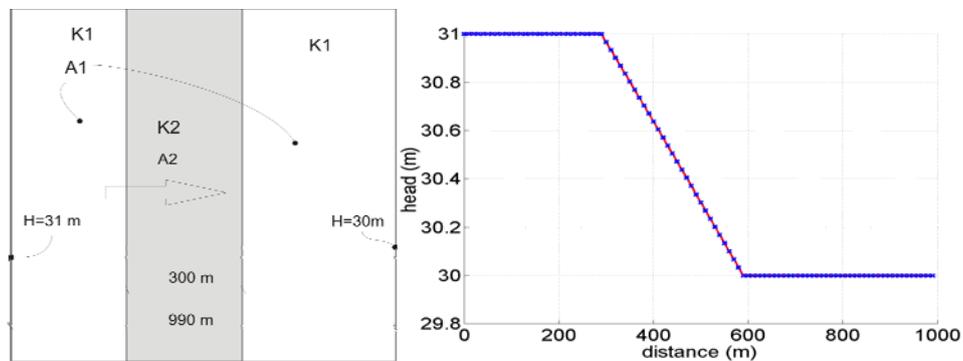


Fig 2 (a) Domain configuration (left).

Fig 2 (b) Numerical (×) and analytical (-) results for $K_1/K_2 = 10^{+8}$ (right).

Robustness of the linear and non-linear system solvers

To complete the non-linear study, we examine in more detail the robustness of the DSCG solver interlooped with the nonlinear Picard solver. First, note that a steady simulation with BigFlow consists of one infinite time step. This is obtained by setting the mass storage term in the linearized equation to zero. The Picard iterations are used to linearize the resulting system.

Let us consider the 1D homogeneous case. In this case the linearized system is tri-diagonal. The CG-based solver should theoretically converge with a number of iterations smaller than or equal to the matrix dimension (Golub & Van Loan, 1989).. This theoretical result was observed experimentally with our double precision simulations using the DSCG solver.

Fig. 3(a) illustrates the results of the CG solver for one outer loop of the Picard iteration. The grid has $1000 \times 1 \times 1$ internal nodes. The results show that convergence is slow until the 999th iteration is reached; then convergence occurs abruptly at the 999th iteration, within machine precision. This behaviour was also observed by Ababou (1996) for linear saturated flow problems.

Fig. 3(b) shows the numerical results for all interlooped iterations (Picard and DSCG). There is an increase in error at the beginning of each new Picard iteration, due to updates of the matrix coefficients. However, this error decreases with iterations, i.e., there is a global convergence of the nonlinear Picard iterations.

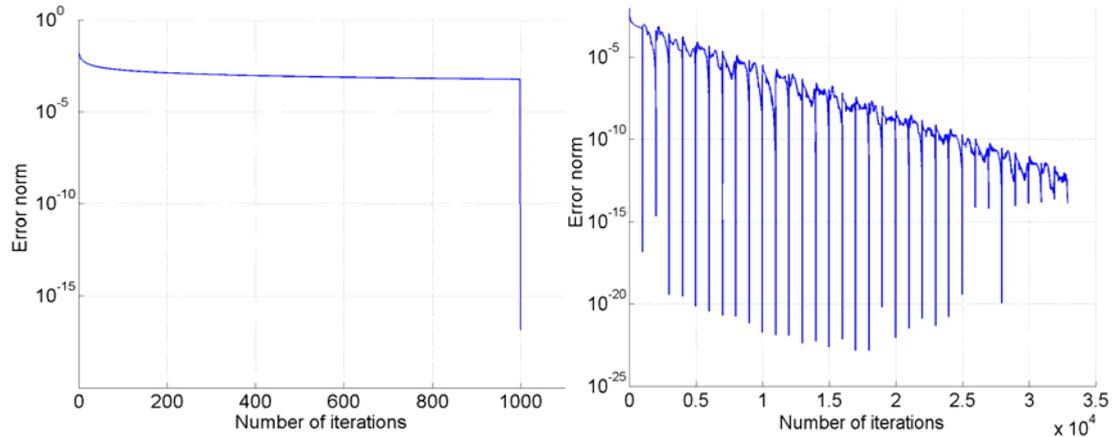


Fig. 3(a) Error norm of the DSCG matrix solver within a single Picard step; notice the abrupt convergence occurring at the 999th iteration (left).

Fig. 3(b) Error norm of the DSCG matrix solver for all Picard iterations (right).

NUMERICAL RESULTS AND ANALYSES

We now analyse the spatial statistics of the seawater wedge (interface elevation $Z_{\text{SALT}}(x,y)$) for the 10 different levels of aquifer variability, as specified in the numerical continuation method. This is shown in Fig. 4(a) and Fig. 4(b).

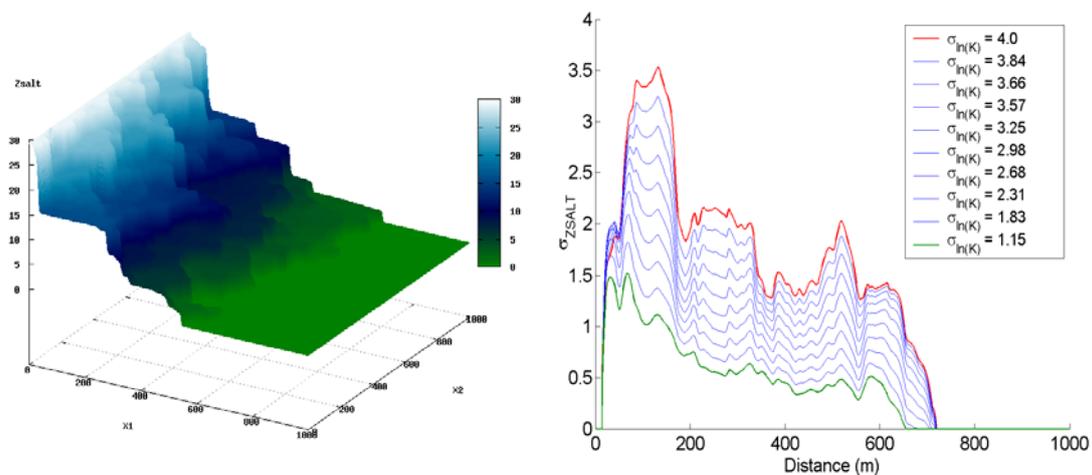


Fig. 4(a) Saltwater/freshwater interface $Z_{\text{SALT}}(x,y)$ for $\sigma_{\text{InK}} = 4.0$ (left).

Fig. 4(b) Transverse profile of $\sigma_{Z_{\text{SALT}}}$ versus distance (x) from seashore, for 10 different values of σ_{InK} ranging from 1.0 to 4.0 (right).

Due to the randomness of the vertically integrated permeability $K(x,y)$, the resulting seawater wedge is very heterogeneous. This can be seen from Fig. 4(a), where $Z_{\text{SALT}}(x,y)$ is shown for the case of largest variability ($\sigma_{\ln K} = 4.0$). In addition, Fig. 4(b) shows the spatial moment $\sigma_{Z_{\text{SALT}}}(x)$ plotted as a function of distance from the seashore, for $\sigma_{\ln K} = 1.0$ up to $\sigma_{\ln K} = 4.0$. This extends results by Ababou & Al-Bitar (2005); they analysed $\sigma_{Z_{\text{SALT}}}(x)$ using a perturbation approximation, valid up to $\sigma_{\ln K} = 1.6$.

CONCLUSIONS AND OUTLOOK

The seawater intrusion problem (sharp interface approach) in randomly heterogeneous coastal aquifers is computationally challenging for three reasons: (1) the problem is nonlinear due to the presence of two unknown surfaces (freshwater and saltwater); (2) large grids are needed in order to compute spatial statistics; (3) the condition of the system becomes worse with both grid size and random permeability contrast ($\sigma_{\ln K}$).

We used different criteria and procedures to control numerical accuracy and performance. Mass balance was close to zero for most random aquifer simulations. Convergence of both inner iterations (CG) and outer iterations (Picard) were carefully controlled via stopping criteria and *a posteriori* analyses of convergence rates. We found that double precision computations were necessary for highly heterogeneous permeabilities. Finally, in order to overcome convergence problems due to large K contrasts ($\sigma_{\ln K} \gg 1$), we introduced a σ -continuation method (homotopy).

The continuation method and other procedures developed in this paper are aimed at a better understanding of $\sigma_{Z_{\text{SALT}}}(x)$, i.e., the variability of seawater intrusion in highly heterogeneous aquifers. A robust perturbation theory is currently being considered for interpreting the results for $\sigma_{\ln K} \gg 1$. A previous perturbation theory (Ababou & Al-Bitar 2005) provided a fairly good fit for $\sigma_{\ln K}$ up to 1.60. Possibly, the correct interpretation of the present numerical experiments requires, for $\sigma_{\ln K} \gg 1$, larger sampling domains (10 million nodes) and/or multiple replicates (Monte-Carlo). Other numerical developments include pumping well modelling, and efficient algorithms to deal with irregular 2D and 3D grid geometry for field applications.

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REFERENCES

- Ababou R (1988) Three-dimensional flow in random porous media. Ph.D. thesis. *M.I.T.*, Cambridge MA, USA.
- Ababou R. (1996) Random Porous Media Flow on Large 3-D Grids: Numerics, Performance, and Application to Homogenization. Chap.1, pp.1-25, in IMA Vol. N° 79 *Mathematics and its Applications: Environmental studies - mathematical, computational and statistical analysis*. M.F.Wheeler ed., Springer, New-York, 410 pp.
- Ababou R. & Al-Bitar A. (2005) Random field approach to seawater intrusion in heterogeneous coastal aquifers: unconditional simulations and statistical analysis. In: *Geostatistics for Environmental Applications*, Renard P., Demougeot-Renard H., Froidevaux R. (eds.), Springer Verlag.
- Ababou R & Trégarot G (2002) Coupled Modeling of Partially Saturated Flows : Macro-Porous Media, Interfaces, and Variability. In: Proc. CMWR 02, *Comput. Meth. Water Resour.*, June 2002, Delft, The Netherlands, Elsevier, 8 pp.
- Ababou R & Bagtzoglou A.C. (1993) BIGFLOW: a Numerical Code for Simulating Flow in Variably Saturated, Heterogeneous Geologic Media - Theory and User's Manual Ver.1.1. *NUREG/CR-6028*, Washington DC., USA.
- Tompson AFB, Ababou R, Gelhar LW (1989) Implementation of the Three-Dimensional Turning Bands Random Field Generator, 2227-2243. *Water Resour. Res.* 25(10).
- Golub G.H. & Van Loan C.F. (1989) *Matrix computations*. 2nd Ed., J. Hopkins Univ. Press, Baltimore, Maryland, 642 pp.