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NUMERICAL SIMULATION OF THE IMPACT OF WATER-AIR FRONTS ON RADIONUCLIDE PLUMES IN HETEROGENEOUS MEDIA

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Abstract. *The goal of this paper is to investigate the interaction of water-air fronts with radionuclide plumes in unsaturated heterogeneous porous media. This problem is modeled by a system of equations that describes both the water-air flow and the radionuclide transport. The water-air flow problem is solved numerically by a mixed finite element combined with a non-oscillatory central difference scheme. For the radionuclide transport equation we use the Modified Method of Characteristics (MMOC). We present the results of numerical simulations for heterogeneous permeability fields taking into account sorption effects.*

keywords: *central difference scheme, Modified Method of Characteristics, mixed finite element method, radionuclide contamination, unsaturated porous medium*

1. Introduction

An important problem arises when a nuclear waste repository is located in subsurface media: the issue of an accidental release of radioactive material through the hydrological environment. Since this complex environment offers difficulties in the prediction of the movement of the radioactive contaminant, investigations concerning the radionuclide transport in unsaturated porous media must be performed to address adequately the problem.

We present a new numerical procedure developed for the problem of two-phase flow with radionuclide transport in an unsaturated two-dimensional porous medium. The immiscible and incompressible phases are water and air. The unsaturated flow and contaminant transport problems can be described by two coupled sets of equations; one set models the two-phase flow and another set governs the contaminant transport within the water phase. This approach was used by Binning, 1994.

The two-phase flow system is expressed in terms of an elliptic equation for a global pressure coupled to a nonlinear conservation law for the water saturation. We solve such system of equations using a precise numerical method which combines a mixed finite element method for the global pressure problem with a second-order, non-oscillatory, central finite difference scheme for the conservation law associated with the water saturation; this numerical procedure was carefully validated by Aquino, 2003. The two-phase flow solution displays a sharp water-air front that represents the transient infiltration of water in the unsaturated zone.

Contaminant transport is typically described by convection-diffusion equations that are dominated by hyperbolic terms. Numerical solution of hyperbolic equations by first-order finite difference schemes may introduces numerical diffusion near sharp fronts; some other methods, based on straightforward higher-order finite differences, may introduce oscillations in the numerical solutions. In the case of radionuclide transport a linear convection-diffusion equation is associated to the radionuclide concentration. We solve this equation using the original *MMOC* procedure (Douglas and Russel, 1982) for the time discretization; a mixed element finite method is used in the approximation of diffusive effects and a domain decomposition iteration (Douglas et al., 1993) is used to handle the resulting linear algebraic problems.

In this paper we perform numerical experiments in order to investigate the interaction of sharp water-air fronts with radionuclide plumes. We will apply our numerical method to simulate an hypothetical scenario of accident involving nuclear contamination. In this accident the radioactive material is dissolved in water and this contaminated solution is transported by the water infiltration in the unsaturated zone. The numerical experiments consider heterogeneous media and the sorption effect of the porous medium on the radionuclide.

2. Governing equations

We study a model that describes water-air flow along with contaminant transport in unsaturated heterogeneous porous media. In this section the governing partial differential equations are presented. We make the following assumptions:

- The fluids are immiscible and incompressible.
- The temperature of the system is considered constant.
- The water-air flow is independent of the contaminant concentration.

2.1. Water-air flow system

Let us describe our model for the water-air flow problem. The equation for the water-phase flow in unsaturated porous media takes the form (Douglas et al., 2000):

$$\frac{\partial}{\partial t}(\phi s_\alpha) + \nabla \cdot \mathbf{u}_\alpha = 0\,, \tag{1}$$

where ϕ is the porosity and s_α the α-phase saturation. In Eq. (1) $\mathbf{u}_\alpha$ is the α-phase velocity given by Darcy's law

$$\mathbf{u}_\alpha = -k\lambda\lambda_\alpha\left(\nabla p_\alpha - \rho_\alpha g \nabla Z\right)\,, \tag{2}$$

where k is the absolute permeability, g is the gravitational constant, p_α is the α-phase partial pressure, ρ_α is the α-phase specific mass, and Z is the depth. The total mobility is defined as $\lambda = (k_{ra}/\mu_a) + (k_{rw}/\mu_w)$, where $k_{r\alpha}$ is the relative permeability, μ_α the viscosity and the relative mobility is defined as $\lambda_\alpha = k_{r\alpha}/\mu_\alpha\lambda$ with $\alpha = w$ (water) or a (air), and we assume that the medium is saturated by water and air, $s_a + s_w = 1$.

Thus, a bit of algebraic manipulation with Eq. (1) leads to the (global) pressure equation (Douglas et al., 2000)

$$\nabla \cdot \mathbf{u} = 0\,, \tag{3}$$

where

$$\mathbf{u} = -k\lambda\left[\nabla p - (\lambda_a\rho_a + \lambda_w\rho_w)\right] g\nabla Z\,. \tag{4}$$

where p is the global pressure. By neglecting capillary pressure forces the saturation equation for the water phase can be written as

$$\phi\frac{\partial s_w}{\partial t} + \nabla \cdot \{\lambda_w[\mathbf{u} + k\lambda\lambda_a(\rho_w - \rho_a)g\nabla Z]\} = 0\,. \tag{5}$$

2.2. Radionuclide transport equation

We assume that a non-volatile radionuclide is only transported by the water phase. Thus, the governing equation of the radionuclide transport depends on the mass balance statement for the water phase.

Let c_w be the concentration of the radionuclide in the water phase and let c_s be the concentration in the solid matrix. Then we can write two balance equations involving c_w and c_s (Bear, 1979). Within the water phase

$$\frac{\partial}{\partial t}(\theta_w c_w) + \nabla \cdot (\mathbf{u}_w c_w) - \nabla \cdot (\theta_w \mathbf{D}\nabla c_w) + \gamma\theta_w c_w = -f(c_w, c_s)\,, \tag{6}$$

and on the solid matrix

$$\frac{\partial}{\partial t}(\theta_s \rho_s c_s) + \gamma \theta_s \rho_s c_s = f(c_w, c_s)\,, \tag{7}$$

where θ_w is the volumetric water content ($\theta_w = \phi s_w$), $\mathbf{u}_w$ is the volumetric flux of the water phase, γ is the radioactive decay constant, $\mathbf{D}$ is the dispersion coefficient tensor, θ_s is the volumetric content of solid matrix ($\theta_s = 1 - \phi$), ρ_s is the specific mass of the solid matrix, and $f(c_w, c_s)$ is the sorption term.

Assuming that the concentrations c_w and c_s are always in equilibrium, this implies that

$$c_s = k_d c_w\,,$$

where k_d is a distribution coefficient.

The two equations above may now be simplified by adding them:

$$\frac{\partial}{\partial t}[(\theta_w + \theta_s \rho_s k_d) c_w] + \nabla \cdot (\mathbf{u}_w c_w) - \nabla \cdot (\theta_w D \nabla c_w) + (\theta_w + \theta_s \rho_s d_d) \gamma\, c_w = 0\,. \tag{8}$$

By expanding the derivatives in the first and second terms of the Equation (8), one gets

$$c_w \frac{\partial \theta_w}{\partial t} + c_w \nabla \cdot \mathbf{u}_w + (\theta_w + \theta_s \rho_s k_d) \frac{\partial c_w}{\partial t} + \mathbf{u}_w \cdot \nabla c_w - \nabla \cdot (\theta_w D \nabla c_w) + (\theta_w + \theta_s \rho_s k_d)\, \gamma\, c_w = 0\,. \tag{9}$$

By making use of the mass balance Equation (1) for the water phase, the first and second terms in the above equation vanish, and then the radionuclide transport equation is given by

$$R(\theta_w) \frac{\partial c_w}{\partial t} + \mathbf{u}_w \cdot \nabla c_w - \nabla \cdot (\theta_w D \nabla c_w) + R(\theta_w)\, \gamma\, c_w = 0\,, \tag{10}$$

where $R(\theta_w) = \theta_w + \theta_s \rho_s k_d$ is defined as the retardation factor.

3. Numerical solution of the water-air flow problem

The water saturation equation, Eq. (5), is solved by a second-order, non-oscillatory, conservative central difference scheme. This scheme is able to solve problems that show sharp fronts in their solution, without solving Riemann problems. The pressure equations, Eq. (3-4), is discretized by mixed finite elements that are suitable to compute accurately the relevant fluxes in heterogeneous permeability fields. The resulting algebraic problems are solved by a preconditioned gradient conjugated method. An operator splitting technique is introduced allowing for a sequential solution of saturation and pressure problems (see Douglas et al., 1997; Douglas et al., 2000).

3.1. Operator splitting

The development of our numerical method will start from Eq. (3)–(5). We will apply an operator splitting technique involving two distinct time steps. As we do not consider here the diffusive part of the saturation equation (because capillarity is neglected), we will only split the pressure calculation from the saturation calculation and we will be led to time steps satisfying $\Delta t_p \geq \Delta t_s$, where the subscripts p and s refer to pressure and saturation, respectively.

We employ locally conservative mixed finite elements to discretize Equations (3) and (4). The discrete equations arising from the application of the lowest index Raviart–Thomas space over squares for one element are (see Douglas et al., 1997; Raviart and Thomas, 1977):

$$\sum_{\beta} u_\beta = 0\,, \tag{11}$$

$$u_\beta = \frac{k_{eff,\beta}\, \lambda_\beta}{h} \left(p - \tilde{p}_\beta + gh\left(\lambda_w \rho_w + \lambda_a \rho_a\right) \nabla Z \cdot \nu_\beta\right)\,, \tag{12}$$

where $\beta = L, R, B, T$ indicate the four edges of an element, $h = \Delta x = \Delta y$ is the length of an element side, $k_{eff,\beta} = 2k\tilde{k}_\beta/(k + \tilde{k}_\beta)$ is the effective permeability between two elements. We use a preconditioned conjugate gradient (PCG) method to solve the velocity–pressure system. The symmetric successive over–relaxation ($SSOR$) method is used for preconditioning the conjugate gradient iterations.

Now, let us turn to the saturation equation, Eq. (5). We indicate a numerical method for the model problem

$$\phi \frac{\partial s_w}{\partial t} + \frac{\partial}{\partial x} f(s_w) + \frac{\partial}{\partial y} g(s_w) = 0\,, \tag{13}$$

to solve Eq. (5). We consider a recently developed numerical method by Nessyahu and Tadmor, 1990 to solve this equation. The method is a second-order, non-oscillatory, conservative central difference scheme. After discretization, the central differencing scheme takes a predictor-corrector form

$$s_{j,k}^{n+\frac{1}{2}} = s_{j,k}^{n} - \frac{1}{2}\left(\alpha_x {f^x}_{j,k}^{n} + \alpha_y {g^y}_{j,k}^{n}\right) , \tag{14}$$

$$s_{j+\frac{1}{2},k+\frac{1}{2}}^{n+1} = \frac{1}{4}\left(s_{j,k}^{n} + s_{j,k+1}^{n} + s_{j+1,k}^{n} + s_{j+1,k+1}^{n}\right) + \frac{1}{16}\left({s^x}_{j,k}^{n} + {s^x}_{j,k+1}^{n} - {s^x}_{j+1,k}^{n} - {s^x}_{j+1,k+1}^{n}\right)$$
$$+\frac{1}{16}\left({s^y}_{j,k}^{n} + {s^y}_{j,k+1}^{n} - {s^y}_{j+1,k}^{n} - {s^y}_{j+1,k+1}^{n}\right) + \frac{\alpha_x}{2}\left(f_{j,k}^{n+\frac{1}{2}} + f_{j,k+1}^{n+\frac{1}{2}} - f_{j+1,k}^{n+\frac{1}{2}} - f_{j+1,k+1}^{n+\frac{1}{2}}\right)$$
$$+\frac{\alpha_y}{2}\left(g_{j,k}^{n+\frac{1}{2}} + g_{j,k+1}^{n+\frac{1}{2}} - g_{j+1,k}^{n+\frac{1}{2}} - g_{j+1,k+1}^{n+\frac{1}{2}}\right) , \tag{15}$$

where $\alpha_x = \Delta t_s/\Delta x$, $\alpha_y = \Delta t_s/\Delta y$ and $\frac{1}{\Delta}\left(\psi^{x\, or\, y}\right)_{j,k}^{n}$ is the numerical derivative of the grid-function $\psi_{j,k}^{n}$ for $\psi = s_w, f, g$

$$\frac{1}{\Delta x}\left(\psi^x\right)_{j,k}^{n} = \frac{\partial}{\partial x}\psi(x = x_j, y = y_k, t = t_n) + \mathcal{O}\left(\Delta x\right) , \tag{16}$$

$$\frac{1}{\Delta y}\left(\psi^y\right)_{j,k}^{n} = \frac{\partial}{\partial y}\psi(x = x_j, y = y_k, t = t_n) + \mathcal{O}\left(\Delta y\right) . \tag{17}$$

To guarantee the desired non-oscillatory property of these approximations our numerical derivatives should satisfy for every grid-function (Nessyahu and Tadmor, 1990)

$$\left(\psi^x\right)_{j,k}^{n} = MinMod\left[\theta\left(\psi_{j+1,k}^{n} - \psi_{j,k}^{n}\right), \frac{1}{2}\left(\psi_{j+1,k}^{n} - \psi_{j-1,k}^{n}\right), \theta\left(\psi_{j,k}^{n} - \psi_{j-1,k}^{n}\right)\right] , \tag{18}$$

where $\theta \in (0, 2)$ stands for a nonlinear limiter, an analogous expression can be written for the y-direction; and the $MinMod[.,.]$ stands for the usual limiter,

$$MinMod\left[x, y\right] = \frac{1}{2}[sgn(x) + sgn(y)].Min(|x|, |y|). \tag{19}$$

At each time level we first reconstruct a piecewise-linear approximation from $\bar{s}(x, y, t) = s_{j,k}(t)$ for $x_{j-\frac{1}{2},k} \leq x \leq x_{j+\frac{1}{2},k}$ and $y_{j,k-\frac{1}{2}} \leq y \leq y_{j,k+\frac{1}{2}}$ (here the over-bar denotes the cell average for $[x_{j,k}, x_{j+1,k}] \times [y_{j,k}, x_{j,k+1}]$); next we evolve in time the piecewise-linear approximation $s(x, y, t + \Delta t_s)$; and finally the resulting solution is projected back into the space of staggered piecewise-constant grid-functions $s_{j+\frac{1}{2},k+\frac{1}{2}}(t + \Delta t_s)$.

4. Numerical solution of the radionuclide transport

We split the linear convection-diffusion equation associated to the radionuclide transport into convective and diffusive problems. The convective problem is solved using the $MMOC$. Mixed finite elements are used in the spatial discretization of the diffusive problem; the linear algebraic problems are handled by a domain decomposition iteration (see Douglas et al., 1993; Douglas et al., 1995).

4.1. Modified method of characteristics

We rewrite the radionuclide transport equation, Eq. (10), in the following form

$$R(\theta_w)\frac{\partial c_w}{\partial t} + \mathbf{u}_w \cdot \nabla c_w - \nabla \cdot \mathbf{v} = g(c_w) , \tag{20}$$

where $\mathbf{v} = \theta_w D \nabla c_w$ and $g(c_w) = -R(\theta_w)\gamma c_w$.

Considering that the flow is essentially along the characteristics associated with the convection $R(\theta_w)\partial c_w/\partial t + \mathbf{u}_w \cdot \nabla c_w$, it is appropriate to introduce differentiation in the characteristic direction τ. Let

$$\psi(\mathbf{x}, \theta_w, \mathbf{u}_w) = \left[R^2(\theta_w) + |\mathbf{u}_w|^2\right]^{\frac{1}{2}} , \tag{21}$$

$$\frac{\partial}{\partial \tau} = \psi^{-1}[R(\theta_w)\frac{\partial}{\partial t} + \mathbf{u}_w \cdot \nabla] , \tag{22}$$

and note that the direction τ is a function of the water content and water volumetric flux, which vary in space and time. It follows easily that the radionuclide transport equation can be written in the form

$$\psi \frac{\partial c_w}{\partial \tau} - \nabla \cdot \mathbf{v} = g(c_w)\,. \tag{23}$$

The $MMOC$ procedure for approximating the directional derivative $\psi \frac{\partial}{\partial \tau}$ is based on backward differencing

$$(\psi \frac{\partial c_w}{\partial \tau})^{n+1}(\mathbf{x}) \approx R(\theta_w^{n+1}) \frac{c_w^{n+1} - c_w^n(\overline{\mathbf{x}}^{n+1})}{\Delta t_p}\,, \tag{24}$$

which allows us to write a discretized form for the radionuclide transport equation

$$R(\theta_w^{n+1}) \frac{c_w^{n+1}(\mathbf{x}) - c_w^n(\overline{\mathbf{x}}^{n+1})}{\Delta t_p} - \nabla \cdot \mathbf{v}^{n+1} = g(c_w^{n+1})\,, \tag{25}$$

where $\mathbf{v}^{n+1} = \theta_w^{n+1} D \nabla c_w^{n+1}$ and

$$\overline{\mathbf{x}}^{n+1} = \overline{\mathbf{x}}(\mathbf{x}, t^{n+1}) = \mathbf{x} - \frac{\Delta t_p}{R(\theta_w^{n+1})} \mathbf{u}_w^{n+1}\,. \tag{26}$$

In this numerical procedure it is not necessary to use extrapolations for θ_w^{n+1} and $\mathbf{u}_w^{n+1}$, since the values have already been obtained from the solution of the water-air flow equations.

5. Numerical experiments

Our numerical experiments are performed in a two-dimensional rectangular domain $\Omega = (0, L_x) \times (0, L_y)$, with boundary conditions $p = 0$ on $y = L_y$, $\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = 0$ on $x = 0, L_x$, where $\mathbf{n}$ is a unit vector normal to the domain boundary. The value of $\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega}$ on $y = 0$ has to be specified.

We present the results of numerical experiments for a physical domain having 16 m $\times$ 32 m discretized by a 64 $\times$ 128 computational grid. Water from rainfall penetrates uniformly into the domain at a constant rate of 1.035 10^{-8} m/s from the top. The following data are held fixed in our experiments: air viscosity $\mu_a = 1.78\ 10^{-5}$ Pa.s, water viscosity $\mu_w = 1.14\ 10^{-3}$ Pa.s, air density $\rho_a = 1.23$ Kg/m^3, water density $\rho_w = 1.0\ 10^3$ Kg/m^3, porosity $\phi = 0.37$, air residual saturation $s_{ra} = 0.2$ and water residual saturation $s_{rw} = 0.0716$. The expressions of the relative permeability function for air and water can be found in Touma and Vauclin, 1986.

The radionuclide considered here is the cesio-237 with an initial concentration of 1.0 Bq in a 4 m $\times$ 4 m region in the physical domain. This initial condition corresponds to a situation where there has been a contaminant release from the radioactive waste repository below the soil surface. In the simulations we use the following parameters: decay constant for the cesio $\gamma = 7.33\ 10^{-10}$ s^{-1} and a constant dispersion coefficient D $= 1.5\ 10^{-9}$ m^2/s.

The numerical experiments use stochastic permeability fields to model heterogeneous formations. These permeability fields were taken to be realizations of self-similar (or fractal) Gaussian random fields (see Glimm et al., 1993 and references therein for the generation of such fields). We consider $\psi(x)$ to be one realization of such random field, and a log-normal permeability field which is given by $k(x) = Me^{S\psi(x)}$, where S is the strength of the heterogeneity and M is the average value for the absolute permeability. In all simulations we have $M = 1.974\ 10^{-14}$ m^2.

5.1. Mass balance error

It is well known that the $MMOC$ procedure is not able to conserve mass (see Douglas et al., 1997), however for miscible displacement problems it has produced accurate numerical solutions with small mass balance errors (Russel and Wheeler, 1983). In order to investigate the influence of water-air fronts on the mass balance of the radionuclide transport, we simulate three physical situations: homogeneous saturated medium and both homogeneous and heterogeneous unsaturated media. The computational domain for the simulations in unsaturated media contains initially 20% water and 80% air. We do not consider either sorption effects or radionuclide decay in this investigation.

The absolute value of the relative mass balance error (ϵ) as a function of the time is shown in the Fig. (1). The results for the homogeneous saturated medium show that the radionuclide mass is adequately conserved with a relative error close to zero. However, for the other situations considered here, the relative error has an increase initially, followed by a decrease in absolute value when the radionuclide plumes are far from the water-air fronts. After a long time this relative error converges to values less than 20%.

The oscillation in the relative mass balance error occurs due to the delay in the radionuclide plume position when compared to the water-air front position (such behavior was also observed by Yeh et al., 1993 and Douglas et al., 1997). Since the radionuclide mass is computed as the product of the water content by the radionuclide concentration, delayed plumes cause large errors in the mass balance. Such a delay is a consequence of the failure of the $MMOC$ to locate precisely the position of the plume.

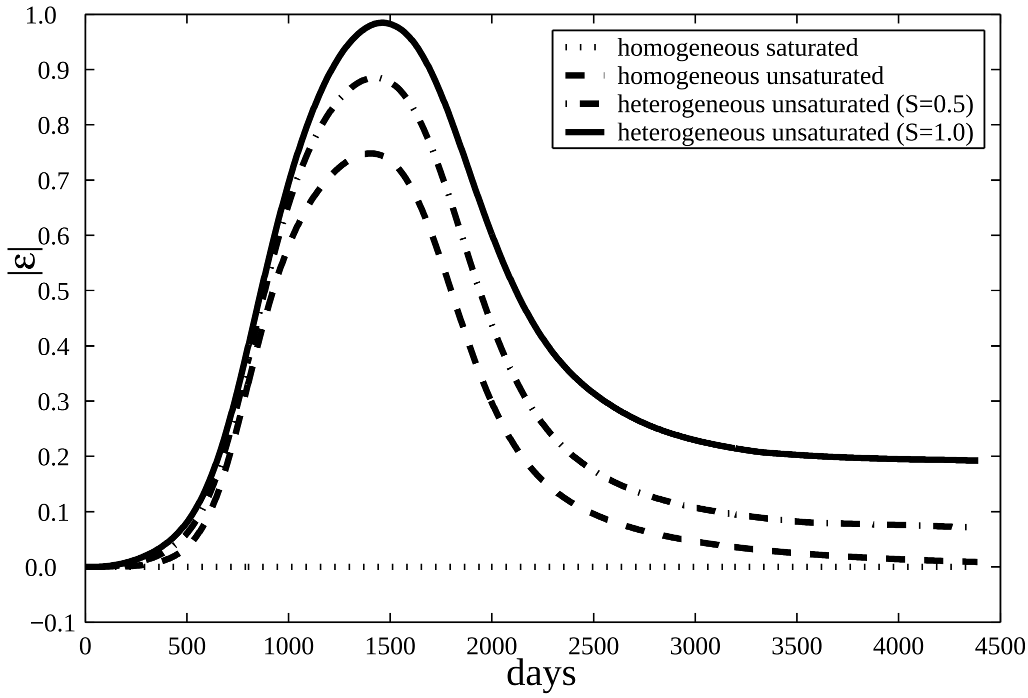

Figure 1: The relative mass balance error curves.

5.2. Weakly heterogeneous unsaturated medium

We investigate the interaction of water-air fronts with radionuclide plumes by considering a permeability field with small variations by setting the strength of the heterogeneity to be $S = 0.5$. We also consider that the radionuclide decay is present in this situation. The pictures of water-air fronts and radionuclide plumes are illustrated in Fig. (2).

5.3. Highly heterogeneous unsaturated medium

Now we simulate our problem considering large variations in the permeability field. For this, the strength of the heterogeneity is set to be $S = 1.0$ and we maintain the radionuclide decay.

The relative mass balance errors produced by the $MMOC$ procedure are higher in this heterogeneous medium. Such a medium generates a highly non-uniform velocity field that introduces some interpolation errors during the $MMOC$ back tracking. This causes numerical diffusion in the radionuclide plume simulation (Yeh et al., 1993. Figure (3) displays the results of this study.

5.4. The sorption effect

Finally, we investigate the interaction of air-water fronts with radionuclide plumes considering heterogeneous unsaturated media, taking into account the sorption effect in the problem. In this simulation, the strength of the heterogeneity is $S = 1.0$ and the sorption term is $k_d = 0.5$.

The result of the simulation is seen in the Fig. (4) where, as expected, we can observe that radionuclide plumes travel with a smaller velocity when the sorption effect is present.

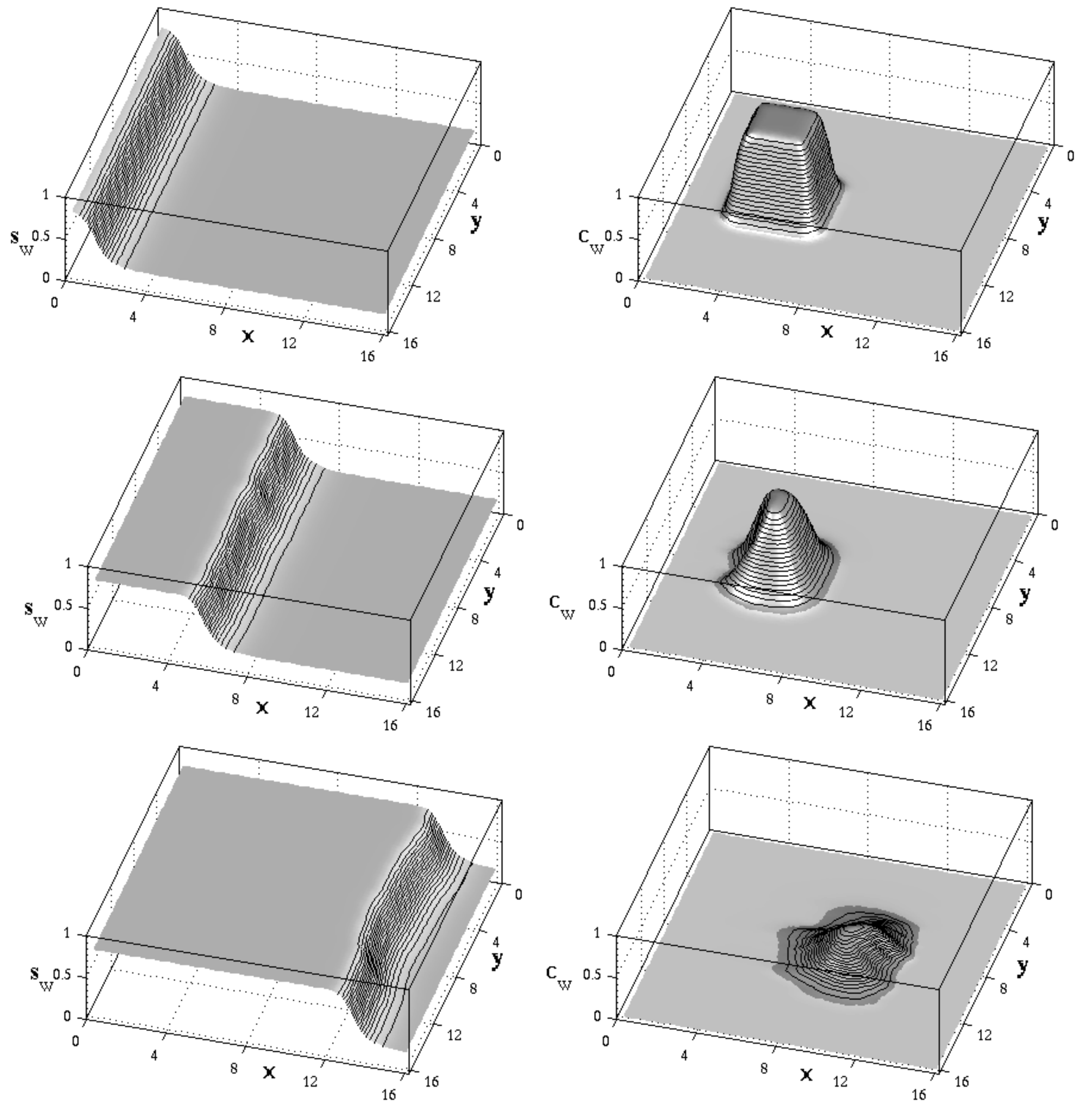

Figure 2: Numerical solution in an heterogeneous medium (M=0.5) at 365, 1460 and 3285 days without sorption effects. Left: water-air front. Right: radionuclide plume.

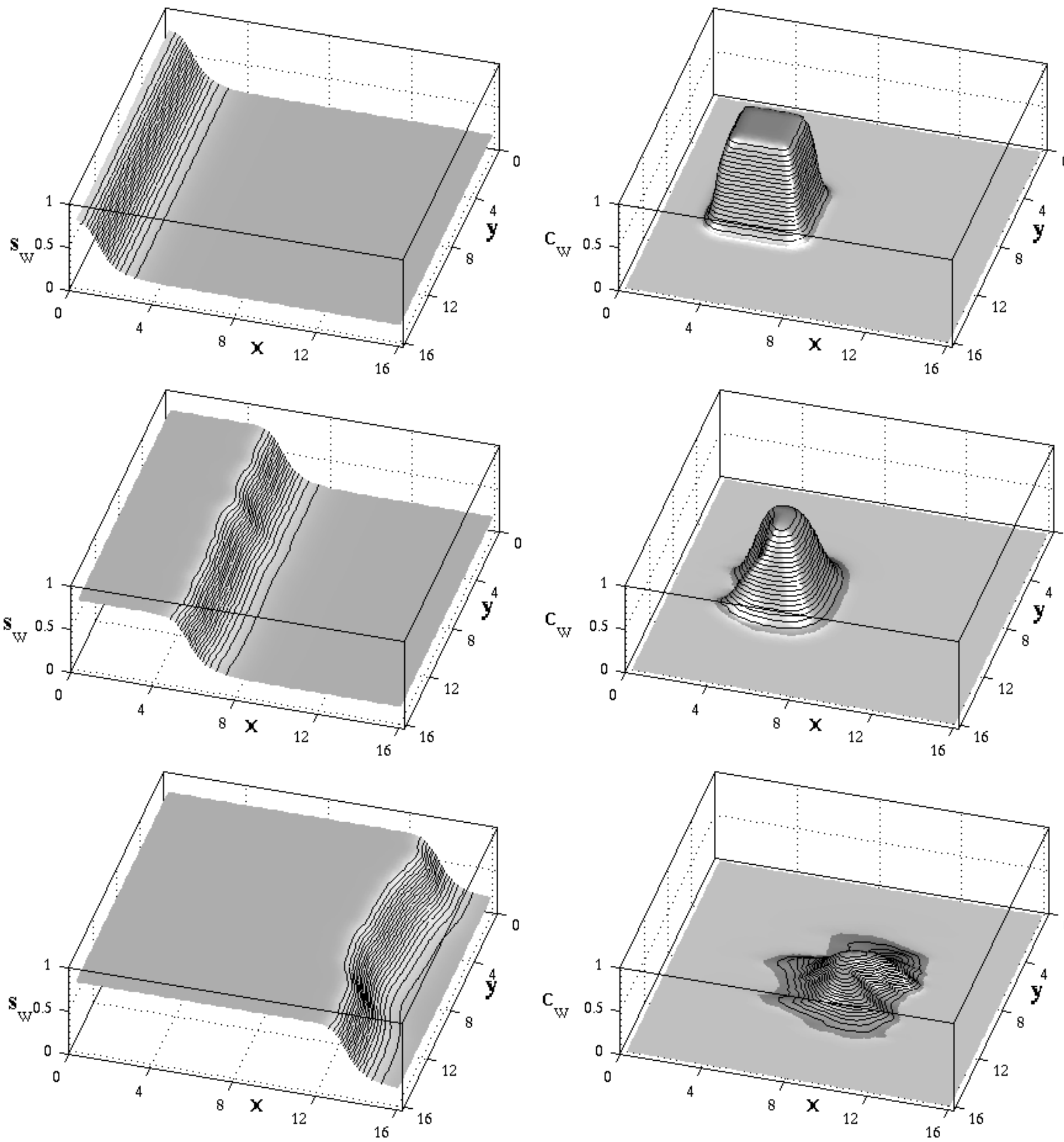

Figure 3: Numerical solution in an heterogeneous medium (M=1.0) at 365, 1460 and 3285 days without sorption effects. Left: water-air front. Right: radionuclide plume.

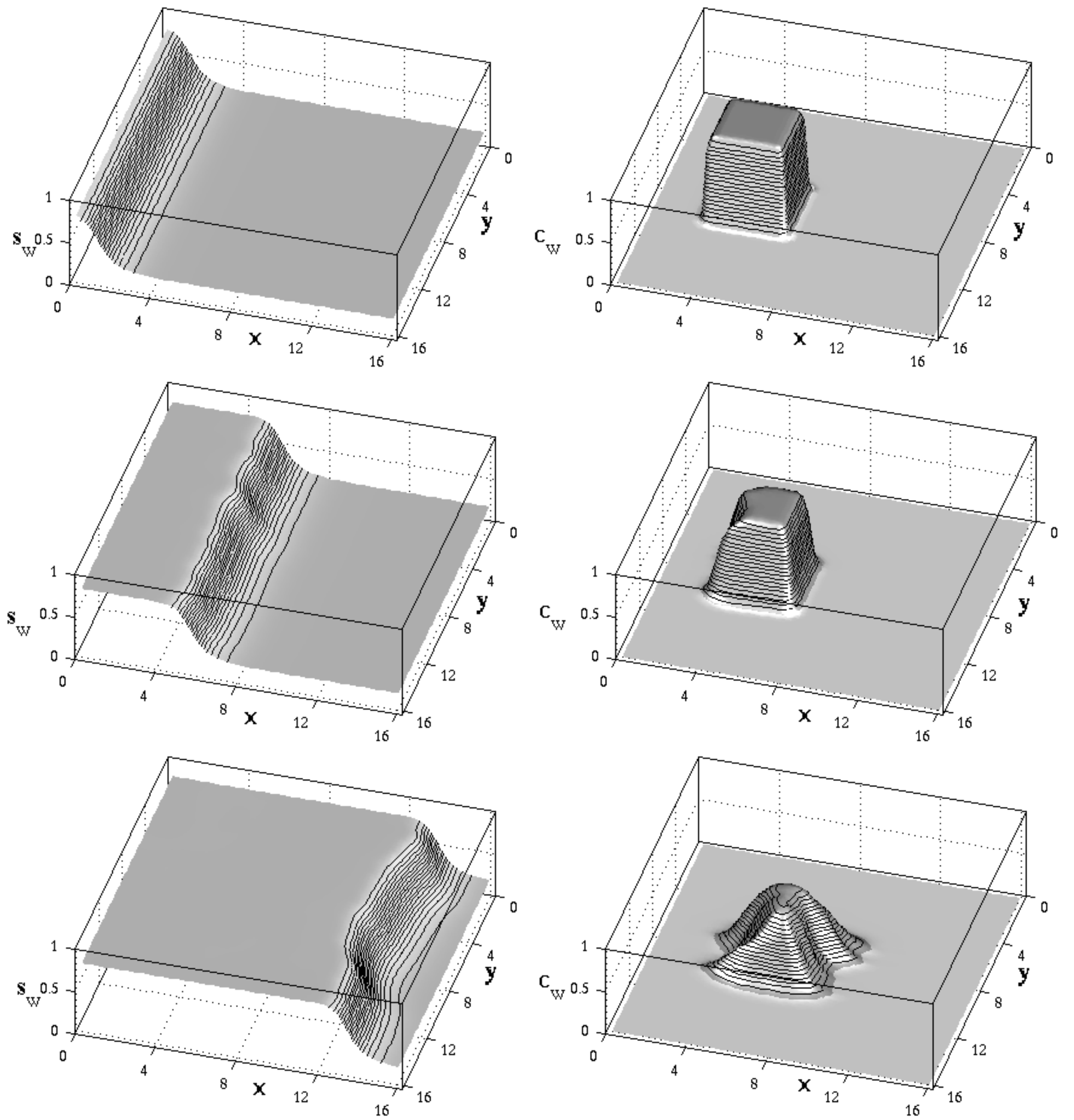

Figure 4: Numerical solution in an heterogeneous medium (M=1.0) at 365, 1460 and 3285 days with sorption effects. Left: water-air front. Right: radionuclide plume.

6. Summary and Conclusions

A two-dimensional numerical method is described to simulate water-air flow and radionuclide transport in unsaturated porous media. Under transient water infiltration solutions of the water-air flow equations display sharp fronts which are propagated in the domain. As long as radionuclide plumes are reached by water-air fronts we find that the $MMOC$ produces large mass balance errors.

To investigate the interaction of water-air fronts with radionuclide plumes numerical simulations were conducted considering heterogeneous permeability fields and sorption effects. Some conclusions based upon the various simulations can be summarized as follows:

- Our numerical scheme to solve the water-air flow problem is computationally efficient and is able to capture accurately sharp fronts in the solutions, even for large grid sizes (Aquino et al., 2004). Thus, we can simulate sharp water-air fronts to investigate the behavior of radionuclide plumes;
- Under transient water infiltration the $MMOC$ procedure produces large oscillations in the relative mass balance error due to the delay in the position of radionuclide plumes;
- We observed the highest relative mass balance errors for the simulations in highly heterogeneous media.

The authors are currently considering the following aspects of the problem at hand:

- The implementation of a Locally Conservative Eulerian-Lagrangian Method (Douglas et al., 2000) for the purpose of conserving the mass locally for the problem of radionuclide transport;
- The impact on the radionuclide plume of the stability-instability problem associated with water-air fronts subject to infiltration and evaporation; a stochastic framework is considered for heterogeneity modeling.

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