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Gas phase appearance and disappearance as a problem with complementarity constraints

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**RESEARCH
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Gas phase appearance and disappearance as a problem with complementarity constraints

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Abstract: The modeling of migration of hydrogen produced by the corrosion of the nuclear waste packages in an underground storage including the dissolution of hydrogen involves a set of nonlinear partial differential equations with nonlinear complementarity constraints. This article shows how to apply a modern and efficient solution strategy, the Newton-min method, to this geoscience problem and investigates its applicability and efficiency. In particular, numerical experiments show that the Newton-min method is quadratically convergent for this problem.

Key-words: Porous media, two-phase flow, dissolution, nuclear waste underground storage, nonlinear complementarity problem, non-smooth function, Newton-min

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Conditions de complémentarité pour l'apparition et la disparition de la phase gazeuse

Résumé : La migration d'hydrogène produit par la corrosion des sites de stockages souterrains des déchets nucléaires avec dissolution de l'hydrogène est formulée comme un ensemble d'équations aux dérivées partielles non-linéaires avec des conditions de complémentarité non-linéaires. Cet article montre comment appliquer une stratégie moderne et efficace, la méthode de Newton-min, pour résoudre ce problème de géosciences. En particulier, les expériences numériques montrent que la méthode de Newton-min se révèle efficace et converge quadratiquement pour ce problème.

Mots-clés : Milieu poreux, écoulement diphasique, dissolution, stockage profond de déchets nucléaires, problème de complémentarité non-linéaire, fonction non-lisse, Newton-min

Contents

1	Introduction	3
2	Problem formulation	4
2.1	Fluid phases	4
2.2	Fluid components	4
2.3	Conservation of mass	5
2.4	Nonlinear complementarity constraints	5
3	Discretization and solution method	6
3.1	A non-smooth system using the Minimum function	6
3.2	Semi-smoothness	7
3.3	The Newton-min algorithm	7
4	Numerical experiment	8
4.1	A problem inspired from the Couplex Gas benchmark	8
4.2	Results and comments	9
4.3	Quadratic convergence	13
5	Conclusion	14

1 Introduction

The couplex-Gas benchmark [22] was proposed by Andra (French National Inventory of Radioactive Materials and Waste) [3] and the research group MoMaS (Mathematical Modeling and Numerical Simulation for Nuclear Waste Management Problems) [21] in order to improve the simulation of the migration of hydrogen produced by the corrosion of nuclear waste packages in an underground storage. This is a system of two-phase (liquid-gas) flow with two components (hydrogen-water). The benchmark generated some interest and engineers encountered difficulties in handling the appearance and disappearance of the phases. The resulting formulation [15] is a set of partial differential equations with nonlinear complementarity constraints. Even though they appear in several problems of flow and transport in porous media like the black oil model presented in [8] or transport problems with dissolution-precipitation [17, 7, 19], complementarity problems are not usually identified as such in hydrogeology and, to circumvent the solution of complementarity conditions, problems are often solved by reformulating the problem as in [6, 1, 2]. However the solution of complementarity problems is an active field in optimization [5, 10, 13] and we draw from the know-how of this scientific community. A similar path is followed in papers like [20, 12, 18]. The application of a semi-smooth Newton method [14, 16], sometimes called the Newton-min algorithm, to solve nonlinear complementarity problem is described. We will demonstrate through a test case, the ability of our model and our solver to efficiently cope with appearance or/and disappearance of one phase.

In the section 2, we introduce the formulation of the problem and in the section 3 we describe the numerical method. In the section 4, we present and discuss a numerical experiment.

2 Problem formulation

This section gives a precise formulation of the mathematical model for the application that was outlined in the introduction. We consider a problem where the gas phase can disappear while the liquid phase is always present.

2.1 Fluid phases

Let ℓ and g be the respective indices for the liquid phase and the gas phase. Darcy's law reads

$$\mathbf{q}_i = -K(x)k_i(s_i)(\nabla p_i - \rho_i g \nabla z), \quad i = \ell, g, \quad (1)$$

where K is the absolute permeability. For each phase $i = \ell, g$, s_i is the saturation and $k_i = \frac{k_{ri}(s_i)}{\mu_i}$ is the mobility with k_{ri} the relative permeability and μ_i the viscosity (assumed to be constant). The mobility k_i is an increasing function of s_i such that $k_i(0) = 0$, $i = \ell, g$. Assuming that the phases occupy the whole pore space, the phase saturations satisfy

$$0 \leq s_i \leq 1, \quad s_\ell + s_g = 1.$$

The phase pressures are related through the capillary pressure law

$$p_c(s_\ell) = p_g - p_\ell \geq 0,$$

assuming that the gas phase is the non-wetting phase. The capillary pressure is a decreasing function of the saturation s_ℓ .

In the following, we will choose s_ℓ and p_ℓ as the main variables since we assume that the liquid phase cannot disappear for the problem under consideration.

2.2 Fluid components

We consider two components, water and hydrogen, identified by the indices $j = w, h$. The mass density of the phase is

$$\rho_i = \rho_w^i + \rho_h^i, \quad i = \ell, g.$$

From M^w and M^h , the water and hydrogen molar masses, we define the molar concentration of phase i :

$$c_i = c_w^i + c_h^i, \quad c_j^i = \frac{s_i \rho_j^i}{M^j}, \quad j = w, h, \quad i = \ell, g. \quad (2)$$

The molar fractions are

$$\chi_h^i = \frac{c_h^i}{c_i}, \quad \chi_w^i = \frac{c_w^i}{c_i}, \quad i = \ell, g. \quad (3)$$

Obviously,

$$\chi_w^i + \chi_h^i = 1, \quad i = \ell, g. \quad (4)$$

We assume that the liquid phase may contain both components, while the gas phase contains only hydrogen, that is the water does not vaporize. In this situation we have

$$\rho_w^g = 0, \quad \rho_g = \rho_h^g, \quad \chi_h^g = \frac{c_h^g}{c_g} = 1, \quad \chi_w^g = 0.$$

For the liquid phase, we assume that the water is the solvent and the hydrogen is the solute and that the quantity of hydrogen dissolved in the liquid is small, that is $c_h^l \ll c_w^l$. So we have

$$\chi_h^l \approx \frac{c_h^l}{c_w^l} = \frac{M^w}{M^h \rho_w^l} \rho_h^l.$$

A third main unknown will be χ_h^l , in addition to s_ℓ and p_ℓ .

2.3 Conservation of mass

We introduce the molecular diffusion flux for the diffusion of hydrogen in the liquid phase

$$j_h^l = -\phi M^h s_\ell c_\ell D_h^l \nabla \chi_h^l \quad (5)$$

where D_h^l is a molecular diffusion coefficient.

Conservation of mass applied to each component, water and hydrogen, gives

$$\begin{aligned} \frac{\partial}{\partial t}(\phi \rho_w^l s_\ell) + \operatorname{div}(\rho_w^l \mathbf{q}_\ell - j_h^l) &= Q_w, \\ \frac{\partial}{\partial t}(\phi s_\ell \rho_h^l + \phi s_g \rho_h^g) + \operatorname{div}(\rho_h^l \mathbf{q}_\ell + \rho_h^g \mathbf{q}_g + j_h^l) &= Q_h. \end{aligned} \quad (6)$$

We assume also that the gas is slightly compressible, that is $\rho_g = C_g p_g$ with C_g the compressibility constant, and that the liquid phase is incompressible, that is ρ_w^l is constant.

2.4 Nonlinear complementarity constraints

Next, we apply Henry's law which says that, at a constant temperature, the amount of a given gas that dissolves in a given type and volume of liquid is directly proportional to the partial pressure of that gas in equilibrium with that liquid.

In the presence of the gas phase, Henry's law reads $H p_g = \rho_h^l$, where $H = H(T) M^h$ with $H(T)$ is the Henry law constant, depending only on the temperature.

There are two possible cases: the gas phase exists: $1 - s_\ell > 0$, Henry's law applies and $H(p_\ell + p_c(s_\ell)) - \rho_h^l = 0$, or the gas phase does not exist, $s_\ell = 1$ and $H(p_\ell + p_c(1)) - \rho_h^l \geq 0$ which says that for a given pressure p_ℓ the concentration ρ_h^l is too small for the hydrogen component to be partly gaseous, or conversely for a given concentration ρ_h^l the pressure p_ℓ is too large for the hydrogen component to be partly gaseous.

These cases can be written as complementary constraints

$$(1 - s_\ell)(H(p_\ell + p_c(s_\ell)) - \rho_h^l) = 0, \quad 1 - s_\ell \geq 0, \quad H(p_\ell + p_c(s_\ell)) - \rho_h^l \geq 0. \quad (7)$$

Finally we end up with a system of nonlinear partial differential equations (conservation equations (6) and Darcy laws (1)) with the nonlinear complementarity constraints (7) describing the transfer of hydrogen between the two phases, the unknowns being s_ℓ , p_ℓ , and χ_h^l . This formulation has the advantage of being valid whether the gas phase exists or not [15].

3 Discretization and solution method

We use a first order Euler implicit scheme for time discretization and cell-centered finite volumes for space discretization. We denote by N , the number of degrees of freedom for s_ℓ , p_ℓ and χ_h^ℓ which is equal to the number of cells. We introduce

- $x \in \mathbb{R}^{3N}$, the vector of unknowns for s_ℓ , p_ℓ , χ_h^ℓ ,
- $\mathcal{H} : \mathbb{R}^{3N} \rightarrow \mathbb{R}^{2N}$, the discretized conservation equations,
- $\mathcal{F} : \mathbb{R}^{3N} \rightarrow \mathbb{R}^N$, the discretized function $1 - s_\ell$,
- $\mathcal{G} : \mathbb{R}^{3N} \rightarrow \mathbb{R}^N$, the discretized function $H(p_\ell + p_c(s_\ell)) - \frac{M^h \rho_w^\ell}{M^w} \chi_h^\ell$.

Then at each time step the problem can be written in compact form

$$\begin{aligned} \mathcal{H}(x) &= 0, \\ \mathcal{F}(x)^\top \mathcal{G}(x) &= 0, \quad \mathcal{F}(x) \geq 0, \quad \mathcal{G}(x) \geq 0, \end{aligned} \tag{8}$$

where the inequalities have to be understood component-wise.

3.1 A non-smooth system using the Minimum function

It is well known that complementarity conditions, consisting of equations and inequalities, can be expressed equivalently by an equation via a complementarity function [10](C-function). Let

$$\begin{aligned} \varphi : \mathbb{R}^N \times \mathbb{R}^N &\rightarrow \mathbb{R}^N \\ (a, b) &\mapsto \min(a, b) \end{aligned}$$

be the minimum function, in which the min operator acts component-wise. This is a C-function, in the sense that it satisfies

$$\varphi(a, b) = 0 \iff a \geq 0, \quad b \geq 0, \quad a^\top b = 0. \tag{9}$$

Other typical scalar C-functions [10] are

- the Fisher-Burmeister function: $\varphi(a, b) = \sqrt{a^2 + b^2} - a - b$,
- $\varphi(a, b) = -ab + \min^2(0, a) + \min^2(0, b)$.

Using this minimum function, we can write the complementarity problem (8) as

$$\begin{aligned} \mathcal{H}(x) &= 0, \\ \varphi(\mathcal{F}(x), \mathcal{G}(x)) &= 0. \end{aligned} \tag{10}$$

Hence, the resulting system of mass conservation (differential) equations and equilibrium conditions is fully free of inequalities (pure set of equations). The only drawback of the introduction of a complementarity problem is that the problem is no longer C^1 , since $\varphi \notin C^1(\mathbb{R}^{2N}, \mathbb{R}^N)$, while the typical assumption for having the local quadratic convergence of Newton's algorithm requires to have a " C^1 function with a Lipchitz-continuous derivative". However, it is well known, especially in the community of optimization, that the assumptions can be weakened in several ways, for example by only assuming strong semi-smoothness. In the next section we give the definition of semi-smoothness from [9, 10].

3.2 Semi-smoothness

Let $\psi : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a locally lipschitz-continuous function. Then, by Rademacher's theorem[10], there is a dense subset $D \subset \mathbb{R}^N$ on which f is differentiable. The B -subdifferential of ψ at a point $x \in \mathbb{R}^N$ is the set

$$\partial_B \psi(x) := \{J \in \mathbb{R}^{N \times N} \mid J = \lim_{k \rightarrow \infty} \psi'(x_k), (x_k) \subset D, x_k \rightarrow x\},$$

where ψ' is the derivative of ψ . The *generalized Jacobian* of ψ at x [9] is the set

$$\partial \psi(x) = \text{co } \partial_B \psi(x),$$

where $\text{co } S$ denotes the convex hull of a set S . Now, the function ψ is said to be semi-smooth at x if ψ is directionally differentiable at x and

$$Jd - \psi'(x; d) = o(\|d\|),$$

for any $d \rightarrow 0$ and for any $J \in \partial \psi(x + d)$, where $\psi'(x; d)$ denotes the directional derivative of ψ at x in the direction of d . Analogously, ψ is called *strongly semi-smooth* at x , if

$$Jd - \psi'(x; d) = o(\|d\|^2).$$

ψ is called (strongly) semi-smooth if ψ is (strongly) semi-smooth at any point $x \in \mathbb{R}^N$.

It is well known that the minimum function and the Fisher-Burmeister function are strongly semi-smooth. One can then solve system (10) using the semi-smooth Newton's method, called the Newton-min method [5, 4] when the min function is used. The Newton-min method can also be regarded as an active set strategy [14].

3.3 The Newton-min algorithm

We now give an exact statement of the Newton-min algorithm for solving the nonlinear system of equation (10).

Below $\partial \varphi(x)$ denotes the generalized Jacobian of φ at a point x . Let Res be the residual of $\psi(x)$ where $\psi(x) := \begin{pmatrix} \mathcal{H}(x) \\ \varphi(x) \end{pmatrix}$ and ε be a stopping criterion for Res.

Let $x^1 \in \mathbb{R}^N$. For $k = 2, 3, \dots$, do the following.

- 1) If $\text{Res} \leq \varepsilon$, stop.
- 2) Define the complementary index sets A^k and I^k by

$$A^k := \{i : \mathcal{G}_i(x^k) < \mathcal{F}_i(x^k)\}, \quad I^k := \{i : \mathcal{G}_i(x^k) \geq \mathcal{F}_i(x^k)\}.$$

- 3) Select an element $\mathcal{J}_x^k \in \partial \varphi(x^k)$ such that its i th line is equal to $\mathcal{F}'_i(x^k)$ [resp. $\mathcal{G}'_i(x^k)$] if $\mathcal{F}_i(x^k) \leq \mathcal{G}_i(x^k)$ [resp. $\mathcal{F}_i(x^k) > \mathcal{G}_i(x^k)$].

4) Let x^{k+1} be a solution to

$$\begin{aligned}\mathcal{H}(x^k) + \mathcal{H}'(x^k)(x^{k+1} - x^k) &= 0, \\ \varphi(x^k) + \mathcal{J}_x^k(x^{k+1} - x^k) &= 0, \quad \mathcal{J}_x^k \in \partial\varphi(x^k).\end{aligned}$$

Note that, as in a smooth Newton method, only one linear system has to be solved at each Newton iteration.

Furthermore the Newton-min method satisfies also a quadratic convergence property. Indeed, a theorem[10] says that if x^* is a solution to the system $\psi(x) = 0$, such that J is nonsingular for all $J \in \partial\psi(x^*)$ (as defined in section 3.2), then for any initial value sufficiently close to x^* , the Newton-min method generates a sequence that converges quadratically to x^* .

We have not yet proved the hypothesis of non-singularity of J for our system but we observed the quadratic convergence in our numerical experiments.

4 Numerical experiment

4.1 A problem inspired from the Couplex Gas benchmark

We consider a one-dimensional core with length $L = 200$ m, initially saturated with liquid ($s_\ell = 1$) and containing no hydrogen ($\chi_h^\ell = 0$). Hydrogen is injected at a given rate on the left. After a while the hydrogen injection is stopped. The problem is then to simulate the migration of hydrogen and to illustrate the gas appearance and disappearance phenomena.

We calculate spatial evolutions of the liquid pressure, the total hydrogen molar density and the the gas saturation along the line. Computations are performed from the initial time up to the stationary state.

The core is supposed to be homogenous porous medium. The capillary pressure function p_c and the relative permeability functions, k_{rl} and k_{rg} , are given by the Van Genuchten-Mualem model [11]:

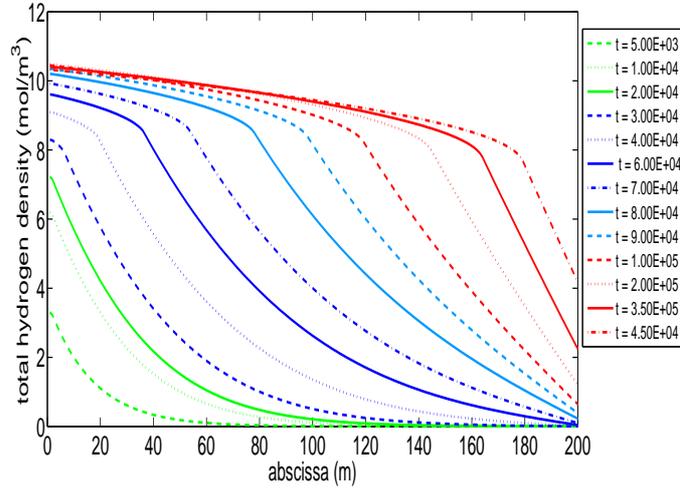
$$\begin{aligned}p_c &= P_r \left(S_{le}^{-1/m} - 1 \right)^{1/n}, \\ k_{rl} &= \sqrt{S_{le}} \left(1 - \left(1 - S_{le}^{1/m} \right)^m \right)^2, \quad k_{rg} = \sqrt{1 - S_{le}} \left(1 - S_{le}^{1/m} \right)^{2m},\end{aligned}$$

with $S_{le} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}$ and $m = 1 - \frac{1}{n}$, and where parameters P_r , n , S_{lr} and S_{gr} depend on the porous medium. The parameters describing the porous medium and the fluid characteristics are given in Table 1. Fluid temperature is fixed to $T = 303$ K.

Initial conditions are $S_\ell(t = 0) = 1$, $\chi_h^\ell(t = 0) = 0$ and $p_\ell(t = 0) = 10^6$ Pa. For boundary conditions on the left, the hydrogen flow rate is given, $\rho_h^\ell \mathbf{q}_\ell + \rho_h^g \mathbf{q}_g + j_h^\ell = 5.57 \cdot 10^{-6}$ kg/m²/year. From this condition, one can deduce the saturation. Still on the left, we impose a zero water flow rate $\rho_w^\ell \mathbf{q}_\ell - j_h^\ell = 0$. On the right, the liquid pressure is given, $p_\ell = 10^6$ Pa, and the liquid saturation is set to $s_\ell = 1$.

Porous medium parameters		Fluid characteristics parameters	
Parameter	Value	Parameter	Value
K	$5 \cdot 10^{-20} \text{ m}^2$	T	303 K
ϕ	0.15 (-)	D_ℓ^h	$3 \cdot 10^{-9} \text{ m}^2/\text{s}$
P_r	$2 \cdot 10^6 \text{ Pa}$	μ_ℓ	$1 \cdot 10^{-9} \text{ Pa}\cdot\text{s}$
n	1.49 (-)	μ_g	$9 \cdot 10^{-9} \text{ Pa}\cdot\text{s}$
S_{lr}	0.4 (-)	$H(T = 303\text{K})$	$7.65 \cdot 10^{-6} \text{ mol/Pa/m}^3$
S_{gr}	0 (-)	M_w	10^{-2} kg/mol
		M_h	$2 \cdot 10^{-3} \text{ kg/mol}$
		ρ_w^ℓ	10^3 kg/m^3

Table 1: Values of porous medium fluid characteristics.

Figure 1: Spatial evolution of hydrogen density at several times t (in years) during hydrogen injection.

4.2 Results and comments

For the numerical simulation below we divided the space interval into 200 intervals of equal length and we used a constant time step of 5000 years. During the simulation, we can identify four important periods, three periods during injection and one period after injection.

During injection (figures 1, 2 and 3): $0 < t < 5.10^5$ years

- Period 1 ($0 < t < 2 \cdot 10^4$ years): only the hydrogen density increases (Figure 1, green curves), while the liquid pressure and the gas saturation stay constant (Figures 2 and 3, green curve); the whole domain is saturated with water ($s_g = 0$).
- Period 2 ($2 \cdot 10^4 \leq t \leq 1.5 \cdot 10^5$ years): at $t = 2 \cdot 10^4$, the gas phase appears

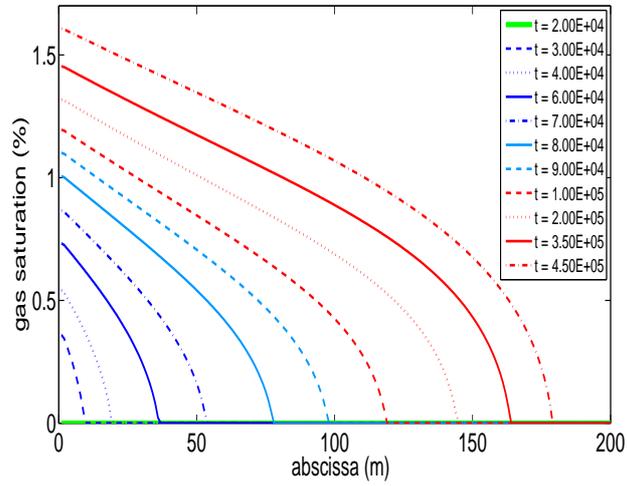


Figure 2: Spatial evolution of gas saturation at several times t (in years) during hydrogen injection.

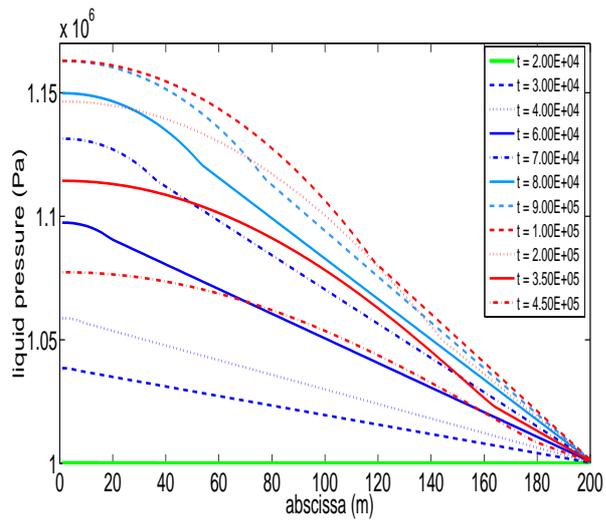


Figure 3: Spatial evolution of liquid pressure at several times t (in years) during hydrogen injection.

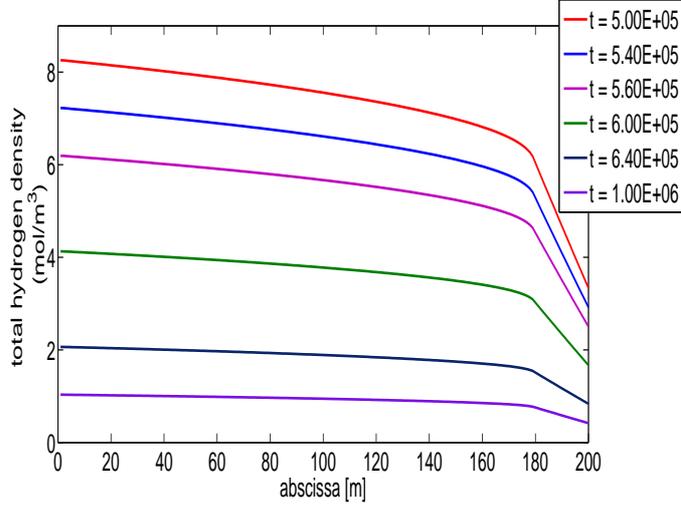


Figure 4: Spatial evolution of hydrogen density at several times t (in years) after hydrogen injection is stopped.

($s_g > 0$). During this period, the liquid pressure increases (Figures 3, blue curves) and pressure gradients are non zero which corresponds to a displacement of both phases. The total hydrogen density and the gas saturation increase (Figures 1 and 2, blue curves) and the unsaturated area grows.

- Period 3 ($1.5 \cdot 10^5 < t < 5 \cdot 10^5$ years): while the total hydrogen density and the gas saturation continue to increase (Figures 1 and 2, red curves); the liquid pressure and the pressure gradient decrease since there is no water injection (Figure 3, red curves).

After injection (Figures 4, 5 and 6):

- Period 4 ($t > 5 \cdot 10^5$ years): cell by cell, starting from the right, the gas saturation decreases and after a while, the gas phase disappears (Figure 5). At the end of the simulation the system reaches a stationary state (Figure 4) and the liquid pressure gradient goes to zero (Figure 6).

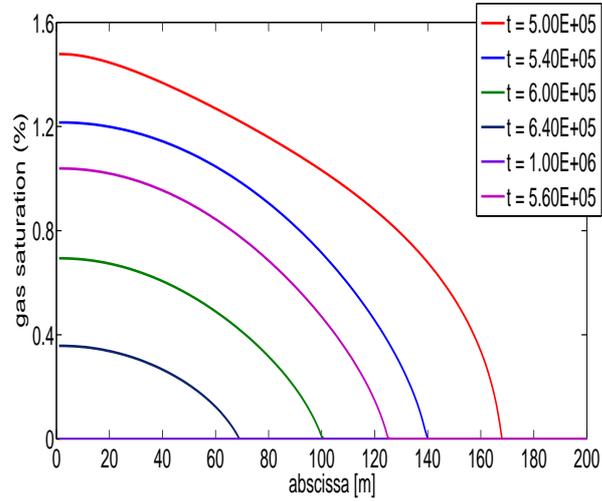


Figure 5: Spatial evolution of gas saturation at several times t (in years) after hydrogen injection is stopped.

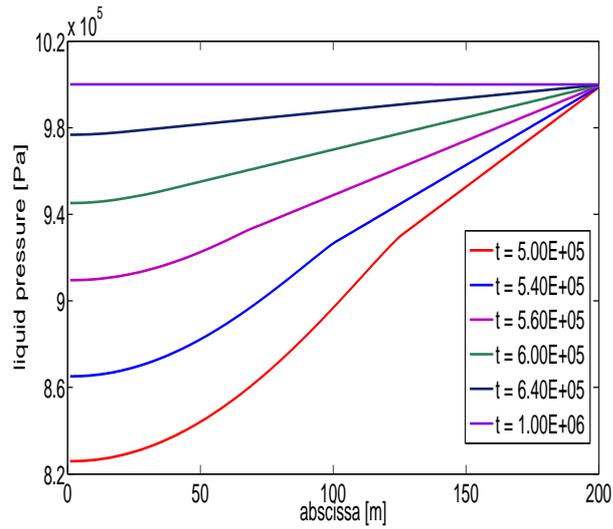


Figure 6: Spatial evolution of liquid pressure at several times t (in years) after hydrogen injection is stopped.

4.3 Quadratic convergence

The figure 7 shows the number of Newton-min iterations per time step for two convergence criterions, $\varepsilon_1 = 1.e-5$ (red curve) and $\varepsilon_2 = 1.e-10$ (blue curve). The points are connected with a straight line. As mentioned at the end of section 3.3, one can expect local quadratic convergence, at least for time steps which are sufficiently small. In Figure 7, we can observe this quadratic convergence. Indeed one can verify in this figure that, at each time step, the residue goes from 1.e-5 to 1.e-10 in one iteration.

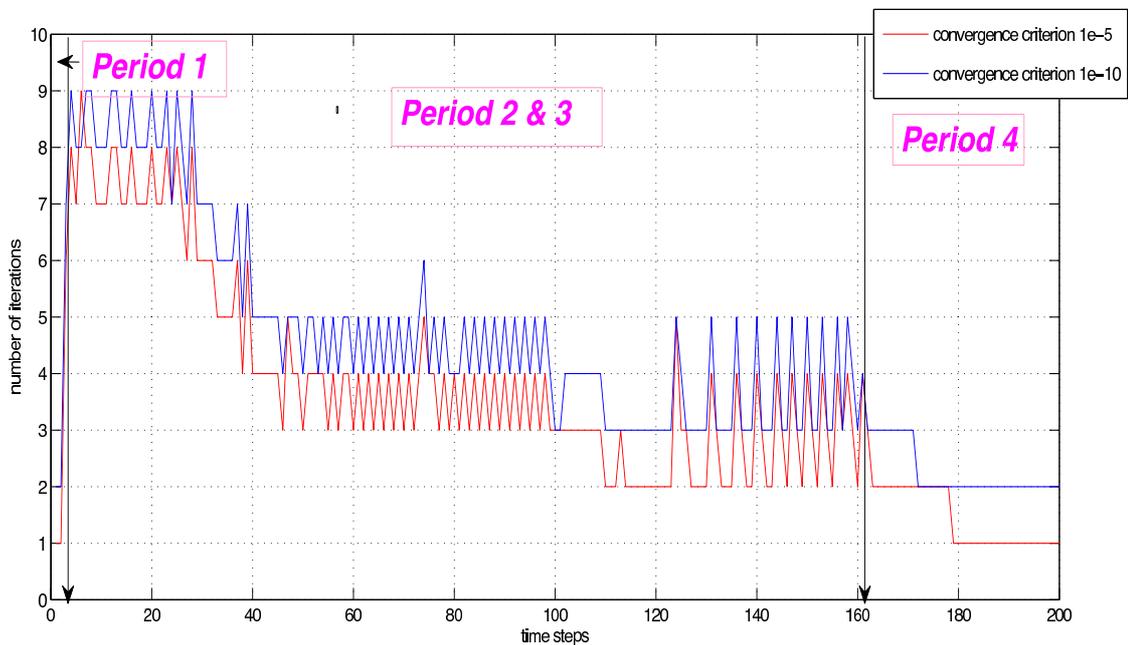


Figure 7: Quadratic convergence of Newton-min: number of Newton-min iterations per time step for two convergence criterions, 1.e-5 (red curve) and 1.e-10 (blue curve).

5 Conclusion

We have studied a solution procedure for a model describing a system of two-phase (liquid-gas) flow in porous media with two components (hydrogen-water) where hydrogen can dissolve in the liquid phase. The problem is formulated as a nonlinear complementarity problem and is solved with the Newton-min method. We considered an example of a Couplex-Gas benchmark and we showed the ability of our solver to describe the appearance and disappearance of the gas phase during the migration of hydrogen. We also discussed the quadratic convergence of the Newton-min method. A theoretical justification for this quadratic convergence and other benchmark examples are under investigation.

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