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Partial Differential Equations

A model of multiphase flow and transport in porous media applied to gas migration in underground nuclear waste repository

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Abstract

We prove existence of solutions for a new model of two compressible and partially miscible phase flow in porous media, applied to gas migration in an underground nuclear waste repository. This model, modeling fully and partially water saturated situations, consist of a coupled system of quasilinear parabolic partial differential equations. We seek a new set of variables in order to obtain a system which belongs to the class of equations considered by Alt and Luckhaus such that it would be possible to use their existence theorem. A simulation of a numerical test case is performed in order to numerically demonstrate the ability of this model to take in account the appearance of one phase. ***To cite this article: F. Smaï, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Résumé

Un modèle d'écoulement et de transport multiphasique en milieu poreux appliqué à la migration de gaz dans un stockage souterrain de déchets nucléaires. On démontre l'existence d'une solution pour un nouveau modèle d'écoulement en milieu poreux de deux phases compressibles et partiellement miscibles en application à la migration de gaz en stockage souterrain de déchets nucléaires. Ce nouveau modèle prend en compte à la fois les régimes saturé et insaturé, il consiste en un système d'équations aux dérivés partielles quasi linéaires parabolique couplé. On cherche un changement de variables qui permet une formulation entrant dans la classe des équations considérées par Alt et Luckhaus ; ce qui permet d'appliquer leur théorème d'existence et ainsi de prouver l'existence d'une solution du modèle. Un test numérique est présenté afin de confirmer la capacité de ce modèle à prendre en compte l'apparition d'une phase. ***Pour citer cet article : F. Smaï, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Version française abrégée

Face aux difficultés constatées par l'exercice Couplex-Gaz (voir [4]), nous avons proposé, dans une précédente publication [2], un modèle d'écoulement compressible multiphasique en milieu poreux pouvant s'appliquer à la migration de gaz dans un stockage souterrain de déchets nucléaires. Une des difficultés essentielle relevé par [4] est l'inaptitude des modèles usuels à prendre en compte simultanément les situations totalement et partiellement saturées en eau ; ce qui amène à des problèmes numériques ou à l'introduction de contraintes numériques non physiques. Le

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principale intérêt de [2] est d'introduire, en s'appuyant sur les principes fondamentaux de la mécanique de fluide et de la thermodynamique, un cadre unifié pour traiter des écoulement totalement et partiellement saturées en eau ; rendant ainsi possible un traitement numérique unifié des situations totalement et partiellement saturé en eau. Les inconnues utilisées initialement dans [2] sont la densité totale d'hydrogène, $X = (1 + (\omega - 1)S_g)R_s$, et la pression de la phase liquide p_l ; où S_g est la saturation en gaz et R_s la concentration d'hydrogène dissout. Cependant, afin de pouvoir appliquer les résultats d'existence de Alt–Luckhaus dans [1], il nous faut introduire un nouveau jeu de variables $\mathbf{u} = (u_1, u_2)$:

$$u_1 = \omega p - r \quad \text{et} \quad u_2 = \ln(r);$$

où le paramètre $\omega = C_v/C_h > 1$ est donné par le modèle (voir équations (7)), $p = \frac{p_l}{p_0}$ et $r = \frac{R_s}{C_h p_0}$ sont respectivement la pression liquide et la densité d'hydrogène dissout adimensionnées. Pour simplifier, on considère le cas d'un milieu poreux homogène et isotrope ; ainsi la perméabilité intrinsèque de la roche, k, et la porosité de la roche, Φ, sont des constantes. Avec les transformations données en (1) et après adimensionnement, le modèle se réécrit sous la forme du système d'équation aux dérivées partielles suivant :

$$\partial_t \mathbf{b}(\mathbf{u}) - \operatorname{div}\big(\bar{\mathcal{A}}\big(\mathbf{b}(\mathbf{u})\big)\nabla\mathbf{u} - \mathcal{B}\big(\mathbf{b}(\mathbf{u})\big)\big) = \mathcal{F} \quad \text{dans }]0,T[\times\Omega,$$
$$\mathbf{b}(\mathbf{u}) = \mathbf{b}^0 \quad \text{sur } \{0\}\times\Omega, \qquad \mathbf{u} = \mathbf{u}^D \quad \text{sur }]0,T[\times\Gamma_D,$$
$$\big(\bar{\mathcal{A}}\big(\mathbf{b}(\mathbf{u})\big)\nabla\mathbf{u} - \mathcal{B}\big(\mathbf{b}(\mathbf{u})\big)\big)\cdot\nu = 0 \quad \text{sur }]0,T[\times(\partial\Omega\setminus\Gamma_D),$$

où $\mathbf{b}$, $\bar{\mathcal{A}}$, $\mathcal{B}$ et $\mathcal{F}$ sont donnés par (5), (6) et (7).

On démontre (Théorème 3.5), à l'aide d'un théorème de Alt–Luckhaus sur les systèmes d'équations différentielles elliptiques–paraboliques quasi linéaires (voir [1]), qu'il existe une solution au problème (2)–(4) sous certaines conditions. Le théorème est applicable si premièrement le terme conservatif dérive d'un potentiel et le tenseur de conductivité non linéaire est elliptique ; et de plus si le terme de flux global satisfait une condition de croissance donnée. Les Lemmes 3.1, 3.2 et 3.3 ci-après fournissent des conditions sous lesquelles ces propriétés sont vérifiées pour le problème (2)–(4).

Enfin, un test numérique est présenté ; il s'agit de simuler numériquement l'injection d'hydrogène dans un milieu poreux homogène entièrement saturé en eau pure. La résolution numérique se décompose en trois étapes : discrétisation implicite en temps ; itérations de Newton pour résoudre le système non linéaire d'équations continues en espace ; discrétisation spatial du système d'équations différentielles linéaires obtenu avec un schéma d'éléments finis mixte-hybride. L'implémentation est effectuée à l'aide du code de calcul Cast3m (voir [5]). Les résultats numériques (voir Fig. 1) sont conformes à la physique du problème ; ils montrent l'accumulation de l'hydrogène en solution dans l'eau jusqu'à ce que, localement, la concentration d'hydrogène dissout soit suffisante pour qu'une phase de gaz apparaisse, créant ainsi une région partiellement saturée. Ensuite, cette région partiellement saturée croît jusqu'à ce que le système atteigne un état stationnaire.

1. Introduction

Motivated by Couplex-Gas (see [4]), in a preceding publication [2], we derived a compositional model of compressible multiphase flow and transport in porous media, with interphase mass transfer in order, to describe the gas migration in an underground nuclear waste repository. In that case, the liquid phase qualified by l is composed of water and dissolved hydrogen and the gas phase qualified by g is composed of vaporized water and hydrogen; the two components are water and hydrogen, qualified by w and h. One of the main difficulty appearing in [4] was the inadequacy of the usual models to take in account both fully and partially water saturated situations; leading to some numerical problems or unphysical numerical constraints. The main interest of [2] is to introduce an unified modeling of fully and partially water saturated porous materials, based on fundamental principles of fluid mechanic and thermodynamic; making possible a unified numerical treatment of fully and partially water saturated situations.

Our aim in this Note is first to prove, under adequate assumptions, the existence of solutions for equations corresponding to this model, and to demonstrate by numerical experiments the ability of this new model to describe both fully and partially water saturated porous materials. For the solutions existence proof, we first rewrite the model ([2]) in new variables such that these new unknowns lead to a conservative term which is rotational, a uniform growth bound for the global flux and ensure ellipticity of the nonlinear conductivity tensor. However both the global flux growth bound and the conductivity tensor ellipticity will be obtain in regions where the hydrogen density is a priori bounded. Finally, these last properties make possible to use the Alt–Luckhaus results from [1], in order to conclude the existence. For the numerical experiments, we numerically simulate injection of hydrogen in a pure water saturated porous media and display evolution of gas saturation S_g, liquid pressure p_l and total hydrogen density X (see Fig. 1). Computations are made using FEM and solving the implicit formulation by an exact Newton procedure; implementation makes use of the modular code Cast3m [5].

2. Setting the problem

The aim of the model developed in [2] was to describe two phase partially miscible flow in porous media, with possible appearance or disappearance of gas phase, like it could happens in an underground nuclear waste repository. Contrary to the classical models (see [3]) where the principal variables are the phase pressures and the saturation, the model in [2] use as principal unknowns $X = (1 + (\omega - 1)S_g)R_s$ the total hydrogen density and p_l the liquid phase pressure, where S_g is the gas saturation and R_s is the dissolved hydrogen density. But, in order to satisfy the conditions of the existence theorem of Alt–Luckhaus (see [1]), we have to find an other set of unknowns $\mathbf{u} = (u_1, u_2)$ such that, in particular, the conservative term of the system derives from a potential. As it is shown in Lemma 3.1, this last property can be obtained by choosing $\mathbf{u}$ as

$$u_1 = \omega p - r \quad \text{and} \quad u_2 = \ln(r), \tag{1}$$

with $\omega = C_v/C_h > 1$ given by equations (7). The new unknowns (u_1, u_2) are then related to $p = \frac{p_l}{p_0}$, the dimensionless liquid pressure, and to $r = \frac{R_s}{C_h p_0}$, the dimensionless dissolved hydrogen density. For sake of simplicity, we consider a homogeneous isotropic porous medium; thus we will denote k the rock intrinsic permeability and Φ the rock porosity which are now two constant scalar. Considering transformations given in (1), we obtain from [2] the dimensionless model:

$$\partial_t \mathbf{b}(\mathbf{u}) - \operatorname{div}\big(\bar{\mathcal{A}}\big(\mathbf{b}(\mathbf{u})\big)\nabla\mathbf{u} - \mathcal{B}\big(\mathbf{b}(\mathbf{u})\big)\big) = \mathcal{F} \quad \text{in }]0, T[\, \times \Omega, \tag{2}$$

$$\mathbf{b}(\mathbf{u}) = \mathbf{b}^0 \quad \text{on } \{0\} \times \Omega, \qquad \mathbf{u} = \mathbf{u}^D \quad \text{on }]0, T[\, \times \Gamma_D, \tag{3}$$

$$\big(\bar{\mathcal{A}}\big(\mathbf{b}(\mathbf{u})\big)\nabla\mathbf{u} - \mathcal{B}\big(\mathbf{b}(\mathbf{u})\big)\big) \cdot \nu = 0 \quad \text{on }]0, T[\, \times (\partial\Omega \setminus \Gamma_D), \tag{4}$$

$$\text{with } \mathbf{b} = (b_1, b_2) = \mathbf{h}(\mathbf{u}) - \mathbf{h}(0) \quad \text{and} \tag{5}$$

$$\mathbf{h} = \begin{pmatrix} -S_g \\ x \end{pmatrix}, \qquad \bar{\mathcal{A}} = \begin{pmatrix} \frac{1}{\omega} k_{r,l} & \frac{r}{\omega} k_{r,l} \\ \frac{r}{\omega} k_{r,l} & r^2(\frac{1}{\omega} k_{r,l} + \beta_1 k_{r,g}) + r\frac{(1-S_g)}{N_c} \end{pmatrix},$$

$$\mathcal{B} = \beta_2 \begin{pmatrix} k_{r,l} \\ k_{r,l} r + \alpha_1 \beta_1 \omega k_{r,g} r^2 \end{pmatrix} \mathbf{e}, \qquad \mathcal{F} = \gamma_2 \begin{pmatrix} \alpha_1 \frac{\mathcal{F}^w}{\rho_g^{std}} \\ \frac{\mathcal{F}^h}{\rho_g^{std}} \end{pmatrix}. \tag{6}$$

The dimensionless total hydrogen density is x, $x = \frac{X}{C_h p_0} = (1 + (\omega - 1)S_g)r$, and the gas saturation, S_g, is given by $S_g = f(r - p)$ where f satisfy $f(0) = 0$, $0 \leqslant f \leqslant 1$ and $f' > 0$ on $\mathbb{R}_+^*$; the relative, liquid and gas, permeability curves $k_{r,l}$ and $k_{r,g}$ are functions of S_g and take values in [0; 1]. The coefficients

$$N_c = \frac{p_0 k}{\Phi D_l^h \mu_l}, \qquad \alpha_1 = C_h p_0 \frac{\rho_g^{std}}{\rho_l^{std}}, \qquad \beta_1 = \frac{\mu_l C_v}{\mu_g C_h}, \qquad \beta_2 = \frac{L g \rho_l^{std}}{p_0}, \qquad \gamma_2 = \frac{L^2 \mu_l}{k C_h p_0^2},$$

$$C_h = \frac{H M^h}{\rho_g^{std}}, \qquad C_v = \frac{M^h}{R\theta \rho_g^{std}}, \qquad t_0 = \frac{\Phi L^2 \mu_l}{p_0 k}, \tag{7}$$

in which we introduce the characteristic pressure and length p_0 and L, depend on the rock intrinsic permeability k, the rock porosity Φ, the molar diffusion coefficient of hydrogen in water D_l^h, the liquid and gas phase viscosities μ_l and μ_g, the standard liquid and gas volume mass ρ_l^{std} and ρ_g^{std}, the gravity acceleration $\mathbf{g} = g\mathbf{e}$, the Henry's law constant H, the hydrogen molar mass M^h, the temperature θ, the universal gas constant R.

The fully water saturated state is now characterized by $r \leqslant p$, according to definition of S_g and properties of f.

3. Existence of a solution

In this section we expose an existence result for the problem (2)–(3)–(4), where $\Omega \in \mathbb{R}^n$ is an open, bounded and connected set with Lipschitz measurable boundary $\Gamma_D \subset \partial\Omega$ and with outward normal ν; $0 < T < \infty$. Definition of a weak solution is given in [1] Section 1.4.

The existence theorem is based on some data properties, namely: the conservative terms derives from a convex potential, the nonlinear conductivity tensor is elliptic and the global flux term satisfies a growth condition. Thanks to the choice of the new unknowns (u_1, u_2), the following three lemmas give conditions under which these properties hold:

Lemma 3.1. *The vector field* $\mathbf{b}$ *is continuous and derives from a potential* $\psi(\mathbf{u}) = \omega F(\frac{(\omega-1)r(u_2)-u_1}{\omega}) + r(u_2) + f(\frac{\omega-1}{\omega})u_1 - (1+(\omega-1)f(\frac{\omega-1}{\omega}))u_2$ *with* $F(\xi) = \int_0^\xi f(\tau)\,\mathrm{d}\tau$, *in the sense that* $\mathbf{b} = \nabla_{\mathbf{u}}\psi$. *Moreover* $\psi(\mathbf{u})$ *is convex.*

Lemma 3.2. *For any fixed* $r_{min} > 0$, $r_{max} > r_{min}$, $k_{min} > 0$ *and* $S_{l,min} > 0$; *if* $\mathbf{u}$ *satisfies* $r_{min} \leqslant r(u_2) \leqslant r_{max}$, $k_{r,l} \geqslant k_{r,min}$ *and* $1 - S_g \geqslant S_{l,min}$, *then* $\bar{\mathcal{A}}(\mathbf{u})$ *is elliptic.*

Lemma 3.3. *For any fixed* $r_{max} > 0$, *if* $\mathbf{u}$ *satisfies* $r(u_2) \leqslant r_{max}$ *then, for any* $\mathbf{v}$, *the relation* $|\bar{\mathcal{A}}(\mathbf{b}(\mathbf{u}))\mathbf{v} - \mathcal{B}(\mathbf{b}(\mathbf{u}))| \leqslant c(1+|\mathbf{v}|)$ *holds with c a constant depending on* r_{max}.

In the following definition, according to [1], we define what we mean by the regularity of Dirichlet and initial conditions:

Definition 3.4. We say that:

1. The Dirichlet condition u^D is regular if $u^D \in L^2(0,T;H^{1,2}(\Omega)) \cap L^\infty(]0,T[\times\Omega)$;
2. The initial condition $\mathbf{b}^0$ is regular if $\Psi(\mathbf{b}^0) \in L^1(\Omega)$ where $\Psi(z) = \sup_{\sigma\in\mathbb{R}^2}(z\cdot\sigma - \psi(\sigma))$ and if there is a measurable function $\mathbf{u}^0$ with $\mathbf{b}^0 = \mathbf{b}(\mathbf{u}^0)$.

Finally, we have the existence theorem:

Theorem 3.5. *Under conditions of Lemmas* 3.1, 3.2 *and* 3.3 *with given* r_{min}, r_{max}, k_{min} *and* $S_{l,min}$ *and assuming that initial and Dirichlet conditions are regular and that* $\partial_t u^D \in L^1(0,T;L^\infty(\Omega))$, *there is a weak solution for problem* (2)–(4).

The proof is a direct application of the existence Theorem 1.7 in [1] from Alt–Luckhaus. Lemmas 3.1, 3.2 and 3.3 ensure that theorem assumptions on the data are fulfilled.

4. Numerical experiment

We will use a quasi-1D scale field simulation, with gas injection in a fully water saturated porous media, in order to numerically test the ability of this model to take in account both the fully and the partially saturated situation. Simulations are done with the modular code Cast3m (see [5]). Note that equations staying valid in both fully and partially water saturated states, there is no need to switch variables/equations following flow state at each node or to introduce residual gas saturation in the model as it is done in simulation based on classical models (see for instance [3]).

The test case follows typical underground waste disposal situations; it consists in a hydrogen injection in a thin piece of host rock containing initially only liquid water and no hydrogen. It corresponds to a horizontal section, so there is no gravity effect, $\mathcal{B} \equiv 0$. Precisely, we have the domain $\Omega = [0m; 200m] \times [-10m; 10m]$ in $\mathbb{R}^2$ with an impervious boundary $\Gamma_{imp} = [0m; 200m] \times \{-10m, 10m\}$, an inflow boundary $\Gamma_{in} = \{0m\} \times [-10m; 10m]$ and an outflow boundary $\Gamma_{out} = \{200m\} \times [-10m; 10m]$. Denoting the water component flux $\phi^w \equiv \mathcal{A}_{11}(\mathbf{u})\nabla u_1 + \mathcal{A}_{12}(\mathbf{u})\nabla u_2$ and the hydrogen component flux $\phi^h \equiv \mathcal{A}_{21}(\mathbf{u})\nabla u_1 + \mathcal{A}_{22}(\mathbf{u})\nabla u_2$, we impose the boundary conditions: $\phi^w \cdot \nu = \phi^h \cdot \nu = 0$ on the impervious boundary Γ_{imp}; $\phi^w \cdot \nu = 0$ and $\phi^h \cdot \nu = Q_d^h$ on the inflow boundary Γ_{in}; $X = 0$ and $p_l = p_{l,out}$ on

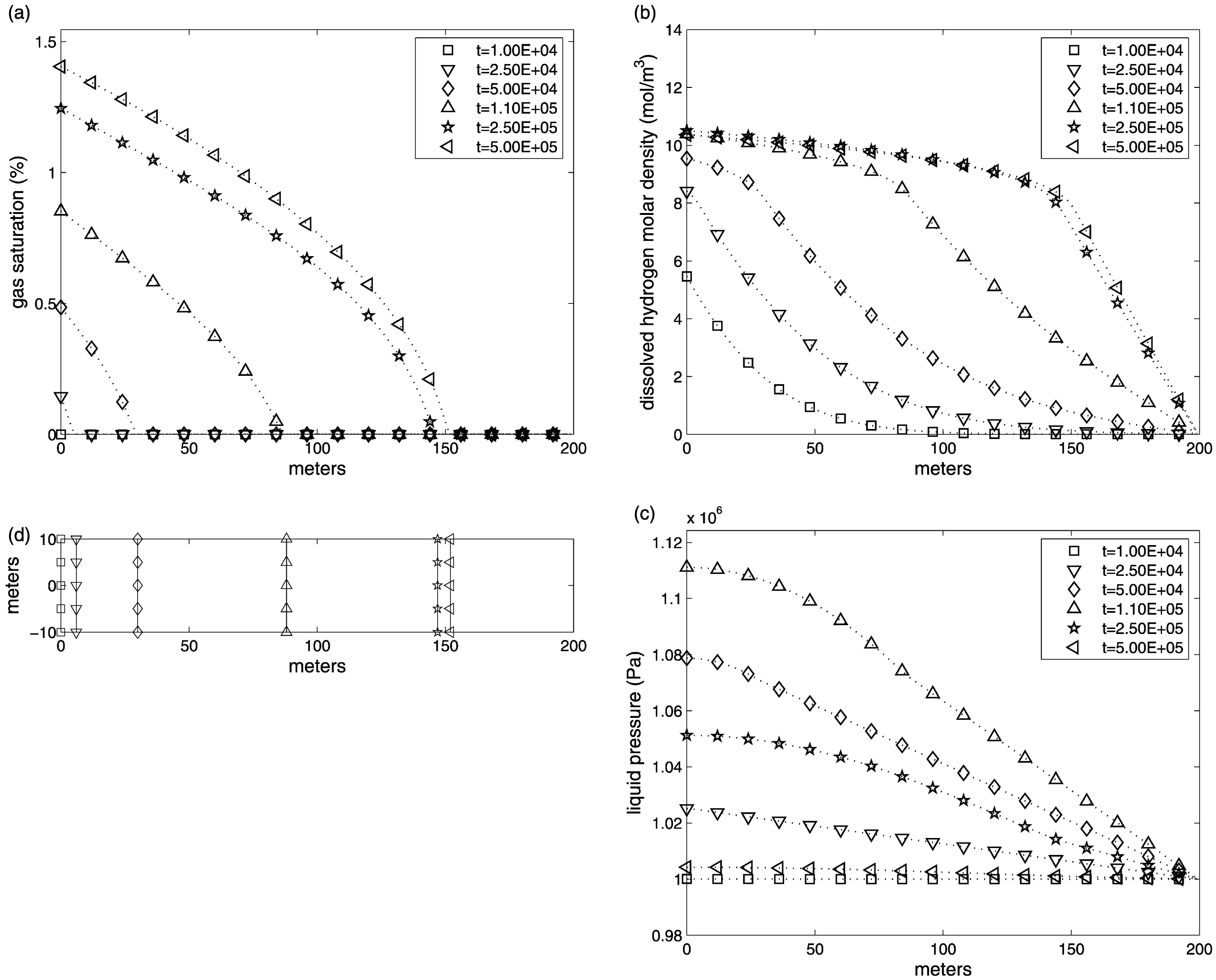

Fig. 1. Each curve represents the spatial evolution in the horizontal direction of (a) gas saturation, (b) dissolved hydrogen molar density and (c) liquid pressure at several time t (in years). In (d) are plotted at different times the saturated/unsaturated gas boundary in Ω.

the outflow boundary Γ_{out}, where Q_d^h and $p_{l,out}$ are fixed to $Q_d^h = 1.5 \times 10^{-5}$ m/years and $p_{l,out} = 10^6$ Pa. The constitutive law $p_c(S_g)$, $k_{r,l}(S_g)$ and $k_{r,g}(S_g)$ are given by the van Genuchten–Mualem model. Following [4], the porous medium parameters and fluid characteristics are the same as in [2] (see Table 1). Simulation is run from $t = 0$ to $T = 5 \times 10^5$ years and, in Fig. 1, we plotted the gas saturation S_g (Fig. 1(a)), the dissolved hydrogen molar density R_s (Fig. 1(b)) and the liquid pressure p_l (Fig. 1(c)) at times $t = 1 \times 10^4$, 2.5×10^4, 5×10^4, 1.1×10^5, 2.5×10^5 and 5×10^5 years. Fig. 1(d) represents, in the whole domain Ω, the saturated/unsaturated boundary at the same time steps.

In a first step ($0 < t < 2.4 \times 10^4$ years; mark $\Box$), all the domain stays fully water saturated (see Figs. 1(a) and 1(d)) and liquid pressure (see Fig. 1(c)) stays uniform in space; only dissolved hydrogen density evolves (see Fig. 1(b)) due to diffusion of dissolved hydrogen in liquid phase; because $r \leqslant p$, in all the domain, all the injected hydrogen is dissolved in the liquid. At $t \approx 2.5 \times 10^4$ years, the hydrogen density has grown enough to satisfy $r > p$ in a part of the domain, the gas phase starts to appear at the inflow boundary (mark ∇) and the unsaturated area expands with the time (marks $\diamondsuit$ and $\triangle$). In the same time, due to presence of gas phase and capillary effect, a liquid pressure gradient appears (see Fig. 1(c)) and, according to generalized Darcy's law, the liquid flows from the inflow boundary Γ_{in} to the outflow boundary Γ_{out}. Hydrogen transport is now operating in three ways: diffusion and convection of the dissolved hydrogen in the liquid phase and flow of gas phase for gaseous hydrogen in partially saturated area. Finally for $t > 1.1 \times 10^5$ years (marks $\star$ and $\triangleleft$), gas saturation (see Fig. 1(a)), dissolved hydrogen density (see Fig. 1(b))

Table 1
Values of porous medium parameters and fluid characteristics.

Porous medium parameters		Fluid characteristics		van Genuchten–Mualem model
Parameter	Value	Parameter	Value	
k	5×10^{-20} m^2	D_l^h	3×10^{-9} m^2/s	$p_c = P_r(S_{le}^{-1/m} - 1)^{1/n}$
Φ	0.15 (−)	μ_l	1×10^{-3} Pa s	$kr_l = \sqrt{S_{le}}(1 - (1 - S_{le}^{1/m})^m)^2$
P_r	2×10^6 Pa	μ_g	9×10^{-6} Pa s	$kr_g = \sqrt{1 - S_{le}}(1 - S_{le}^{1/m})^{2m}$
n	1.49 (−)	$H(\theta = 303\text{ K})$	7.65×10^{-6} mol/Pa/m^3	$S_{le} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}$
S_{lr}	0.4 (−)	M^w	10^{-2} kg/mol	$m = 1 - \frac{1}{n}$
S_{gr}	0 (−)	M^h	2×10^{-3} kg/mol	
θ	303 K	ρ_l^{std}	10^3 kg/m^3	
		ρ_g^{std}	8×10^{-2} kg/m^3	

and partially saturated area (see Fig. 1(d)) continue to increase toward a stationary state; but liquid pressure goes down and tends toward a uniform stationary state (see Fig. 1(c)). This liquid pressure decrease is due to the absence of water injection on the inflow boundary Γ_{in}. In fact, at stationary state, water mass conservation equation becomes $\mathrm{div}(k_{r,l} \nabla p) = 0$; thus, from boundary conditions, liquid pressure is spatially uniform at the stationary state.

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