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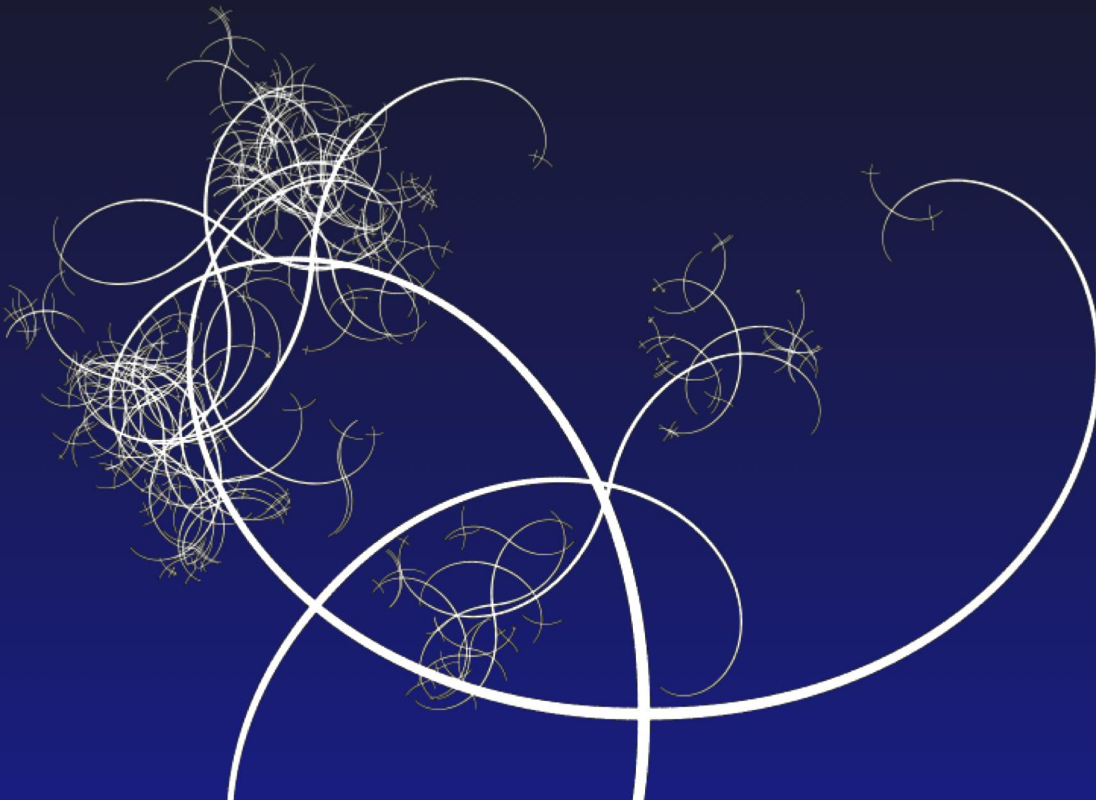

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MODELING CAPILLARY HYSTERESIS IN UNSATURED POROUS MEDIA

GÉRARD GAGNEUX AND OLIVIER MILLET

This paper deals with the modeling of cyclic hysteresis phenomena for flows in unsaturated porous media, using a dynamic regularization process of Sobolev type. The addition of a kinematic regularizing term of third-order partial derivatives, depending on a strictly positive, small real parameter, enables us to capture the missing information of the ill-posed hysteresis phenomena via Rankine–Hugoniot and “entropy” inequalities. When this parameter tends to zero, an oriented hysteresis loop, corresponding to the realistic problem modeled, emerges from the flow of an associated auxiliary ordinary differential equation.

1. Introduction

The modeling of moisture transport in partially saturated porous media is of major importance for civil engineering, soil physics, and pharmaceutical applications. The hysteresis effects, often neglected in the modeling as they are difficult to be taken into account, play a central role in the imbibition and drying process.

In this paper, we propose an original modeling of cyclic hysteresis phenomena in partially saturated porous media, in the simplified case of water–air flows. The approach used is based on the artificial introduction of an unstable spinodal interval and on Sobolev’s method of dynamic regularization, inspired by the works of P. I. Plotnikov [1996; 1994], publicized by L. C. Evans and M. Portilheiro [2004; Evans 2004]. The hysteresis graph is replaced by Cartesian curves and an artificial spinodal interval generating instabilities, with associated attractive–repulsive dynamics.

The additional information to describe the hysteresis effects is introduced on the form of entropy-type inequalities. This way, the asymptotic limit of viscous approximate solutions generates effects of irreversibility and enables us to recover the expected hysteresis loop.

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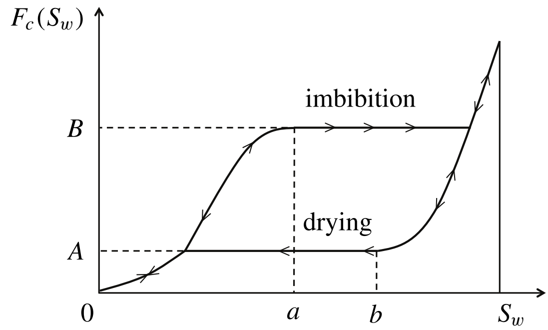

Figure 1. Graph of F_c representing the hysteresis loop during an imbibition-drying process.

2. The physical problem

2.1. ***Richards equation.*** The flow of two fluid phases (water–air flow), isothermal and immiscible, in an unsaturated porous medium is considered. To focus on the study of the hysteresis effects, in particular irreversibility, the gravity is neglected and the porous medium is assumed to be homogeneous and isotropic.[1] Moreover, the water vapor in the gas phase is neglected and the air pressure is assumed to be constant and equal to the atmospheric pressure.[2]

The water saturation S_w is classically governed by a Richards equation,

$$\varphi \frac{\partial S_w}{\partial t} - \Delta \Theta_c(S_w) = 0, \tag{1}$$

where φ denotes the porosity of the porous medium considered. We assume that the residual saturation of each fluid is equal to zero.

Even if the mathematical analysis of this equation is now well stated [Gagneux and Madaune-Tort 1995; Lions 1969], it ignores the hysteresis and dynamic effects that play a major role in the behavior of unsaturated porous media.

2.2. ***Hysteresis modeling.*** The capillary hysteresis effects can be modeled with a multivalued operator F_c whose oriented graph F_c of $\mathbb{R}^2$ is represented in Figure 1. The circulation sense depends both on the values of S_w and on the sign of $\frac{\partial S_w}{\partial t}$. It characterizes the imbibition and drying phases, through the differential inclusion[3]

$$0 \in \left\{ \varphi \frac{\partial S_w}{\partial t} - \Delta F_c\left(S_w, \operatorname{sign}\left(\frac{\partial S_w}{\partial t} \right) \right) \right\}. \tag{$\mathcal{P}_{\text{hyst}}$}$$

[1] The analysis holds also for the anisotropic case.

[2] It is equivalent to assume that the gas phase moves fast and is connected to outside.

[3] In the sense of [Aubin and Cellina 1984].

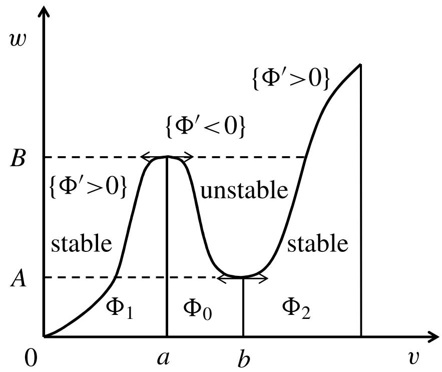

Figure 2. The spinodal interval $[a, b]$ and the unstable part of the graph of Φ.

It is equivalent to search a pair (S_w, q_w) with $q_w \in \left\{F_c\left(S_w, \operatorname{sign}\left(\frac{\partial S_w}{\partial t}\right)\right)\right\}$ which satisfies

$$\varphi \frac{\partial S_w}{\partial t} - \Delta q_w = 0 \tag{2}$$

associated to a Cauchy initial condition $S_{w(0)}$ and Neumann homogeneous boundary conditions. To simplify the problem without loss of generality, we will consider in the following a normalized porosity $\varphi = 1$ (this is always possible using a homothetical time scaling, when φ is constant).

In a first step, using a mathematical artifice, we replace the part of the graph F_c representing the loop by a cubic Cartesian curve Φ (Figure 2). Then, to approach problem $(\mathscr{P}_{\text{hyst}})$, a nonlinear monotone diffusion equation with an ad hoc "spinodal" interval $]a, b[$ is introduced. The graph F_c is replaced on $]a, b[$ by a cubic spline function, denoted Φ_0, whose slope is strictly negative everywhere on $]a, b[$ and assuring a $\mathscr{C}^1$ continuity at (a, B) and (b, A) with the preserved part.

The graph F_c is decomposed by splitting its domain of definition into three distinct parts. This leads us to introduce three injective functions, Φ_0, Φ_1 and Φ_2, defined on $[a, b]$, $[0, a]$ and $[b, 1]$, respectively. We denote by β_0, β_1 and β_2 their respective inverse functions and by Φ the numerical function of class $\mathscr{C}^1$ on $[0, 1]$ whose graph is the joining of the graphs of Φ_0, Φ_1 and Φ_2.

This substitution enables us to give sense to the initial formal problem in a suitable mathematical functional framework, via the initial–boundary value system

$$\begin{cases} \dfrac{\partial v}{\partial t} - \Delta\Phi(v) = 0 & \text{in } Q =]0, T[\times \Omega, \\ \dfrac{\partial \Phi(v)}{\partial n} = 0 & \text{on } \Sigma =]0, T[\times \Gamma, \\ v(0) = S_{w(0)} & \text{in } \Omega, \end{cases} \tag{P_Φ}$$

where Ω denotes a bounded domain of $\mathbb{R}^d$, $d \geq 1$, with a Lipschitz boundary Γ and an associated external unit normal vector n. The new forward–backward problem (P_Φ) with variable parabolicity direction is ill posed without any supplementary information, because of the nonmonotonic function Φ. The dynamic regularization process that follows will enable us to regularize the problem. Note that a problem similar to (P_Φ) has been studied in [Smarrazzo and Tesei 2010; 2012; Smarrazzo 2008].

3. Dynamic regularization process of Sobolev type

The classical notations that follow are introduced. Let Ω be a bounded domain of $\mathbb{R}^d$ whose boundary Γ is a Lipschitz manifold of dimension $d-1$. For $T > 0$, we write $Q =]0, T[\, \times \Omega$, $\Sigma =]0, T[\, \times \Gamma$ and let Δ be the Laplacian operator[4] of $\mathbb{R}^d$. We denote by $H^s(\Omega)$, $s \in \mathbb{R}$, the classical Hilbert spaces [Lions and Magenes 1968]. For all $\varepsilon > 0$, the embedding of $H^s(\Omega)$ into $H^{s-\varepsilon}(\Omega)$ is compact. Moreover, we identify $L^2(\Omega) = H^0(\Omega)$ to its dual, so that the dual of $H^1(\Omega)$, denoted $H^1(\Omega)'$, can be identified to an superspace of $L^2(\Omega)$ with $H^1(\Omega) \hookrightarrow L^2(\Omega) \hookrightarrow H^1(\Omega)'$, the embeddings being dense and continuous. In addition, an initial state $S_{w(0)} \in L^\infty(\Omega)$ satisfying $0 \leq S_{w(0)} \leq 1$ a.e. in Ω is given.

The dynamical regularization process of Sobolev type used is based on "artificial viscosity". A parameter $\lambda > 0$ is introduced in the initial ill-posed problem (P_Φ), which is transformed into the third order boundary problem

$$\begin{cases} \dfrac{\partial v_\lambda}{\partial t} - \Delta\Phi(v_\lambda) - \lambda\Delta\dfrac{\partial v_\lambda}{\partial t} = 0 & \text{in } Q =]0, T[\, \times \Omega, \\ \dfrac{\partial}{\partial n}\left(\Phi(v_\lambda) + \lambda\dfrac{\partial v_\lambda}{\partial t}\right) = 0 & \text{on } \Sigma =]0, T[\, \times \Gamma, \\ v_\lambda(0) = S_{w(0)} & \text{in } \Omega. \end{cases} \qquad (P_\Phi)_\lambda$$

We then introduce the auxiliary dynamical unknown w_λ defined by

$$w_\lambda = \Phi(v_\lambda) + \lambda\frac{\partial v_\lambda}{\partial t}, \tag{3}$$

or equivalently

$$\frac{\partial v_\lambda}{\partial t} = \frac{w_\lambda - \Phi(v_\lambda)}{\lambda}, \quad t > 0. \tag{4}$$

Note that the dynamics created by (4) drive the system onto stable parts of the graph, as we will see in the sequel.

[4]In the sense of distributions.

Problem $(P_\Phi)_\lambda$ may be rewritten as

$$\begin{cases} \dfrac{\partial v_\lambda}{\partial t} - \Delta w_\lambda = 0 & \text{in } Q =]0, T[\times \Omega, \\ \dfrac{\partial w_\lambda}{\partial n} = 0 & \text{on } \Sigma =]0, T[\times \Gamma, \\ v_\lambda(0) = S_{w(0)} & \text{in } \Omega. \end{cases} \tag{5}$$

Equivalently, for nearly all t, w_λ is a solution of the elliptic problem parametrized in time[5]

$$\begin{cases} w_\lambda - \lambda \Delta w_\lambda = \Phi(v_\lambda) & \text{in } \Omega,\ t > 0, \\ \dfrac{\partial w_\lambda}{\partial n} = 0 & \text{on } \Gamma,\ t > 0. \end{cases} \tag{6}$$

The "$-$ Laplacian" operator (denoted again $-\Delta$) specifically associated with homogeneous Neumann boundary conditions on Γ is obviously a nonbounded operator from $L^2(\Omega)$ into L^2 (Ω) whose domain is $H^2(\Omega)$. We introduce the Yosida regularization $-\Delta_\lambda := -\Delta(J_\lambda) = (I - J_\lambda)/\lambda$ and its resolvent $J_\lambda = (I - \lambda\Delta)^{-1}$. According to (6), it follows that

$$w_\lambda = J_\lambda \Phi(v_\lambda). \tag{7}$$

Problem $(P_\Phi)_\lambda$ can be formulated again in a well-posed form[6] for the operator $-\Delta_\lambda \Phi$ in $L^2(\Omega)$:

$$\begin{cases} \dfrac{\partial v_\lambda}{\partial t} - \Delta_\lambda \Phi(v_\lambda) = 0, & t \in]0, T[, \\ v_\lambda(0) = S_{w(0)} & \text{in } L^2(\Omega) \text{ and a.e. in } \Omega. \end{cases} \tag{P_λ}$$

The following proposition summarizes the properties of the solutions of (P_λ):

Proposition 1. *Let us denote by $g : \mathbb{R} \to \mathbb{R}$ a Lipschitz nondecreasing function, a so-called "entropy function", and let*

$$G(r) = \int_0^r g(s)\,ds, \quad G_\Phi(r) = \int_0^r g(\Phi(s))\,ds, \quad g_{1/2}(r) = \int_0^r \sqrt{g'(s)}\,ds, \quad r \in \mathbb{R}. \tag{8}$$

From the Rademacher theorem [Evans and Gariepy 1992], *g' is a bounded Borelian representative of the derivative of g in its class.*

For all $\lambda > 0$, the solution v_λ of (P_λ) associated to w_λ has the following properties:

(i) *Estimations using entropy inequations* (*for each entropy function g*):

$$\frac{\partial}{\partial t} G_\Phi(v_\lambda) \le \operatorname{div}(g(w_\lambda)\nabla w_\lambda) - g'(w_\lambda)|\nabla w_\lambda|^2 \quad \text{in } Q. \tag{9}$$

[5] According to an observation of [Evans and Portilheiro 2004].

[6] Thanks to the Cauchy–Lipschitz–Picard theorem via a first-order differential equation with given initial condition.

Using the function G defined in (8), *the last inequality can be rewritten as*

$$\frac{\partial}{\partial t} G_\Phi(v_\lambda) \le \Delta(G(w_\lambda)) - G''(w_\lambda)|\nabla w_\lambda|^2 \quad \textit{in } Q.$$

The following inequalities hold:

$$\int_\Omega G_\Phi(v_\lambda(t,x))\,dx \le \int_\Omega G_\Phi(v_\lambda(s,x))\,dx \le \int_\Omega G_\Phi(S_{w(0)})\,dx, \qquad t > s > 0,$$

$$\|g_{\frac{1}{2}}(w_\lambda)\|^2_{L^2([0,T];H^1(\Omega))} \stackrel{\text{def}}{=} \int_Q g'(w_\lambda)|\nabla w_\lambda|^2\,dx\,dt \le C_g, \qquad C_g = C(g).$$

(ii) *We have the following uniform a priori estimates*:

$$\begin{aligned} \|v_\lambda\|_{L^\infty(Q)} + \|w_\lambda\|_{L^\infty(Q)} &\le C_1, \\ \|w_\lambda\|_{L^2([0,T];H^1(\Omega))} + \sqrt{\lambda}\left\|\frac{\partial v_\lambda}{\partial t}\right\|_{L^2(Q)} &\le C_2, \\ \left\|\frac{\partial v_\lambda}{\partial t}\right\|_{L^2([0,T];(H^1(\Omega))')} &\le C_3. \end{aligned}$$

The frame constants depend on the extremum values of Φ *and* $S_{w(0)}$.

Proof. The general principle of the proof of this proposition may be found in [Evans 2004, p. 427]. This classical computation is somewhat akin to an entropy flux calculation for a hyperbolic conservation law, through choices of nondecreasing functions g (see also [Gagneux and Millet 2015] for more details). We note that the inequality (9) is straightforward from the following relation, for any function Φ:

$$\frac{\partial}{\partial t} G_\Phi(v_\lambda) - \operatorname{div}(g(w_\lambda)\nabla w_\lambda) = -g'(w_\lambda)|\nabla w_\lambda|^2 - \big(g(w_\lambda) - g(\Phi(v_\lambda))\big)\frac{w_\lambda - \Phi(v_\lambda)}{\lambda} \tag{10}$$

stated in [Evans and Portilheiro 2004; Evans 2004; Plotnikov 1996]. □

4. Study of capillary effects

4.1. ***Generalized "entropic" solutions.*** It follows from the uniform estimates of Proposition 1 that we can find subsequences $\{v_{\lambda_k}\}$ and $\{w_{\lambda_k}\}$ and a pair[7] (v, w) such that, as $\lambda_k \to 0$,

$$v_{\lambda_k} \rightharpoonup v \quad \text{in } L^\infty(Q) \text{ weakly-}*, \tag{11}$$

$$\frac{\partial v_{\lambda_k}}{\partial t} \rightharpoonup \frac{\partial v_\lambda}{\partial t} \quad \text{in } L^2\big([0,T];(H^1(\Omega))'\big) \text{ weakly}, \tag{12}$$

$$w_{\lambda_k} \rightharpoonup w \quad \text{in } L^\infty(Q) \text{ weakly-}* \text{ and in } L^2([0,T];H^1(\Omega)) \text{ weakly}, \tag{13}$$

[7] A vanishing viscosity limit.

and

$$w_{\lambda_k} - \Phi(v_{\lambda_k}) \to 0 \quad \text{in } L^p(Q) \text{ strongly, for any finite } p.$$

Furthermore, we can assume that[8]

$$v_{\lambda_k} \to v \quad \text{in } C^0([0,T]; H^1(\Omega)') \text{ strongly.} \tag{14}$$

The associated Cauchy condition is given by

$$\begin{cases} v(0,\cdot) = S_{w(0)} & \text{in } H^1(\Omega)', \text{ a.e. in } \Omega, \\ 0 \le v(t,\cdot) \le 1 & \text{in } \Omega,\ t>0, \\ \displaystyle\int_\Omega v(t,x)\,dx = \int_\Omega S_{w(0)}(x)\,dx, & t>0. \end{cases}$$

In addition, the pair[9] (v, w) belongs to the functional frame

$$\begin{cases} v \in L^\infty(Q) \cap C^0([0,T]; H^1(\Omega)'), \\ \dfrac{\partial v}{\partial t} \in L^2([0,T]; H^1(\Omega)'), \\ w \in L^\infty(Q) \cap L^2([0,T]; H^1(\Omega)), \end{cases}$$

and is a solution of the boundary value problem

$$\begin{cases} \dfrac{\partial v}{\partial t} - \Delta w = 0 & \text{in } \mathscr{D}'(Q) \text{ and } L^2([0,T]; H^1(\Omega)'), \\ \dfrac{\partial w}{\partial n} = 0 & \text{on } \Sigma, \\ v(0,\cdot) = S_{w(0)} & \text{a.e. in } \Omega. \end{cases}$$

Because of the nonmonoticity of Φ, the information (11)–(14) is not sufficient to conclude that $w = \Phi(v)$, as we will see in what follows.

Let us denote by Ξ the complementary of the set of points of $\mathscr{L}^{d+1}$-approximate continuity of v according to the rigorous definition of the shock wave [Evans and Gariepy 1992; Gagneux and Madaune-Tort 1995]. The set Ξ is Borelian and $\mathscr{L}^{d+1}$-negligible because v is in $L^\infty(Q)$.

Let us assume that Ξ is a countable union of smooth hypersurfaces Ξ^i of $\mathbb{R}^{d+1}$ which admit a unit normal vector $\nu^i = (\nu^i_1, \dots, \nu^i_d, \nu^i_{d+1}) = (\tilde{\nu}^i, \nu^i_{d+1})$.

Using the usual notations for jumps in hyperbolic scalar laws and for the Hausdorff measure $\mathscr{H}^d$, very informally, the pair (v, w) satisfies the Rankine–Hugoniot and entropy conditions for all i, integrating by parts locally in a vicinity of a given transition interface via appropriate smooth functions with compact support:

$$\begin{aligned} \nu^i_{d+1}[v] = \tilde{\nu}^i.[\nabla w] \quad \text{and} \quad [w] = 0 \quad & \mathscr{H}^d\text{-a.e. on } \Xi^i, \\ \nu^i_{d+1}[G_\Phi(v)] - \tilde{\nu}^i.[\nabla w] g(w) \le 0 \quad & \mathscr{H}^d\text{-a.e. on } \Xi^i. \end{aligned} \tag{15}$$

8 From a classical compactness result of J. A. Dubinskii [Lions 1969, pp. 141-142].

9 The pair (v, w) is called a *generalized solution* of the problem (P_Φ).

Relation (15) may be written in the form

$$\nu^i_{d+1}\big([G_\Phi(v)] - g(w)[v]\big) \le 0 \quad \mathcal{H}^d\text{-a.e. on } \Xi^i \tag{16}$$

with the notations (8) for the definition of g (entropy function) and G_Φ. In this form, relation (16) will be very useful to highlight the further developments.

4.2. ***Associated hysteresis effects.*** The analysis of hysteresis effects relies on the following proposition:

Proposition 2. *There exist three $\mathcal{L}^{d+1}$-measurable and bounded functions*, Λ_0, Λ_1 *and* Λ_2, *that are representative of the respective influence of the three branches of the graph of* Φ^{-1} (*in the sense of the set theory*) *through the functions* β_0, β_1 *and* β_2. *Moreover*, *we have*

$$0 \le \Lambda_i \le 1 \qquad \text{and} \qquad \sum_{i=0}^{2} \Lambda_i = 1 \quad \mathcal{L}^{d+1}\text{-a.e. in } Q.$$

In addition, *when* λ_k *tends to* 0^+,

$$\mu(v_{\lambda_k}) \text{ converges to } \sum_{i=0}^{2} \Lambda_i \mu(\beta_i(w)) \text{ in } L^\infty(Q) \text{ weakly-}*$$

for any numerical continuous function μ. *In addition*, *we have the following strong convergences*:

$$w_{\lambda_k} \text{ and } \Phi(v_{\lambda_k}) \text{ converge to } w \text{ in } L^p(Q) \text{ strongly for any finite } p.$$

Finally, *for any Lipschitz nondecreasing function* g, *we have the entropy relation in the sense of the measures in* Q

$$\frac{\partial}{\partial t}\bigg(\sum_{i=0}^{2} \Lambda_i\, G_\Phi(\beta_i(w))\bigg) \le \operatorname{div}(g(w)\nabla w) - g'(w)|\nabla w|^2 \quad \text{in } Q. \tag{17}$$

Proof. The difficult technical proof of this proposition is not detailed here and can be found in [Evans and Portilheiro 2004; Evans 2004; Plotnikov 1996; 1994] with some adjustments. □

When Λ_0 is equal to zero everywhere,[10] the method provides a response corresponding to the initial problem, thanks to the information contained in the complementary entropy relation (17). That is the main goal of the following proposition, based on the complementary information on the entropy given by (15)–(16), which enables us to determine the sense of circulation of the hysteresis loop.

[10]That corresponds in the final result to the neutralization of the decreasing part of the cubic introduced artificially to create a repulsive region.

Proposition 3. *In the framework of Proposition 2, we assume that*

$$\Lambda_0 = 0 \quad in\ Q, \qquad \Lambda_1 = 1 \quad in\ Q_1 \qquad and \qquad \Lambda_2 = 1 \quad in\ Q_2,$$

where Q_1 and Q_2 are two open subsets of the cylinder Q, with a Lipschitz interface $\Sigma_{1,2} = \overline{Q}_1 \cap \overline{Q}_2$ admitting a unit normal vector $\nu = (\nu_{1,\dots,}\nu_d, \nu_{d+1})$ of $\mathbb{R}^d \times \mathbb{R}$, oriented into Q_1.

Using the notations of Figure 2, the problem can be written more precisely as a problem with free surface:

$$\begin{cases} v = \beta_1(w) \ and \ \dfrac{\partial v}{\partial t} - \Delta\Phi_1(v) = 0 \quad in\ Q_1, \\ v = \beta_2(w) \ and \ \dfrac{\partial v}{\partial t} - \Delta\Phi_2(v) = 0 \quad in\ Q_2. \end{cases} \tag{18}$$

As a consequence of the information contained in the Rankine–Hugoniot and entropy relations (15)–(16), *which are justified here along the shock wave $\Sigma_{1,2}$, the sign of the component ν_{d+1} of the normal vector ν, i.e., its orientation during the time, is specified by the relations*

$$\begin{cases} \nu_{d+1} = 0 \quad if\ A < w < B, \\ \nu_{d+1} \geq 0 \quad if\ w = A, \\ \nu_{d+1} \leq 0 \quad if\ w = B. \end{cases} \tag{19}$$

4.3. ***Interpretation of the results.*** According to Proposition 3, the expected hysteresis effect is well described by the pair (v, w), the generalized solution of (P_Φ). The change of the expression of the state law, which governs the diffusion process according to the values of the reduced saturation, is given by (18). Moreover, relation (19) reveals that the interface $\Sigma_{1,2}$ evolves only if w takes the value A or B (see Figure 1).

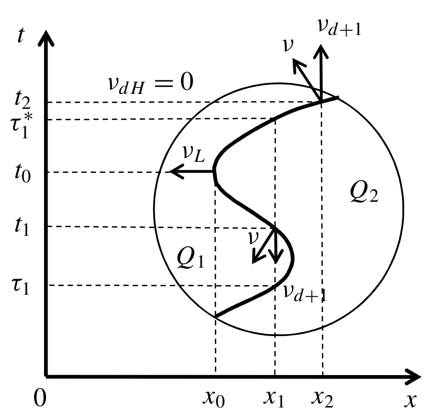

Figure 3. More general case illustrating Proposition 3.

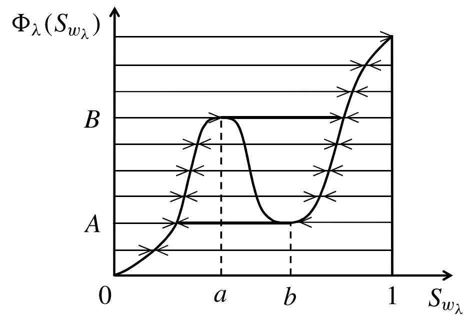

Figure 4. Flow of the auxiliary ordinary differential equation and emergence of the hysteresis effects when $\lambda \to 0$.

To illustrate the resulting hysteretic behavior, let us consider the generic example of Figure 3 on the previous page, zooming on a time interval representing three possible states of the point x_1 at three different times. We focus on the possible states corresponding to the abscissa x_1.

At the point (t_1, x_1), we have a jump from Q_1 to Q_2, $w = B$, and we are in the imbibition phase (see also Figure 1). On the contrary, at the point (t_2, x_2), we have a jump from Q_2 to Q_1, $w = A$, and we are in the drainage phase.

Therefore, the entropy method linked to the Sobolev regularization leads to a hysteresis loop similar to that obtained for Stefan's supercooling problem [Evans 2004]. The flow of the auxiliary ordinary differential equation (3) leads to hysteresis effects when $\lambda \to 0$ (Figure 4).

5. Conclusion

The hysteresis phenomena of flows in unsaturated porous media has been modeled with success, using the artificial introduction of an unstable spinodal interval and on a dynamic regularization process of Sobolev type.

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