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# A PHASE-BY-PHASE UPSTREAM SCHEME THAT CONVERGES TO THE VANISHING CAPILLARITY SOLUTION FOR COUNTERCURRENT TWO-PHASE FLOW IN TWO-ROCKS MEDIA

#### BORIS ANDREIANOV AND CLÉMENT CANCÈS

ABSTRACT. We discuss the convergence of the upstream phase-by-phase scheme (or upstream mobility scheme) towards the vanishing capillarity solution for immiscible incompressible two-phase flows in porous media made of several rock types. Troubles in the convergence where recently pointed out in [S. Mishra & J. Jaffré, Comput. Geosci., 2010] and [S. Tveit & I. Aavatsmark, Comput. Geosci, 2012]. In this paper, we clarify the notion of vanishing capillarity solution, stressing the fact that the physically relevant notion of solution differs from the one inferred from the results of [E. F. Kaasschieter, Comput. Geosci., 1999]. In particular, we point out that the vanishing capillarity solution depends on the formally neglected capillary pressure curves, as it was recently proven in by the authors [B. Andreianov & C. Cancès, Comput. Geosci., 2013]. Then, we propose a numerical procedure based on the hybridization of the interfaces that converges towards the vanishing capillarity solution. Numerical illustrations are provided.

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#### 1. MOTIVATIONS OF THE PAPER

Computing the solution of multiphase flows in porous media is a crucial issue for several important applications, like oil-engineering, nuclear waste repository management or CO2 sequestration in aquifers.

Among the numerous numerical methods proposed for solving related problems, the so-called *phase-by-phase upstream* or *upstream mobility* scheme occupies a particularly important place. Indeed, it is robust, physically motivated, and quite easy

to implement (see e.g. [AS79, BJ91]). Its convergence is guaranteed in the simple case of incompressible two-phase flows governed by the so-called *Buckley-Leverett* equation in a homogeneous porous media, both for computing the vanishing capillarity limit [Sam88, BJ91] with an explicit scheme and for solving the model in presence of capillary diffusion [EHM03] in an implicit version of the scheme.

Nevertheless, in the case of heterogeneous rocks, some of its straightforward generalizations may produce unexpected results, at it has been pointed out in several recent works [MJ10, TA12, TMA13]. In particular, the version of the scheme proposed in [MJ10] and [TA12] fails to capture the "expected" solution in the case of a rock discontinuity. In this paper, we give two explanations for this lack of convergence.

- (1) Firstly, it turns out that convergence of the scheme is closely related to the preservation of some crucial steady states, and the schemes that are not able to preserve them may converge to a limit different from the expected one.
- (2) Secondly, even when a scheme guarantees convergence to the "expected" solution, the notion of "expected" solution suggested in the paper [Kaa99] and used in several subsequent works is not, in general, the physically relevant one.

In view of these two difficulties, the goals of this paper are twofold.

#### (1) Establishing a firm theoretical background.

This is the purpose of §2. We clarify the notion of vanishing capillarity solution (which is the physically relevant solution) for the Buckley-Leverett equation in heterogeneous rocks. This relies on the previous study carried out by the authors [AC13], where it has been pointed out that even if capillarity seems to be neglected, the vanishing capillarity solution in a heterogeneous medium strongly depends on the capillary pressure curves.

### (2) Designing schemes that capture the physically relevant solution.

This point is developed in §3. We propose a simple (and physically motivated) way to correct the phase-by-phase upstream scheme so that it preserve some particular steady states. This allows the scheme to converge towards the vanishing capillarity solution. Notice that, in view of previous point, it is mandatory to know the capillary pressure curves in order to identify the steady states to be preserved.

We exhibit numerical results in §4 as an evidence of the relevance of the method.

The goal of this paper is not to detail the mathematical proofs (the proofs can all be found in references, mainly in [AC13] and [AC]), but to take benefits of these theoretical results for explaining and correcting the convergence troubles observed in [MJ10] and [TA12]. We restrict our study to the one-dimensional framework; natural extensions to the more complicated multidimensional framework can be designed, e.g, along the guidelines proposed in [ABC13], although the current state of the art does not allow for a theoretical analysis of the problem.

#### 2. Understanding the vanishing capillarity solution

2.1. **Description of the model with capillary diffusion.** Let us first recall the equations governing an incompressible immiscible two-phase flow in a one-dimensional porous medium. For the sake of clarity, we adopt notations referring to a situations where we are interested in the flow of oil (subscript o) and water (subscript w). Denoting by  $\phi$  the porosity of the medium,  $s_{\alpha}$  the saturation of the

phase  $\alpha$ , and  $v_{\alpha}$  its filtration speed ( $\alpha \in \{o, w\}$ ), the conservation of mass yields

$$\phi \partial_t s_\alpha + \partial_x v_\alpha = 0.$$

The filtration speeds  $v_{\alpha}$  for each phase are governed by the Darcy-Muskat law

(2) 
$$v_{\alpha} = -K\eta_{\alpha}(s_{\alpha}) \left(\partial_{x} p_{\alpha} - \rho_{\alpha} g\right),$$

where K denotes the permeability of the rock,  $\eta_{\alpha}$  is the mobility of the phase  $\alpha$ ,  $p_{\alpha}$  its pressure,  $\rho_{\alpha}$  its density and g is the projection of the gravity on the direction of the axis x. The functions  $\eta_{\alpha}$  are assumed to be Lipschitz continuous, non-decreasing, and to satisfy  $\eta_{\alpha}(0) = 0$ . More precisely, there exists two irreducible saturations  $s_{o,r} \in [0,1)$  and  $s_{w,r} \in [0,1)$  satisfying  $s_{o,r} + s_{w,r} < 1$  and such that

$$\eta_{\alpha}(s_{\alpha}) = 0 \text{ if } s \leq s_{\alpha,r}, \qquad \eta_{\alpha}(s_{\alpha}) > 0 \text{ if } s > s_{\alpha,r}.$$

We assume that the two-phase fluid occupies the whole pore volume, leading to the constitutive relation

$$(3) s_o + s_w = 1,$$

while we assume the following capillary pressure relation (which expresses equilibrium of the interface between the two fluids at the pore scale):

$$(4) p_o - p_w = \pi(s_o),$$

where  $\pi$  is an increasing function that we call *capillary pressure profile*.

Thanks to relation (3), we can eliminate one saturation from the system, setting

$$(5) s := s_o, \quad s_w = 1 - s.$$

For the sake of notation clarity, we denote in the sequel

$$\underline{s} = s_{o,r}, \quad \overline{s} = 1 - s_{w,r}.$$

Summing up (1) for  $\alpha = o, w$  we find that the total flow rate

$$q := v_o + v_w$$

does not depend on space. For the sake of simplicity, we will assume that it also does not depend on time and that it is given beforehand (at this point, the situation in the multi-dimensional case is much more complicated, see in particular [ABC13]).

According to the recent contribution [CP12] (see also [BLS09, CGP09]), the definition of the phase pressure  $p_{\alpha}$  is ambiguous where  $\eta_{\alpha}(s_{\alpha}) = 0$ , so that the inverse of the capillary pressure function  $\pi^{-1}$  must be extended in a continuous way by the constant values  $\underline{s}$  and  $\overline{s}$  outside of the interval  $(\pi(\underline{s}), \pi(\overline{s}))$ . This extension, still denoted by  $\pi^{-1}$ , is illustrated on Figure 1.

Now we can use the classical reformulation of the problem (1)–(6) (see e.g. [CJ86]) that leads to the single degenerate parabolic equation

(7) 
$$\phi \partial_t s + \partial_x f(s) = \partial_x \left( \lambda(s) \partial_x \pi(s) \right),$$

where the nonlinearities f and  $\lambda$  are given by the formulas

(8) 
$$\lambda(s) = K \frac{\eta_o(s)\eta_w(1-s)}{\eta_o(s) + \eta_w(1-s)}, \qquad f(s) = q \frac{\eta_o(s)}{\eta_o(s) + \eta_w(1-s)} + \lambda(s)(\rho_o - \rho_w)g.$$

The typical behavior of the function f is illustrated on Figure 2. For classical models used in oil-engineering, the flux function f is bell-shaped, i.e.

(9) there exists 
$$\sigma \in [\underline{s}, \overline{s}]$$
 such that  $f'(s)(\sigma - s) > 0$  for all  $s \in (\underline{s}, \overline{s}) \setminus \{\sigma\}$ .

Despite the condition (9) is not mandatory for our study (we refer to [AC] for a generalization), it simplifies the analysis. Therefore, we will assume that (9) holds in this paper.

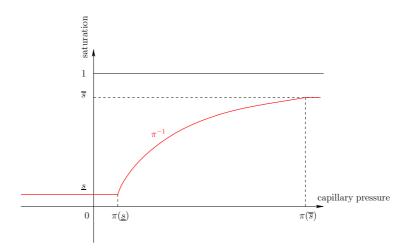


FIGURE 1. The inverse  $\pi^{-1}$  of the capillary pressure function  $\pi$  is extended by constants outside of the interval  $(\pi(\underline{s}), \pi(\overline{s}))$ . This approach is equivalent to the one, proposed in [BLS09, CGP09], that consists in extending the capillary pressure function into a maximal monotone graph.

Finally, we suppose that the initial saturation is known, namely that

(10) 
$$s(x, t = 0) = s_{\text{ini}}(x) \in [\underline{s}, \overline{s}], \text{ for } x \in \mathbb{R}.$$

Remark 2.1. In the definition (8) of the convective flux function f, two distinct components are in competition. The first one corresponds to the effect of the total convection of the fluid, and it drags both phases in the same sense contrarily to the second component, corresponding to buoyancy, that produces a countercurrent flow.

**Remark 2.2.** In order to study mathematically the problem (7),(10) many authors use the so-called Kirchhoff transform  $\theta(s)$ , defined by

$$\theta(s) = \int_{\underline{s}}^{s} \lambda(a) \pi'(a) da,$$

so that, at least formally,  $\lambda(s)\partial_x\pi(s)=\partial_x\theta(s)$ . The physical meaning of the Kirchhoff transform is not clear, so that we will avoid its explicit introduction despite it was instrumental for establishing important theoretical results omitted in this paper.

2.2. Vanishing capillarity solution in a single rock porous medium. In many applications, one can be tempted to neglect the effects of the capillary diffusion (produced by the right-hand side of (7)). The idea can be understood thanks to a very simple scaling argument, meaning that the time and space scales considered for observing the dynamic of the flow are much larger than the scales where diffusion may have an important effect. From a mathematical point of view, the scaling consists in changing t into  $t/\epsilon$  and x into  $x/\epsilon$  in (7) for a small parameter  $\epsilon > 0$ , which leads to the equation

(11) 
$$\phi \partial_t s^{\epsilon} + \partial_x f(s^{\epsilon}) = \epsilon \partial_x \left( \lambda(s^{\epsilon}) \partial_x \pi(s^{\epsilon}) \right).$$

The vanishing capillarity model is then obtained as the limit, as  $\epsilon \to 0$ , of the model (11).

In order to give a precise physical significance to the vanishing capillarity limit model, one has to understand the relation between limits of solutions ( $s = \lim_{\epsilon \to 0} s^{\epsilon}$ )

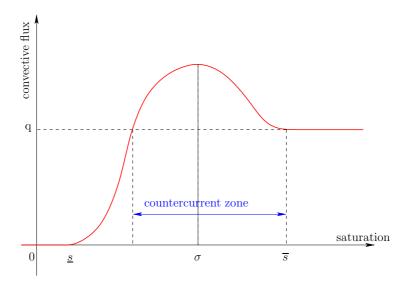


FIGURE 2. The convective flux function f is in general bell-shaped (although this is not mandatory in our study, see [AC]). For a saturation s that satisfies f(s) > q, the two phases move in opposite senses, leading to the so-called countercurrent flow.

and the formal limit of equation (11). Taking formally the limit  $\epsilon \to 0$  in (11) provides the hyperbolic Buckley-Leverett equation

(12) 
$$\phi \partial_t s + \partial_x f(s) = 0, \qquad s(\cdot, 0) = s_{\text{ini}}.$$

One may expect that  $s = \lim_{\epsilon \to 0} s^{\epsilon}$  is the solution of (12) with the appropriate initial data; in fact, the situation is much more delicate. In our setting, the vanishing capillarity limit s will be a solution of the limiting (hyperbolic) Buckley-Leverett equation (which we call the *vanishing capillarity solution*). It is what we consider as the *physically relevant solution*, but it is not the unique solution of the equation. All the other solutions should be disregarded, being artifacts of the theory; and they must be carefully avoided in numerical computations.

Indeed, regarding equation (12) it is well known (see e.g. [Ole63] for the case of vanishing viscosity solutions) that, even for a smooth datum  $s_{\rm ini}$ , the classical (continuously differentiable) solutions of (12) may develop discontinuities after a finite time. For this reason, considering solutions in the distributional sense — one calls them "weak solutions" — is mandatory. Further, the problem (12) may admit an infinite number of different weak solutions for the same initial datum; it is understood that all these solutions except one (the vanishing capillarity solution) are non-physical. An admissibility criterion based on "entropy dissipation" has to be added for selecting the unique vanishing capillarity solution. Following Kruzhkov [Kru70], this criterion can be explicitly stated as follows:

(13) 
$$\phi \partial_t |s - \kappa| + \partial_x \left( \operatorname{sign}(s - \kappa) (f(s) - f(\kappa)) \right) \le 0, \quad \forall \kappa \in [\underline{s}, \overline{s}].$$

Here and in the sequel, entropy inequalities are understood in the weak (disctributional) sense. Let us stress that (13), called the *Kruzhkov entropy criterion*, is an

<sup>&</sup>lt;sup>1</sup>To be precise, the criterion was introduced for the case of "vanishing viscosity", which corresponds to  $\lambda=1$  and  $\pi=Id$  and which is physically relevant, e.g., for the Burgers equation. But it turned out that in a homogeneous rock, the same notion is suitable for describing the vanishing capillarity limit irrespective of the shape of the functions  $\lambda(\cdot)$  and  $\pi(\cdot)$ . We will see that the situation is drastically different at interfaces between different rocks.

intrinsic criterion: namely, one can check that a given function s is an admissible solution without checking that s is the limit of unknown solutions  $s^{\epsilon}$  corresponding to small capillarity  $\epsilon > 0$ . The family of inequalities (13) means that there is a contraction between the solution s and the obvious constant steady state  $\kappa$  (roughly speaking, the  $L^1$  distance between  $s(t, \cdot)$  and  $\kappa$  is decreasing with time).

The Kruzhkov entropy criterion leads to the same solution as the so-called *Lax criterion* that is easy to visualize, in the case of discontinuous piecewise regular solutions. The Lax criterion claims that the characteristic curves can enter a discontinuity but cannot leave it. This can be interpreted by the following very simple claim which, in some models, is directly related to the second principle of thermodynamics: the discontinuity can destroy but it cannot generate information. We illustrate the Lax criterion on Figure 3.

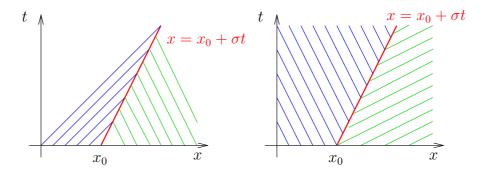


FIGURE 3. We illustrate on both figures a discontinuity of the solution traveling with speed  $\sigma$  (red line). On the left figure, the characteristic curves (red and green lines) enter the discontinuity, so that the Lax criterion is fulfilled. On the contrary, the characteristic curves leave the discontinuity on the right figure, violating the Lax criterion. Such a discontinuity is said to be *undercompressive*. In the two-rocks' setting we will focus on, an undercompressive discontinuity may occur at x=0, with the speed  $\sigma=0$ .

2.3. The case of a two-rocks porous medium. Let us stress that in a homogeneous rock, the intrinsic characterization (13) of the vanishing capillarity limit does not retain any information on the capillary pressure profile  $\pi$ . This means that the capillarity forces can be fully neglected; this also means that when  $\epsilon$  is small, solutions  $s^{\epsilon}$  of model (11) corresponding to different profiles  $\pi$  are close to each other because they are close to some common limit s (which is the Kruzhkov entropy solution of (12)).

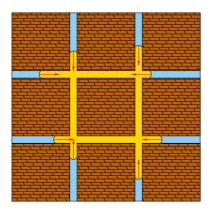
The case of a two-rocks domain is considerably more complicated, and we first go back to the pore scale to illustrate that capillary forces play a major role in this configuration. As noticed in [AMPP12] and illustrated on Figure 4, it is natural to neglect the macroscopic contribution of capillarity in the case of a homogeneous rock, but capillary forces can not be neglected at the interface between different rocks. Therefore, we have to bear in mind that capturing the singular effect located at the interface may be necessary for computing the physically relevant solution.

This singular effect linked to capillarity was first pointed out by the second author in the case where the capillary pressure only depends on space but not on the saturation. In this particular case, it was pointed out in [Can10a, Can10b] (see also [Can10c]) that, in the case of a countercurrent flow, the solution may change following the orientation of buoyancy with respect to capillarity. Later, in [AC13]

we have shown that in general, the full knowledge of the capillary pressure curve is necessary to identify the vanishing capillarity solution, that is the limit as  $\epsilon$  tends to 0 of the solution of the problem with  $\epsilon$ -capillary diffusion

(14) 
$$\phi(x)\partial_t s^{\epsilon} + \partial_x f(s^{\epsilon}; x) = \epsilon \partial_x \left( \lambda(s^{\epsilon}; x) \partial_x \pi(s^{\epsilon}; x) \right)$$

(now, with x-dependent discontinuous at x=0 nonlinearities  $f(\cdot), \lambda(\cdot), \pi(\cdot)$  and parameter  $\phi$ ).



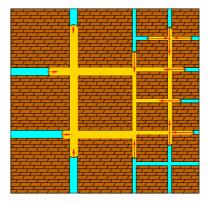


FIGURE 4. At the pore scale, the capillary pressure is an increasing function of the curvature of the interface between the two fluids. The wetting angle, i.e. the angle appearing at the point (on a line, in 3d) where the two phases and and rock grain meet, is fixed by the fluid and the rock properties; smaller is the pore, greater is the capillary pressure. Nevertheless, in a regular configuration, there is a natural balance of the resulting capillary forces applied on a droplet of non-wetting fluid (in yellow), so that capillarity forces have a small macroscopic effect (left figure). This natural balance is lost (right figure) when the droplet is placed on the interface between two rocks with different physical parameters (characteristic pore size, wetting angle, etc.).

2.3.1. A model case with two adjacent rocks. Let us now come back to the macroscopic description of the problem, extending to the heterogeneous case the modeling of the problem. We restrict ourselves to the case of a single interface located at x=0, the generalization to a finite number of interfaces being straightforward. We also assume, for the sake of simplicity, that the subdomains  $\{x<0\}$  (denoted by  $\Omega_l$ ) and  $\{x>0\}$  (denoted by  $\Omega_r$ ) are homogeneous. For every relation involving a space dependent quantity (e.g.,  $\varphi(x)$ ) that is valid separately in each of the two subdomains, we will use the double subscripting (e.g.,  $\varphi_{l,r}$ ), but we will keep the notation s for the saturation defined in  $\mathbb{R} = \overline{\Omega_l \cup \Omega_r}$ .

Let us put forward a hyperbolic Buckley-Leverett model for this case. We will see that, firstly, it captures the vanishing capillarity limit of the more precise parabolic Buckley-Leverett model (see Theorem A.1 in Appendix). Secondly, it can be discretized in a rather straightforward way (see §3).

First, notice that  $f_{l,r}$  are *compatible* in the sense that

(15) 
$$f_l(\underline{s}_l) = f_r(\underline{s}_r) = 0, \qquad f_l(\overline{s}_l) = f_r(\overline{s}_r) = q.$$

In each of the subdomains  $\Omega_{l,r}$ , the relation (12) remains valid, i.e.

(16) 
$$\phi_{l,r}\partial_t s + \partial_x f_{l,r}(s) = 0, \quad x \neq 0,$$

and more precisely, we recover the Kruzhkov inequalities (13), which now are localized away from the interface:

$$(17) \ \phi_{l,r}\partial_t |s-\kappa| + \partial_x \left( \operatorname{sign}(s-\kappa)(f_{l,r}(s) - f_{l,r}(\kappa)) \right) \le 0, \ x \ne 0, \ \forall \kappa \in [\underline{s}_{l,r}, \overline{s}_{l,r}].$$

The above equation (17) characterizes the flow within the homogeneous rocks  $\Omega_{l,r}$ .

2.3.2. Interface conditions for two-rocks' medium. Now let us focus on the transmission conditions across the interface. Denote by  $s_{l,r}$  the one-sided values of the saturation s at the interface. The principle of mass conservation imposes the flux transmission condition

$$(18) f_l(s_l) = f_r(s_r),$$

which is the well-known Rankine-Hugoniot condition for a zero-speed discontinuity. Here again, for a given initial datum  $s_{\rm ini}$ , there may exist an infinite number of solutions (see [AMG05, BKT09]) fulfilling (10), (17) and (18), so that an adapted entropy criterion must be added to select the physically relevant solution. A consequence of the singular effect at the interface between the two rocks (see the discussion at the pore scale, Fig. 4) is that one has to allow this interface to "generate information", which means that some undercompressive discontinuities should be allowed at x=0. Therefore, the Lax criterion is not suitable anymore for fully describing the expected behavior of the vanishing capillarity solution on the interface between different rocks, and original admissibility criteria for undercompressive discontinuities have to be put forward.

In order to obtain the interface admissibility condition suitable for characterization of the vanishing capillarity solution, in this paper we have chosen to focus on the transmission condition on the capillary pressure which is the second quantity that would remain continuous at the interface. Indeed, in the physical model, one would expect that the one-sided values of the saturation  $s_{l,r}$  have to be linked by the following pressure transmission condition:

(19) there exists 
$$p \in [-\infty, +\infty]$$
 such that  $s_l = \pi_l^{-1}(p)$  and  $s_r = \pi_r^{-1}(p)$ ,

which means that  $\pi_l(s_l) = \pi_r(s_r)$ . While this second interface transmission condition can be enforced into the parabolic model (the case  $\epsilon > 0$ ), see in particular [BDvD03, CGP09, Can09, CP12, BCH13], in the scaled hyperbolic Buckley-Leverett model ( $\epsilon = 0$ ) the pressure transmission condition is, at a first glance, incompatible with the flux transmission condition (18). Indeed, the passage to the limit  $\epsilon \to 0$  in the scaling procedure leads to a loss of information (a gradual interface layer that may be present in  $s^{\epsilon}$  for  $\epsilon > 0$  gives rise to a pure jump in  $s = \lim_{\epsilon \to 0} s^{\epsilon}$  at the limit  $\epsilon = 0$ ). Also from the purely mathematical perspective, due to the fact that the equation governing the flow is hyperbolic the pressure transmission condition (19) cannot be imposed literally. Having in mind the mathematical theory of hyperbolic conservation laws, it is natural to impose (19) in a weaker (generalized) sense inspired from the work of Bardos, le Roux and Nédélec [BlRN79].

In order to make this sense explicit, let us introduce the exact Godunov solver for the flux functions  $f_{l,r}$ :

(20) 
$$G_{l,r}(a,b) = \begin{cases} \min_{s \in [a,b]} f_{l,r}(s) \text{ if } a \leq b, \\ \max_{s \in [b,a]} f_{l,r}(s) \text{ if } a \geq b. \end{cases}$$

With this notation, the generalized pressure-and-flux transmission condition at the interface x = 0 writes as follows:

(21) there exists 
$$p \in [-\infty, +\infty]$$
 such that  $f_l(s_l) = G_l(s_l, \pi_l^{-1}(p)) = G_r(\pi_r^{-1}(p), s_r) = f_r(s_r).$ 

To be precise, (21) is understood pointwise at the interface x=0, i.e.,  $s_{l,r}(\cdot)$  and  $p(\cdot)$  in (21) are t-dependent functions. This is nothing but saying that  $s\mathbf{1}_{x<0}$  is the solution in the sense of [BlRN79] to conservation law in  $\Omega_l$  with the Dirichlet condition  $\pi_l^{-1}(p)$  at  $x=0^-$ , that  $s\mathbf{1}_{x>0}$  is the solution in the sense of [BlRN79] to conservation law in  $\Omega_r$  with the Dirichlet condition  $\pi_r^{-1}(p)$  at  $x=0^+$ , while the common value p expresses the (generalized) pressure transmission across the interface and the common value  $f_{l,r}(s_{l,r})$  ensures the flux transmission.

In relation with condition (21), we will say that the quantities  $\pi_{l,r}^{-1}(p)$  are onesided expected values of the saturation at the interface making the capillary pressure continuous, while the quantities  $s_{l,r}$  are the effective values of the saturation. Roughly speaking, the transitions between the effective values  $s_{l,r}$  and the expected values  $\pi_{l,r}^{-1}(p)$  are due to the interface layers that develop in  $s^{\epsilon}$ , for small non-zero values of  $\epsilon$ .

Obviously, condition (21) is more restrictive than condition (18). Actually, (18) (along with (16)) only guarantees that s is a weak solution of the mass conservation equation

(22) 
$$\phi(x)\partial_t s + \partial_x f(s; x) = 0, \quad x \in \mathbb{R},$$

$$\phi(x) = \phi_l \mathbf{1}_{x<0} + \phi_r \mathbf{1}_{x>0}, \ f(\cdot; x) = f_l(\cdot) \mathbf{1}_{x<0} + f_r(\cdot) \mathbf{1}_{x>0}$$

and (21) plays the role of an entropy condition for (22) at the interface.

In conclusion, on the basis of the above modeling arguments we arrive to the following precise notion of solution for the hyperbolic Buckley-Leverett model (22) corresponding to capillary pressure profiles  $\pi_{l,r}$ .

**Definition 2.1** (vanishing capillarity solution). A function  $s \in L^{\infty}(\Omega \times \mathbb{R}_+; [\underline{s}, \overline{s}])$  is a vanishing capillarity solution of (22) if it satisfies Kruzhkov entropy inequalities (17) away from the interface, and if the generalized pressure-and-flux transmission condition (21) at the interface holds pointwise for a.e.  $t \in [0, T]$ .

The name "vanishing capillarity solution" is formally justified by the above analysis, and it is rigorously justified by the result of Theorem A.1 in Appendix.

Remark 2.3. Note that the formulation (21), in the particular case  $\pi_l = \pi_r = Id$  (this is the case of vanishing viscosity limit) was used in [Die09] as an equivalent formulation of the " $\Gamma$ -condition" used as admissibility condition at the interface. The idea to use the " $\Gamma$ -condition" also appeared, at the numerical level, in the early work [CCJ87].

2.3.3. A study of steady states and adapted entropies. In the case of a homogeneous domain, the celebrated Kruzhkov's theory allows to characterize the vanishing capillarity solution by expressing in (13) its contraction w.r.t. the constant steady states  $\kappa$ . In the two-rocks model, the constant states  $\kappa$  are not steady states anymore because of the flux discontinuity. Instead, one has to rely upon a well-chosen family of piecewise constant steady states  $\kappa(x)$  of the form

(23) 
$$\kappa(x) = \kappa_l \mathbf{1}_{x<0} + \kappa_r \mathbf{1}_{x>0}.$$

While the function  $\kappa$  defined in (23) clearly satisfies (17), it must satisfy (21) to be a steady state in the sense of Definition 2.1. This means that  $(\kappa_l, \kappa_r)$  has to belong to the set  $\mathcal{G}_{\pi}^*$  defined by

(24) 
$$\mathcal{G}_{\pi}^* = \{ (s_l, s_r) \in [\underline{s}_l, \overline{s}_l] \times [\underline{s}_r, \overline{s}_r] \mid (s_l, s_r) \text{ fulfill } (\underline{21}) \}.$$

This set plays a central role in the analysis of vanishing capillarity solutions. Firstly, according to Definition 2.1, for almost all t > 0 we have  $(s_l(t), s_r(t)) \in \mathcal{G}_{\pi}^*$ , where

 $s_{l,r}$  are one-sided traces from  $\Omega_{l,r} \times \mathbb{R}_+$  on  $\{x = 0\} \times \mathbb{R}_+$  of s, in the sense that for all T > 0,

$$\lim_{h \to 0} \frac{1}{h} \int_0^T \int_{-h}^0 |s(x,t) - s_l(t)| dx dt = 0 = \lim_{h \to 0} \frac{1}{h} \int_0^T \int_0^h |s(x,t) - s_r(t)| dx dt.$$

Moreover, following the idea of [BJ97, AP05, BKT09] the family of steady states (23) associated with couples  $(\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^*$  allows to extend the Kruzhkov type-entropy inequalities (17), set up separately in  $\Omega_l$  and in  $\Omega_r$ , to the whole domain  $\mathbb{R} = \overline{\Omega_l \cup \Omega_r}$ . To this end, one uses the adapted entropies  $s \mapsto |s - \kappa(x)|$ :

**Proposition 2.2** (adapted entropy inequalities). A function s is a vanishing capillarity solution in the sense of Definition 2.1 if and only if, for all  $(\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^*$ ,

(25) 
$$\phi(x)\partial_t |s - \kappa(x)| + \partial_x \left( \operatorname{sign}(s - \kappa(x))(f(s; x) - f(\kappa(x); x)) \right) \le 0,$$
 where  $\kappa(x) = \kappa_t \mathbf{1}_{x < 0} + \kappa_r \mathbf{1}_{x > 0}.$ 

Note that formulation (25) is the main tool used in the proof of convergence of the numerical scheme described in the below section. Proposition 2.2 is in fact a general property in the setting of discontinuous-flux conservation laws, see [AKR11]. An additional characterization of solutions is given in Theorem A.1 in the Appendix, where the link with vanishing capillarity limits is made rigorous.

Now, define  $\mathcal{E}_{\pi} \subset \mathcal{G}_{\pi}^*$  by

(26) 
$$\mathcal{E}_{\pi} = \left\{ (\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^* \mid \kappa_{l,r} = \pi_{l,r}^{-1}(p) \text{ for some } p \right\},$$

then the set  $\mathcal{E}_{\pi}$  is associated with steady states (23) that yield a constant capillary pressure field in  $\overline{\Omega_l \cup \Omega_r}$ . The subset  $\mathcal{E}_{\pi}$  of  $\mathcal{G}_{\pi}^*$  consists in the intersection of the set

(27) 
$$\mathcal{F} = \{ (s_l, s_r) \in [\underline{s}_l, \overline{s}_l] \times [\underline{s}_r, \overline{s}_r] \mid f_l(s_l) = f_r(s_r) \}$$

(couples satisfying the flux transmission condition (18)) with the set

(28) 
$$\mathcal{P} = \{ (\pi_l^{-1}(p), \pi_r^{-1}(p)), \text{ for } p \in [-\infty, +\infty] \}$$

(those satisfying the pressure transmission condition (19)). Note that the combination of (18) and (19) is much stronger than the generalized flux-and-pressure transmission condition (21). Notice also that every steady state(23) with  $(\kappa_l, \kappa_r) \in \mathcal{E}_{\pi}$  is an evident limit of vanishing capillarity approximations because it fulfills (14) for every  $\epsilon > 0$ .

As a consequence of (15),  $\mathcal{E}_{\pi}$  contains the extremal values  $(\underline{s}_{l}, \underline{s}_{r})$  and  $(\overline{s}_{l}, \overline{s}_{r})$ , but it can also contain some additional intermediate couples that play a central role in the characterization of the solution. In particular,  $\mathcal{P}$  can cross the subset  $\mathcal{U}$  of  $\mathcal{F}$ , made of the stationary undercompressive discontinuities, defined by

$$\mathcal{U} = \{(s_l, s_r) \in \mathcal{F} \mid s_l > \sigma_l \text{ and } s_r < \sigma_r\};$$

the set  $\mathcal{U}$  is the graph of a continuous strictly decreasing function. The set  $\mathcal{P}$  is a maximal monotone graph joining  $(\underline{s}_l,\underline{s}_r)$  for  $p=-\infty$  to  $(\overline{s}_l,\overline{s}_r)$  for  $p=+\infty$ . Therefore it follows from the monotonicity argument that either  $\mathcal{P}\cap\mathcal{U}=\emptyset$ , or  $\mathcal{P}\cap\mathcal{U}$  is reduced to a single couple denoted by  $(s_l^\pi,s_r^\pi)$ . As explained in [AC13], different configurations lead to very different behavior of the solution s at the interface, because the set  $\mathcal{G}_\pi^*$  of the possible traces depends on the couple  $(s_l^\pi,s_r^\pi)$  selected by intersecting  $\mathcal{P}$  and  $\mathcal{U}$ . Let us introduce

$$\mathcal{O} = \mathcal{F} \setminus \mathcal{U}$$

the set of the overcompressive and Lax-regular discontinuities (cf. [BKT09, Figure 1.2]). We have the following alternative.

<sup>&</sup>lt;sup>2</sup>Such traces  $s_{l,r}$  exist thanks to a result of Panov [Pan07] and thanks to assumptions (9) that imply flux non-degeneracy.

- (A) If  $\mathcal{P} \cap \mathcal{U} = \emptyset$ , then  $\mathcal{G}_{\pi}^* = \mathcal{O}$ . In this case, illustrated on Figure 5(A), the vanishing capillarity solution coincides with the so-called *optimal entropy solution* highlighted by Kaasschieter [Kaa99] and used in several subsequent works.
- (B) Assume now that  $\mathcal{P} \cap \mathcal{U} = (s_l^{\pi}, s_r^{\pi})$ , set  $\overline{F} = f_{l,r}(s_{l,r}^{\pi})$ , and define  $\mathcal{O}^{\overline{F}} = \{(s_l, s_r) \in \mathcal{O} \mid f_{l,r}(s_{l,r}) \leq \overline{F}\}$ . Then  $\mathcal{G}_{\pi}^* = \mathcal{O}^{\overline{F}} \cup (s_l^{\pi}, s_r^{\pi})$ . In this case, illustrated on Figure 5(B), the vanishing solution is not the optimal entropy solution anymore. In particular, the fact that the state  $(s_l^{\pi}, s_r^{\pi})$  is an admissible undercompressive state generates a constraint on the flux across the interface (cf. [CG07, AGS10, AC12]), i.e.,

$$(29) (s_l, s_r) \in \mathcal{G}_{\pi}^* \implies f_{l,r}(s_{l,r}) \leq \overline{F} = f_{l,r}(s_{l,r}^{\pi}).$$

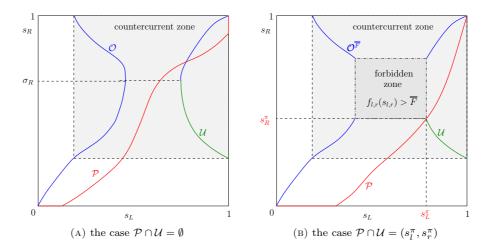


FIGURE 5. Geometrical construction of the set  $\mathcal{G}_{\pi}^*$  in the  $(s_l, s_r)$ plane. The dependence of  $\mathcal{G}_{\pi}^*$  w.r.t. the capillary pressure profiles  $\pi_{l,r}$  comes from its dependence w.r.t. the curve  $\mathcal{P}$  defined in (28).

**Remark 2.4.** In the early work of Kaasschieter, the configuration where  $\mathcal{E}_{\pi}$  contains non-trivial elements, as in configuration (B), is considered as "merely coincidental" and neglected, leading to the erroneous conclusion that, in general, the vanishing capillarity solution coincides with the optimal entropy solution, i.e.  $\mathcal{G}_{\pi}^* = \mathcal{O}$ .

#### 3. Description of the numerical scheme

The goal of this section is to take advantage of the mathematical characterization of the vanishing capillarity solution of §2 and to build a numerical scheme, derived from the widely used the phase-by-phase upstream scheme, that converges towards the physically relevant vanishing capillarity solution. According to the discussion of the previous section, explicit use of nonlinearities  $\pi_{l,r}$  in the scheme is mandatory on the interface between the two rocks.

First, in §3.1 we recall the phase-by-phase upstream scheme in the well-known case of a homogeneous domain. This scheme will be used in each of the homogeneous rocks  $\Omega_{l,r}$ . Second, in §3.2 using one additional unknown we enforce the physical coupling of the schemes written in  $\Omega_{l,r}$  across the interface. This strategy leads to the obtention of a monotone well-balanced scheme preserving the set  $\mathcal{G}_{\pi}$  defined in (26) of the steady states with constant capillary pressure. The  $L^{\infty}$ -stability and

convergence of the scheme are stated in  $\S 3.3$ . Extension to higher order methods are shortly discussed in  $\S 3.4$ .

For the sake of clarity, we only present the case of uniform time and space discretizations, avoiding the introduction of more complex notations. However, the generalization of the scheme to the case of non-uniform discretizations is straightforward.

3.1. The case of a homogeneous porous medium. In what follows, we denote by  $\Delta x$  and  $\Delta t$  the space and time discretization steps, respectively. The cell numbered by j+1/2 is located between the "edges" (that are just breakpoints, since we are in 1D)  $x_j = j\Delta x$  and  $x_{j+1} = x_j + \Delta x = (j+1)\Delta x$ . The discrete solution  $s_h$  is defined as the piecewise constant function

(30) 
$$s_h(x,t) = s_{j+1/2}^{n+1} \quad \text{if } (x,t) \in (x_j, x_{j+1}) \times (n\Delta t, (n+1)\Delta t],$$

where the quantities  $\left(s_{j+1/2}^{n+1}\right)_{j,n}$  are obtained via the time-explicit numerical scheme

$$(31) \ \phi \frac{s_{j+1/2}^{n+1} - s_{j+1/2}^n}{\Delta t} \Delta x + \operatorname{Up}(s_{j+1/2}^n, s_{j+3/2}^n) - \operatorname{Up}(s_{j-1/2}^n, s_{j+1/2}^n) = 0, \quad j \in \mathbb{Z},$$

initialized with some values  $s_{j+1/2}^0 \in [0,1]$  such that  $\sum_j s_{j+1/2}^0 \mathbf{1}_{(x_j,x_{j+1})} \to s_{\text{ini}}$  a.e. on  $\mathbb{R}$  as  $\Delta x \to 0$ ; for the theoretical analysis, we choose the values

(32) 
$$s_{j+1/2}^{0} = \frac{1}{\Delta x} \int_{x_{j}}^{x_{j+1}} s_{\text{ini}}(x) dx.$$

In (31), Up:  $[\underline{s}, \overline{s}]^2 \to \mathbb{R}$  is the phase-by-phase upstream flux function, whose expression relies on the particular structure (8) of the flux function f. Namely, given a couple of states  $(a, b) \in [\underline{s}, \overline{s}]^2$ , we set

(33) 
$$\operatorname{Up}(a,b) = \frac{\eta_o^{\star}}{\eta_o^{\star} + \eta_w^{\star}} \left[ q + K(\rho_o - \rho_w) \eta_w^{\star} \right],$$

where the superscript " $\star$ " for  $\eta_{o,w}$  reflects the upstream choice in each phase:

(34) 
$$\eta_o^{\star} = \begin{cases} \eta_o(a) & \text{if } q + K(\rho_o - \rho_w) \eta_w^{\star} \ge 0, \\ \eta_o(b) & \text{if } q + K(\rho_o - \rho_w) \eta_w^{\star} \le 0, \end{cases}$$

(35) 
$$\eta_w^{\star} = \begin{cases} \eta_w(1-a) & \text{if } q + K(\rho_w - \rho_o)\eta_o^{\star} \ge 0, \\ \eta_w(1-b) & \text{if } q + K(\rho_w - \rho_o)\eta_o^{\star} \le 0. \end{cases}$$

Let us briefly discuss the definition and the convergence of this scheme.

Remark 3.1. Despite the upwinding in formulas (34)–(35) seems to be implicit, a very simple physical argument developed in [BJ91] allows to make the calculation of (33) explicit. Indeed, buoyancy make both phases move in opposite senses, while the global convection make them move in the same direction. Then, for a given q, there is one phase for which both contributions are oriented in the same sense, and therefore its upwinding direction is known a priori. Then, the upwinding direction of the other phase stems from (34)–(35).

**Remark 3.2.** Three properties are required for justifying convergence of finite volume schemes with two-point flux: consistency, monotonicity and uniform Lipschitz continuity (see, e.g., to [CM80, GR91, EGH00] for the convergence proofs). We recall that the above phase-by-phase upstream scheme does satisfy the three properties. Indeed, first, in view of (8) the numerical flux function  $Up(\cdot, \cdot)$  in (33) is consistent, i.e.,

$$(36) Up(s,s) = f(s).$$

Second, as proven in [BJ91],  $Up(\cdot, \cdot)$  is monotone non-decreasing in a, non-increasing in b, and third, it is Lipschitz continuous w.r.t. both variables. More precisely, there exist positive quantities  $L^+$  and  $L^-$  such that

$$(37) 0 \le \partial_a \operatorname{Up}(a,b) \le L^+, -L^- \le \partial_b \operatorname{Up}(a,b) \le 0, \quad \forall (a,b) \in [\underline{s},\overline{s}]^2.$$

This allows to claim that, under the appropriate CFL condition, the scheme converges towards the unique entropy solution s of (10)–(12) as the discretization step tends to 0, namely

(38) 
$$s_h \to s \text{ in } L^1_{loc}(\mathbb{R} \times \mathbb{R}_+) \quad \text{ as } \quad \Delta x, \Delta t \to 0 \text{ provided } \frac{(L^+ + L^-)\Delta t}{\phi \Delta x} \le 1$$

where s is the solution of (12) in the sense (13).

3.2. Transmission conditions on the interface between different rocks. Now, we assume that the porous medium is discontinuous at  $x_0 = 0$  (it consists of two different rocks  $\Omega_{l,r}$  meeting at x = 0), and that the rocks  $\Omega_{l,r}$  are homogeneous. For the same meshes as those described in §3.1 (in particular, the mesh breakpoint corresponding to j = 0 now coincides with the rocks' interface x = 0), general Finite Volume scheme with two-point fluxes on boundaries between volumes takes the form

(39) 
$$\phi_{j+1/2} \frac{s_{j+1/2}^{n+1} - s_{j+1/2}^{n}}{\Delta t} \Delta x + F_{j+1} \left( s_{j+1/2}^{n}, s_{j+3/2}^{n} \right) - F_{j} \left( s_{j-1/2}^{n}, s_{j+1/2}^{n} \right) = 0$$

with  $\phi_{j+1/2} = \phi_{l,r}$  if  $x_{j+1/2} \in \Omega_{l,r}$ . Since the vanishing capillarity solution satisfies the usual admissibility conditions away from the interface x = 0, we want to stick to the phase-by-phase upstream scheme of §3.1 (which is consistent with these classical admissibility conditions) for computing the numerical fluxes at the breakpoints  $x_j$  for  $j \neq 0$  at each time step  $n\Delta t$ . Therefore, we simply set

(40) 
$$F_j\left(s_{j-1/2}^n, s_{j+1/2}^n\right) = \begin{cases} \operatorname{Up}_l(s_{j-1/2}^n, s_{j+1/2}^n) & \text{if } j < 0, \\ \operatorname{Up}_r(s_{j-1/2}^n, s_{j+1/2}^n) & \text{if } j > 0, \end{cases}$$

where the numerical fluxes  $\operatorname{Up}_{l,r}$  are deduced in a straightforward way from (33) in the case of piecewise constant x-dependent parameters K,  $\eta_o$  and  $\eta_w$ .

In order to fully define the Finite Volume scheme (39) we now have to focus on the numerical treatment of the interface, i.e., define the interface flux function  $F_0(\cdot,\cdot)$ . The formula for  $F_0$  that we propose is based on the introduction of an additional "pressure" variable at the interface, as suggested by the transmission condition (21). Notice that this can be seen as a kind of hybridization of the scheme on the rocks' interface. To this end, we just replace the exact Riemann solvers  $G_{l,r}$  appearing in (21) by the approximate Riemann solvers<sup>3</sup> Up<sub>l,r</sub>. This leads to solving at each time step the following scalar nonlinear equation on the unknown p:

(41) find 
$$p^n$$
 such that  $\operatorname{Up}_l\left(s_{-1/2}^n, \pi_l^{-1}(p^n)\right) = \operatorname{Up}_r\left(\pi_r^{-1}(p^n), s_{1/2}^n\right)$ ,

and then, given the so obtained value that we call  $p^n$ , we define

$$(42) F_0\left(s^n_{-1/2}, s^n_{1/2}\right) := \operatorname{Up}_l\left(s^n_{-1/2}, \pi^{-1}_r(p^n)\right) \equiv \operatorname{Up}_r\left(\pi^{-1}_r(p^n), s^n_{1/2}\right).$$

 $<sup>^3</sup>$ As proved in [ABC13, Prop. 2.4], any monotone consistent Lipschitz continuous Riemann solvers  $R_{l,r}$  can be used for approximation of vanishing capillarity solution. The best (least diffusive) approximation can be obtained, as usual, using the Godunov fluxes  $G_{l,r}$ ; but we stick to the choice of fluxes  $\operatorname{Up}_{l,r}$ , in order to simplify the implementation of the scheme.

**Remark 3.3.** For all  $a, b \in [0, 1]$ , the function

(43) 
$$p \in \mathbb{R} \mapsto \Psi_{a,b}(p) := \operatorname{Up}_{l}\left(a, \pi_{l}^{-1}(p)\right) - \operatorname{Up}_{r}\left(\pi_{l}^{-1}(p), b\right)$$

is a continuous non-increasing function, moreover,

$$\lim_{p \to -\infty} \Psi_{a,b}(p) \ge 0, \qquad \lim_{p \to -\infty} \Psi_{a,b}(p) \le 0$$

(this can be checked as in [AC13, Appendix A.2]). Therefore, equation (41) always admits at least one solution  $p^n$ . While this solution  $p^n$  might be non-unique (because  $\Psi_{a,b}$  can be constant on intervals), actually the corresponding flux value  $F_0\left(s_{-1/2}^n, s_{1/2}^n\right)$  is uniquely defined. As a consequence of the fact that  $\Psi_{a,b}$  can be constant on intervals, solving the equation  $\Psi_{a,b}(p) = 0$  with the Newton method might lead to severe difficulties. Taking advantage of the monotonicity of  $\Psi_{a,b}$ , we suggest to solve the problem thanks to the regula falsi method, whose convergence is ensured, moreover, the convergence is superlinear at least in the situations where  $\Psi_{a,b}$  is smooth in a vicinity of the solution.

To sum up, the above arguments lead to the following definition of the numerical flux  $F_0$ :

(44) 
$$F_0(a,b) = \operatorname{Up}_l(a, \pi_l^{-1}(p)) \equiv \operatorname{Up}_r(\pi_r^{-1}(p), b)$$
 for  $p$  that solves  $\Psi_{a,b}(p) = 0$ , where  $\Psi_{a,b}$  is defined by (43).

Now, let us investigate the properties of the so defined numerical flux  $F_0$ . A remarkable property of the hybridization technique is that the resulting two-point numerical flux  $F_0$  inherits the crucial monotonicity and Lipschitz continuity properties of the numerical fluxes  $\operatorname{Up}_{l,r}$ . More precisely, we have the following proposition, whose proof is detailed in [AC].

**Proposition 3.1.** Let  $L_{l,r}^{\pm}$  be positive quantities such that

$$0 \le \partial_a \operatorname{Up}_{l,r}(a,b) \le L_{l,r}^+, \qquad -L_{l,r}^- \le \partial_b \operatorname{Up}_{l,r}(a,b) \le 0,$$

then  $F_0$  is Lipschitz continuous and its a.e. partial derivatives satisfy

$$0 \le \partial_a F_0(a,b) \le L_l^+, \qquad -L_r^- \le \partial_b F_0(a,b) \le 0.$$

The above proposition leads to the following CFL condition for our scheme:

(45) 
$$\frac{\Delta t}{\Delta x} \le \min\left(\frac{\phi_l}{L_l^+ + L_l^-}, \frac{\phi_r}{L_r^+ + L_r^-}, \frac{\phi_l}{L_l^+ + L_r^-}, \frac{\phi_r}{L_l^+ + L_r^-}\right),$$

Further, notice that in the homogeneous case, the classical consistency property implies the well-balance property: namely, the constant states are equilibria of the scheme. This is not longer true in the two-rocks' case because  $f_l \neq f_r$ . The corresponding steady states are now piecewise constant function  $\kappa(x)$  defined by (23) for  $(\kappa_l, \kappa_r)$  belonging to  $\mathcal{G}_{\pi}^*$ . In contrary to the exact Godunov solver, the hybridized phase-by-phase upstream numerical flux (44) does not preserve in general all the elements of  $\mathcal{G}_{\pi}^*$ , i.e., one may have

$$F_0(\kappa_l, \kappa_r) \neq f_l(\kappa_l) \equiv f_r(\kappa_r)$$
 for certain  $(\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^*$ .

Nevertheless, the scheme preserves exactly the subset  $\mathcal{E}_{\pi}$  of  $\mathcal{G}_{\pi}^{*}$ , that is fundamental in the characterization of the solution. Since it preserves these fundamental equilibria, the scheme is said to be  $\mathcal{E}_{\pi}$ -well-balanced. This notion is made explicit in the following proposition.

**Proposition 3.2.** The interface flux  $F_0$  defined by (44) is  $\mathcal{E}_{\pi}$ -well-balanced, i.e.,

$$F_0(\kappa_l, \kappa_r) = f_l(\kappa_l) \equiv f_r(\kappa_r)$$
 for all  $(\kappa_l, \kappa_r) \in \mathcal{E}_{\pi}$ .

Actually, in the case (B) of § 2.3.3 the result of Proposition 3.2 is sufficient to justify convergence of the scheme.

In order to ensure the convergence of the scheme in all possible configurations, we also check that all the steady states (23) with  $(\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^*$  are recovered at the limit of the scheme, when the discretization parameters tend to 0. This leads to the notion of  $\mathcal{G}_{\pi}^*$ -consistency introduced in Proposition 3.3 below, whose proof is given in [AC] for a general situation (see [ABC13] for the idea of the proof in the case of bell-shaped fluxes).

**Proposition 3.3.** The scheme is  $\mathcal{G}_{\pi}^*$ -consistent, i.e. for all  $(\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^*$ , there exists a steady discrete solution  $\kappa_h(x) = \sum_{j \in \mathbb{Z}} k_{j+1/2} \mathbf{1}_{(x_j, x_{j+1})}(x)$  such that

$$f_{l,r}(\kappa_{l,r}) = F_j(\kappa_{j-1/2}, \kappa_{j+1/2}), \quad \forall j \in \mathbb{Z},$$

and such that  $\kappa_h \to \kappa \equiv \kappa_l \mathbf{1}_{x<0} + \kappa_r \mathbf{1}_{x>0}$  in  $L^1_{loc}(\mathbb{R})$  as  $\Delta x \to 0$ .

3.3. Stability and convergence of the scheme. As a consequence of Proposition (3.1), we can claim that under the CFL condition (45), the scheme is monotone,

$$(46) s_{j+1/2}^n \geq \check{s}_{j+1/2}^n \quad \forall j \in \mathbb{Z} \quad \Longrightarrow \quad s_{j+1/2}^{n+1} \geq \check{s}_{j+1/2}^{n+1} \quad \forall j \in \mathbb{Z}$$

where  $s_{j+1/2}^{n+1}$  is given by (31) and  $\check{s}_{j+1/2}^{n+1}$  is given by

$$\phi_{j+1/2} \frac{\check{s}_{j+1/2}^{n+1} - \check{s}_{j+1/2}^{n}}{\Delta t} \Delta x + F_{j+1} \left( \check{s}_{j+1/2}^{n}, \check{s}_{j+3/2}^{n} \right) - F_{j} \left( \check{s}_{j-1/2}^{n}, \check{s}_{j+1/2}^{n} \right) = 0.$$

Since the constant states  $(\underline{s}_{i+1/2})_{i\in\mathbb{Z}}$  and  $(\overline{s}_{i+1/2})_{i\in\mathbb{Z}}$ , defined by

(47) 
$$\underline{s}_{j+1/2} = \underline{s}_{l,r}, \quad \overline{s}_{j+1/2} = \overline{s}_{l,r} \quad \text{if } x_{j+1/2} \in \Omega_{l,r},$$

are steady solutions of the scheme (recall that  $(\underline{s}_l, \underline{s}_r)$  and  $(\overline{s}_l, \overline{s}_r)$  belong to  $\mathcal{G}_{\pi}$ ), we deduce from (46) that the scheme is  $L^{\infty}$ -stable:

$$(48) \underline{s}_{l,r} \leq s_{j+1/2}^n \leq \overline{s}_{l,r}, \quad \forall n \geq 0, \forall j \in \mathbb{Z} \text{ s.t. } x_{j+1/2} \in \Omega_{l,r}.$$

To sum up, the scheme we propose is

(1) physical bounds preserving, i.e.

$$\underline{s}(x) \leq s_h(x,t) \leq \overline{s}(x)$$
, for almost all  $(x,t) \in \mathbb{R} \times \mathbb{R}_+$ ;

(2) monotone and Lipschitz continuous, i.e., there exist positive constants  $L^+$ and  $L^-$  such that

$$0 \le \partial_a F_j(a, b) \le L^+, \quad -L^- \le \partial_b F_j(a, b) \le 0, \quad \forall j \in \mathbb{Z};$$

- (3) bulk-consistent, i.e.  $\operatorname{Up}_{l,r}(s,s)=f_{l,r}(s)$  for all  $s\in[\underline{s}_{l,r},\overline{s}_{l,r}];$ (4)  $\mathcal{E}_{\pi}$ -well-balanced at the interface in the sense of Proposition 3.2;
- (5)  $\mathcal{G}_{\pi}^*$ -consistent in the sense of Proposition 3.3.

Therefore, it follows from the theoretical study carried out in [AC] that it converges under a CFL condition that is slighly more restrictive than (45). More precisely, we will assume in Theorem 3.4 that there exists  $\zeta \in (0,1)$  such that

(49) 
$$\frac{\Delta t}{\Delta x} \le \zeta \min \left( \frac{\phi_l}{L_l^+ + L_l^-}, \frac{\phi_r}{L_r^+ + L_r^-}, \frac{\phi_l}{L_l^+ + L_r^-}, \frac{\phi_r}{L_l^+ + L_r^-} \right).$$

**Theorem 3.4.** Let  $s_h$  be the numerical solution defined by (30), (32), (39), (40) and (42), then

$$s_h \to s$$
 in  $L^1_{loc}(\mathbb{R} \times \mathbb{R}_+)$  as  $\Delta x, \Delta t \to 0$  provided (49) holds,

where s is the unique vanishing capillarity solution in the sense of Definition 2.1.

3.4. **High resolution schemes.** Since it is well known that monotone finite volume schemes for solving scalar conservation laws can not be more accurate than first order (see e.g. [LeV02]), the scheme presented in §3.2 may fail to capture in a sharp way the features of the solutions to (16), (18) and (21).

To avoid the introduction of excessive diffusion in the scheme in the case of a homogeneous porous medium, one of the most popular approach introduced in [vL79] consists in replacing the numerical flux  $\operatorname{Up}(s^n_{j-1/2}, s^n_{j+1/2})$  used in (31) by  $\operatorname{Up}(s^n_{j,-}, s^n_{j,+})$ , where the values  $s^n_{j,-}$  and  $s^n_{j,+}$  are one-sided reconstructions of the saturation on both sides of the edge  $x_j$  obtained by piecewise polynomial reconstructions of the saturation. In what follows, we denote by

(50) 
$$\mathcal{R}: \begin{cases} \left[\underline{s}, \overline{s}\right]^{\mathbb{Z}} \to \left(\mathbb{R}^{2}\right)^{\mathbb{Z}} \\ \left(s_{k+1/2}^{n}\right)_{k \in \mathbb{Z}} \mapsto \begin{pmatrix} \mathcal{R}_{j,-} \left(\left(s_{k+1/2}^{n}\right)_{k \in \mathbb{Z}}\right) \\ \mathcal{R}_{j,+} \left(\left(s_{k+1/2}^{n}\right)_{k \in \mathbb{Z}}\right) \end{pmatrix}_{j \in \mathbb{Z}} = \begin{pmatrix} s_{j,-}^{n} \\ s_{j,+}^{n} \end{pmatrix}_{j \in \mathbb{Z}}$$

a general reconstruction operator providing one-sided edge saturations from the cell-centered saturations.

For example, for constructing a formally second order in space and total variation diminishing (TVD) scheme in the case of a homogeneous porous medium, one can use some reconstructions based on the so-called minmod slope limiter, as suggested in [BJ91]. More precisely, defining

$$\operatorname{minmod}(a, b) = \begin{cases} 0 \text{ if } \operatorname{sign}(a) \neq \operatorname{sign}(b), \\ \operatorname{sign}(a) \operatorname{min}(|a|, |b|) \text{ otherwise,} \end{cases} \quad \forall (a, b) \in \mathbb{R}^2,$$

one can choose

$$\begin{cases} s_{j,-}^n = s_{j-1/2}^n + \frac{\Delta x}{2} \text{minmod} \left( \frac{s_{j-1/2}^n - s_{j-3/2}^n}{\Delta x}, \frac{s_{j+1/2}^n - s_{j-1/2}^n}{\Delta x} \right), \\ s_{j,+}^n = s_{j+1/2}^n - \frac{\Delta x}{2} \text{minmod} \left( \frac{s_{j+1/2}^n - s_{j-1/2}^n}{\Delta x}, \frac{s_{j+3/2}^n - s_{j+1/2}^n}{\Delta x} \right), \end{cases}$$

defining by the way the reconstruction operator  $\mathcal{R}$  (50). Other high resolution reconstructions can be found for example in the books [LeV02, Tor09].

#### 4. Numerical results

In this section, we provide numerical results for illustrating our purpose. All the numerical results have been obtained with Scilab [Sci].

4.1. Capturing the undercompressive shocks. In this section, our aim is to give a strong evidence that our scheme captures physically relevant solutions that the former versions of the scheme proposed in [AJG04, MJ10, TA12] fail to capture. Recall (see Remark 2.4) that the notion of optimal entropy solution is not always appropriate, it was however the starting point in the interpretation of numerical results proposed in the works [MJ10, TA12].

In our test case called TEST CASE 1 in what follows, we have set  $\phi_l = \phi_r = .1$ ,  $\underline{s}_l = \underline{s}_r = 0$ ,  $\overline{s}_l = \overline{s}_r = 1$ ,  $q = 10^{-3}$ , g = -9, 81,  $\rho_0 = 0.87$ ,  $\rho_w = 1$ ,  $k_o(s) = s^2$ ,  $k_w(s) = (1-s)^2$ ,  $\mu_o = 5 \times 10^{-3}$ ,  $\mu_w = 10^{-3}$ ,  $\eta_{o,l}(s) = \eta_{o,r}(s) = \frac{k_o(s)}{\mu_o}$ ,  $\eta_{w,l}(s) = \eta_{w,r}(s) = \frac{k_w(s)}{\mu_w}$ ,  $K_l = 3 \times 10^{-4}$ ,  $K_r = 10^{-4}$ , and the capillary pressure functions are defined by

(51) 
$$\pi_{l,r}(s) = P_{l,r} - \ln(1-s),$$

the entry pressures  $P_{l,r}$  being set at  $P_l = 0$ ,  $P_r \in \{1, 2, 3\}$ . The generalized inverse  $\pi_{l,r}^{-1}$  of  $\pi_{l,r}$  is then given by

$$\pi_{l,r}^{-1}(p) = 1 - \exp(\min(0, P_{l,r} - p)).$$

We plot on Figure 6 the capillary pressure functions  $\pi_{l,r}$  and the convective flux functions  $f_{l,r}$  corresponding to the above choice of parameters.

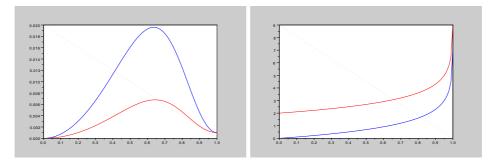


FIGURE 6. TEST CASE 1: On the left figure, we have plotted the convective flux functions  $f_l$  (blue solid line) and  $f_r$  (red solid line). The flux functions are bell-shaped, and satisfy  $f_l(0) = f_r(0) = 0$ ,  $f_l(1) = f_r(1) = q = 10^{-3}$ . On the right figure, we have plotted the unbounded capillary pressure functions  $\pi_l$  (blue solid line) and  $\pi_r$  (red solid line) defined by (51). We refer to the online version of the article for the color figures.

The interface has been placed at x = 0.5, and the initial data  $s_0$  is given by

$$s_0(x) = 0.8\mathbf{1}_{x<0.3}(x) + 0.1\mathbf{1}_{x>0.3}(x).$$

The solution  $s_h$  is computed on the set  $[-1,1] \times [0,4]$  thanks to the scheme described in §3, and compared to the solution  $\tilde{s}_h$  obtained via the scheme proposed in [AJG04, MJ10, TA12], where the interface flux is treated thanks to the upstream flux without hybridization procedure. In the computations, we have set  $\Delta x = \Delta t = 10^-3$ .

As one can see on Figures 7, the solution without hybridization at the interface does not predict the physically relevant undercompressive shock at the interface in the cases  $P_r = 2$  or  $P_r = 3$ , overestimating by the way the quantity of oil overpassing the interface between the rocks. The undercompressive discontinuity at x = 0.5 appears clearly on Figure 8, where we have plotted the solution  $s_h$  of the hybridized scheme in the (x,t) plane.

4.2. Numerical homogenization: capillary forces play a major role. Obtaining effective equations governing the flow in the case of a periodic heterogeneous porous medium has been the purpose of numerous works. In the case where capillary diffusion is not neglected, let us for example mention the contributions [BH95, vDMP02, Sch08, HOS13].

The case where capillary diffusion is neglected, i.e., the so-called *vanishing capillarity limit* is more intricate, and no mathematical results are available up to our knowledge. In [MHM10], a formal upscaling of the hyperbolic Buckley-Leverett equation with gravity in a periodic layered porous media was proposed. Since it was based on Kaasschieter's work [Kaa99], the singular effects linked to capillarity pointed out in §2 were not taken into account. In this section, we provide a numerical evidence that these effects have a strong influence on the upscaled model.

Let us now define the so-called TEST CASE 2, corresponding to a periodic layered porous medium. The porous medium is made of the apposition of cells  $(C_k)_{k\in\mathbb{Z}}$ , each cell  $C_k$  being made of two rocks  $\Omega_l$  and  $\Omega_r$ , the physical characteristics in  $\Omega_{l,r}$  being the same as those considered in TEST CASE 1. The initial data is given by  $s_0 = 0.81_{x<0} + 0.11_{x>0}$ .

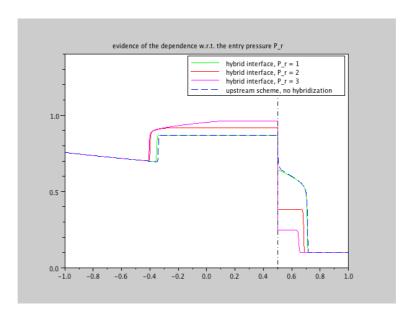


FIGURE 7. TEST CASE 1: Solutions of the hybrid scheme (solid lines) corresponding to different values of the entry pressure  $P_r$ , i.e.,  $P_r=1$  (green line),  $P_r=2$  (red line), and  $P_r=3$  (magenta line) plotted at time t=2. The blue dashed line corresponds to the numerical solution of the scheme without hybridization. It appears that the solution without hybridization coincides with the solution for  $P_r=1$ . This comes from the fact that for  $P_r=1$ , we are in the case (A) described in §2.3.3 while the case (B) occurs for  $P_r=2$  or  $P_r=3$ . We refer to the online version of the article for the color figures.

From a numerical point of view, we consider 100 cells  $C_k$ , each of them containing 10 numerical cells  $(x_j, x_{j+1})$ . We solve numerically the problem

$$\phi \partial_t s + \partial_x f(s; x) = 0, \qquad s(x, 0) = s_0(0)$$

by using the hybridized flux (42) at each rock discontinuity (the subscript l and r being switched one edge over two). The solution is then compared with the one provided by the scheme without hybridization. The solution we obtain have an highly oscillating behavior (see Figure 10), but we consider their mean values on the cells  $C_k$  by setting

$$S_k^n = \int_{C_k} s_h(x, n\Delta t) dx.$$

Hence, we obtain a numerically homogenized solution  $S_h$  defined by

$$S_h(x,t) = S_k^n$$
 if  $(x,t) \in C_k \times [n\Delta t, (n+1)\Delta t)$ .

The function  $S_h$  is plotted on Figure 11, where it is compared to the solution obtained by numerical homogenization, but without using hybridization of the interface. It appears clearly that the behaviors of both solutions widely differ, so that, once again, the capillary forces shall not be neglected in the computations at rocks interfaces.

Remark 4.1. Only few mathematical results are available for the homogenization of scalar conservation laws with space-depending flux functions. In particular, notice

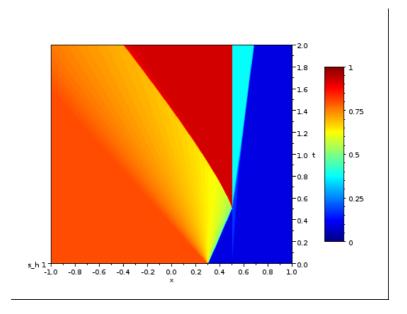


FIGURE 8. TEST CASE 1: The solution  $s_h$  of the hybridized upstream scheme plotted in the (x,t) plane for  $P_r = 2$ . The undercompressive wave, created at  $t \simeq 0.5$  by the interface, appears to be propagated in both domains.

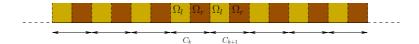


FIGURE 9. Test case 2: The layered porous medium is made of a periodic apposition of two different rocks with different physical characteristics.

that the configuration proposed in Test case 2 does not enter the theory proposed by E [E92] and Dalibard [Dal09].

# Appendix A. Equivalent definitions for the vanishing capillarity solution

Let us provide an equivalent reformulation of admissibility condition (17),(21) which will play only an auxiliary role in our study (the notions introduced are instrumental for some proofs, but they are not needed for description and implementation of the scheme). This section can be omitted by a reader not interested in deeper theoretical considerations.

As mentioned in §2.3.3, it is possible to obtain a complete description of the set  $\mathcal{G}_{\pi}^*$  where the one-sided traces  $(s_l, s_r)$  live as soon as one knows the set  $\mathcal{P}$  (defined via (28) thanks to the capillary pressure profile  $\pi_{l,r}$ ) and the set  $\mathcal{F}$  (defined via (27) thanks to the flux functions  $f_{l,r}$ ). Then, as pointed out in Proposition 2.2, the vanishing capillarity solution s satisfies a contraction property with respect to all steady states  $\kappa(x) = \kappa_l \mathbf{1}_{x<0} + \kappa_r \mathbf{1}_{x>0}$  as soon as  $(\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^*$ , i.e., for all

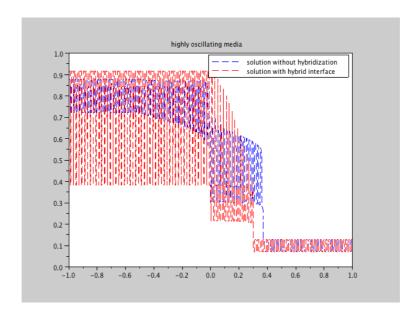


FIGURE 10. TEST CASE 2: Saturation profile in a layered porous medium. The solution of the phase-by-phase upstream scheme without hybridization (dashed blue line) strongly differs from the vanishing capillarity solution computed with the scheme (39)–(42) (solid red line), which is the physically relevant solution.

$$\psi \in \mathcal{C}_{c}^{\infty}(\mathbb{R} \times \mathbb{R}_{+}) \text{ with } \psi \geq 0, \text{ one has}$$

$$\iint_{\mathbb{R} \times \mathbb{R}_{+}} |s(x,t) - \kappa(x)| \partial_{t} \psi(x,t) dx dt + \int_{\mathbb{R}} |s_{0}(x) - \kappa(x)| \psi(x) dx$$

$$(52) + \iint_{\mathbb{R} \times \mathbb{R}_{+}} \operatorname{sign}(s(x,t) - \kappa(x)) (f(s(x,t);x) - f(\kappa(x);x)) \partial_{x} \psi(x,t) dx dt \geq 0.$$

Taking advantage of the recent developments of the theory on scalar conservation laws with discontinuous fluxes (see e.g. [Tow00, SV03, KRT03, AP05, AMG05, BKT09] in the *bell-shaped* case and [Die09, AKR11] for general flux functions) and in the theory of two-phase flows with discontinuous capillary pressures (see e.g. [BDvD03, CGP09, Can09, Can10a, Can10b, AC13]), we can state the following theorem, which justifies the use of the terminology *vanishing capillarity solution* in Definition 2.1.

**Theorem A.1.** Let the nonlinearities  $\pi_{l,r}$ ,  $f_{l,r}$  and the initial data  $s_0$  be given, then the following assertions are equivalent:

- (A) s is the unique vanishing capillarity solution in the sense of Definition 2.1;
- (B)  $s \in L^{\infty}(\mathbb{R} \times \mathbb{R}_{+})$  with  $\underline{s}(x) \leq s(x,t) \leq \overline{s}(x)$  for almost all  $(x,t) \in \mathbb{R} \times \mathbb{R}_{+}$ , and s satisfies (52) for all  $\kappa(x) = \kappa_{l} \mathbf{1}_{x<0} + \kappa_{r} \mathbf{1}_{x>0}$  with  $(\kappa_{l}, \kappa_{r}) \in \mathcal{G}_{\pi}^{*}$  and all  $\psi \in \mathcal{C}_{c}^{\infty}(\mathbb{R} \times \mathbb{R}_{+})$  with  $\psi \geq 0$ ;
- (C)  $s = \lim_{\epsilon \to 0} s^{\epsilon}$  where  $s^{\epsilon}$  is the unique solution (in the sense of [Can09]) to problem (10),(14) with capillarity parameter  $\epsilon > 0$ .

Despite the fact that we will not provide here a complete proof (this is the purpose of the papers [AC13, ABC13, AC]), let us briefly justify the equivalence between the three notions of solution stated in Theorem A.1.

First, using the general tools developed for scalar conservation laws with discontinuous flux functions (see for example [AKR11] for an axiomatized approach of

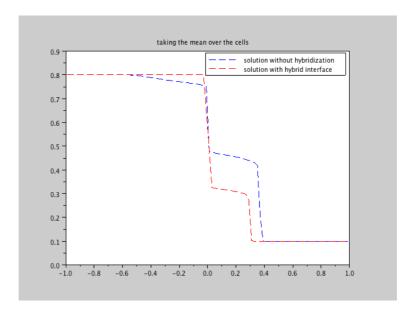


FIGURE 11. TEST CASE 2: Mean saturation profiles  $S_h$  for the layered porous medium. The solution computed without hybridizing the interfaces (blue dashed line) provides a wrong amplitude and a wrong propagation speed compared to the solution obtained with the scheme (39)–(42) (solid red line) designed to capture the vanishing capillarity solution.

the problem based on the "maximality" and " $L^1$ -dissipativity" properties of  $\mathcal{G}_{\pi}^*$ ), we can claim that there exists at most one solution in the sense of Definition 2.1, i.e., in the sense (A).

The fact that (A) is equivalent to (B) is the purpose of Proposition 2.2, and is proved in [AKR11] in the general axiomatized setting.

Finally, let us prove that (C) is equivalent to (A) and (B). As proved in [Can09] (see also [AC13]), localized contraction principles (called Kato inequalities) can be derived for the problem with non-zero capillarity parameter  $\epsilon$ . More precisely, let  $s^{\epsilon}$  and  $\check{s}^{\epsilon}$  be two mild solutions (see [AC13] for the precise definition of the notion of *mild solution*) of the problem (14) corresponding to initial data  $s_0$  and  $\check{s}_0$  respectively, then

(53) 
$$\partial_t |s^{\epsilon} - \check{s}^{\epsilon}| + \partial_x \left( \operatorname{sign}(s^{\epsilon} - \check{s}^{\epsilon}) (f(s^{\epsilon}; x) - f(\check{s}^{\epsilon}; x)) \right) \le \mathcal{R}_{\epsilon},$$

where  $\lim_{\epsilon \to 0} \mathcal{R}_{\epsilon} = 0$  in the distributional sense. Let  $(\kappa_l, \kappa_r) \in \mathcal{G}_{\pi}^*$  then there exists a steady state  $\kappa^{\epsilon}(x)$  of (14) tending to  $\kappa_l \mathbf{1}_{x<0} + \kappa_r \mathbf{1}_{x>0}$  as  $\epsilon \to 0$ . Choosing  $\check{s}^{\epsilon} = \kappa^{\epsilon}$  in (53) and letting  $\epsilon$  tend to 0 provides that  $s = \lim_{\epsilon \to 0} s^{\epsilon}$  is a  $\mathcal{G}_{\pi}^*$ -entropy solution, so that (C) implies (B). Now, since there exists a unique function s satisfying (B), it suffices to show that there exists a function s such that  $s = \lim_{\epsilon \to 0} s^{\epsilon}$ . This can be done for example as in [AC13, Appendix A.1] by adapting the BV<sub>loc</sub>-argument of [BGKT08]; also the result of our Theorem 3.4 justifies the existence.

To conclude, let us stress that the three notions of solution (A), (B), and (C), which are shown to be equivalent in Theorem A.1, have their own interest. Indeed, the definition (C) provides the physical sense of the vanishing capillarity solution, but is not easy to use in practice. On the other hand, the definition (B) is central for the analysis of the problem, e.g., for proving the convergence of a numerical scheme (cf. [AC]). Finally, the definition (A) (or Definition 2.1) is the one we have

used for designing the numerical scheme, replacing the exact Godunov solvers  $G_{l,r}$  appearing in (21) by the monotone approximate Riemann solvers  $\operatorname{Up}_{l,r}$  in (42).

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