Limit boundary conditions for finite volume approximations of some physical problems

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Abstract

In the industrial context, Finite Volume schemes are used to compute an approximation of the solution of a system of equations set on a certain domain. When this domain is bounded, some numerical boundary conditions have to be implemented in order to complete the computation of the Finite Volume scheme. This is a tricky step in the elaboration of the scheme, which is still not mastered. In fact, at a closer sight, it appears that there is a deep interaction between the understanding of the physical phenomena at the boundary of the domain and the implementation of the numerical boundary conditions. Unfortunately, this link is not always completely intelligible and a reason for this lack of clarity is the fact that, whereas the continuous equation satisfied by the limit of the numerical solution is known, the boundary conditions satisfied by this very limit are not well-understood. The purpose of this paper is to clarify this point in three industrial situations of one-dimensional two-phase flows.

1 Introduction

We consider the case of three problems of multi-phase flow in a one dimensional domain, arising in the oil engineering setting: the waterflood of a core extracted from an actual oil reservoir, the multi-phase flow in a pipe, and the separation of phases in a distillation column. In these problems, the one-dimensional domain can be horizontal, tilted of vertical. For each of these cases, the conservation equations (of mass and momentum) lead to a coupled system of equations. Under some simplifications in an incompressible two-phase setting, the engineer can then draw a finite volume scheme whose unknowns are the discrete values of the volumic ratio of the phase one within the two phases. In particular, the boundary conditions for the numerical scheme are set in accordance to the physical device. We show in section 5 that, for these three industrial cases, the resulting finite volume scheme comes down to the following set of equations:

$$\frac{h}{k}[u_i^{n+1} - u_i^n] + G(u_i^n, u_{i+1}^n) - G(u_{i-1}^n, u_i^n) = 0, \; \forall i = 2, \dots, I-1, \; \forall n \in \mathbb{N}, \tag{1}$$

$$\frac{h}{k}[u_1^{n+1} - u_1^n] + G(u_1^n, u_2^n) - \bar{f}^n = 0, \text{ with } \bar{f}^n = \frac{1}{k}\int_{nk}^{(n+1)k} \bar{f}(t)dt, \; \forall n \in \mathbb{N}, \tag{2}$$

$$\frac{h}{k}[u_I^{n+1} - u_I^n] + f(u_I^n) - G(u_{I-1}^n, u_I^n) = 0, \; \forall n \in \mathbb{N}, \tag{3}$$

and

$$u_i^0 = \frac{1}{h}\int_{(i-1)h}^{ih} u_0(x)dx, \; \forall i = 1, \dots, I, \tag{4}$$

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where the hypotheses on the data and the notations are the following ones:

Hypotheses and notations (HN) :

1. *The one dimensional domain is defined by* $(0, L)$ *with* $L > 0$*, the number of grid blocks is* $I \in \mathbb{N}_*$*, the space step is* $h = \frac{L}{I}$ *and the time step is* $k > 0$*.*

2. *The function* $G \in \mathcal{C}^0([0,1] \times [0,1], \mathbb{R})$ *is a Lipschitz continuous function, which is non decreasing w.r.t. its first argument and non increasing w.r.t. its second argument. In the general case, the function G which verifies these properties is said to be a monotonous numerical flux, consistent with the function* $g \in \mathcal{C}^0([0,1], \mathbb{R})$ *defined by* $g(a) = G(a, a)$ *for all* $a \in [0, 1]$*.*

3. *This function g is assumed to verify the following properties:* $g(0) = 0$ *and, setting* $\alpha = g(1)$*, there exists* $a_\star \in (0, 1]$ *such that* $g(a_\star) = \alpha$*, the function g is nondecreasing on* $(0, a_\star)$ *and* $g(a) \geq \alpha$ *for all* $a \in [a_\star, 1]$*.*

4. *The function* $f \in \mathcal{C}^0([0,1], \mathbb{R}_+)$ *is Lipschitz continuous, nondecreasing and such that* $f(0) = 0$ *and* $f(1) = \alpha$*.*

5. *We denote by* $\mathcal{L}$ *a Lipschitz constant either for G and f.*

6. *The function* $u_0 \in L^\infty(0, L)$ *is such that* $u_0(x) \in [0, 1]$ *for a.e.* $x \in (0, L)$*.*

7. *The function* $\bar{f} \in L^\infty(\mathbb{R}_+)$ *is such that* $\bar{f}(t) \in [0, \alpha]$ *for a.e.* $t \in \mathbb{R}_+$*. We denote by* $\overline{u}$ *a (possibly non uniquely defined) function of* $L^\infty(\mathbb{R}_+)$ *satisfying*

$$g(\overline{u}(t)) = \bar{f}(t) \quad \textit{and} \quad \overline{u}(t) \in [0, a_\star] \quad \textit{for a.e. } t \in \mathbb{R}_+. \tag{5}$$

8. *We then denote by* $u_{h,k}$ *the numerical solution, defined a.e. in* $(0, L) \times \mathbb{R}_+$ *through the scheme (1)-(4) by*

$$u_{h,k}(x, t) = u_i^n, \ \forall x \in ((i-1)h, ih), \ \forall t \in (nk, (n+1)k), \ \forall i = 1, \ldots, I, \ \forall n \in \mathbb{N} \tag{6}$$

The figure 1 presents a possible choice for the functions g and f.

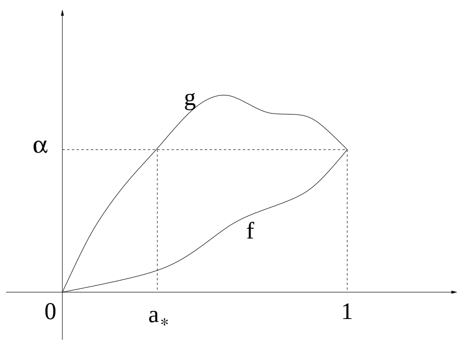


Figure 1: Shape of the functions f and g

The equation (2) expresses the fact that the ratio between the two phases is known for the injected fluid at $x = 0$.
Let us detail the issue at stake in Equation (3). It is interesting to notice that two different requirements can govern the derivation of this equation in the elaboration of the finite volume scheme. Indeed, we will see that the numerical implementation of the boundary conditions is naturally known (for dictated by

physical arguments) in the examples of two-phase flow in porous media or separation of phases in binary distillation column. In fact, in those two examples, it is the boundary conditions satisfied by the solution of the continuous model (obtained by passing to the limit in the equations of the scheme) which are not so clear. Conversely, in the study of a two-phase flow in a pipe, it appears that the boundary condition which should be satisfied by the limit solution of the scheme is known and clearly designed. It is the way to implement it numerically which raises difficulties. The main theorem of this paper (Theorem 1) helps to predict the boundary conditions satisfied by the solution of the continuous equation from the numerical boundary conditions satisfied by the solution of the scheme, or the converse operation.
Notice that, under hypotheses and notations (HN), it is always possible to find some values $\overline{u}^n$ such that $g(\overline{u}^n) = \bar{f}^n$, and such that the values $\overline{u}^n$ can be used to define a discrete time dependent function, strongly convergent to the function $\overline{u}$. Furthermore, one can build a monotonous numerical flux G_0 consistent with g such that $G_0(a,b) = g(a)$, for all $(a,b) \in [0,a_\star] \times [0,1]$. We can thus replace, in (2), $\bar{f}^n$ by $G_0(\overline{u}^n, u_1^n)$, for all $n \in \mathbb{N}$. This lead to the numerical boundary condition:

$$\frac{h}{k}[u_1^{n+1} - u_1^n] + G(u_1^n, u_2^n) - G_0(\overline{u}^n, u_1^n) = 0, \; \forall n \in \mathbb{N}, \tag{7}$$

If, furthermore, we assume that there exist a real value $\overline{\overline{u}} \in [0,1]$ and some function G_I such that G_I is a monotonous numerical flux consistent with g and such that

$$G_I(a, \overline{\overline{u}}) = f(a), \;\; \forall a \in [0,1], \tag{8}$$

we can then replace, in (3), the value $f(u_I^n)$ by $G_I(u_I^n, \overline{\overline{u}})$. This leads to the numerical boundary condition:

$$\frac{h}{k}[u_I^{n+1} - u_I^n] + G_I(u_I^n, \overline{\overline{u}}) - G(u_{I-1}^n, u_I^n) = 0, \; \forall n \in \mathbb{N}, \tag{9}$$

The equations (1), (4), (7) and (9) then define a monotonous three-point finite volume scheme in which the numerical flux depends on the interface. For such a finite volume scheme, with such numerical boundary conditions, it is proven in [Vov02] that $u_{h,k}$ converges as $h \to 0$ and $k \to 0$, under a CFL condition, to the weak entropy solution u of a nonlinear scalar hyperbolic problem with boundary conditions, formally given by:

$$u_t(x,t) + (g(u))_x(x,t) = 0, \;\; \text{for a.e. } (x,t) \in (0,L) \times \mathbb{R}_+, \tag{10}$$

$$u(x,0) = u_0(x), \;\; \text{for a.e. } x \in (0,L), \tag{11}$$

$$g(u(0,t)) = \bar{f}(t), \;\; \text{for a.e. } t \in \mathbb{R}_+, \tag{12}$$

and

$$g(u(L,t)) = \overline{\overline{u}}, \;\; \text{for a.e. } t \in \mathbb{R}_+. \tag{13}$$

The correct mathematical interpretation of the boundary conditions (12) and (13) is recalled below (Theorem 1).

However, we stress the fact that, in general, the relation (8) cannot hold for any functions g and f satisfying hypotheses and notations (HN) (such as those encountered in the industrial cases). Indeed, the equation (8) implies $f(\overline{\overline{u}}) = g(\overline{\overline{u}})$ because of the consistency of G_I with g (this equality is at least satisfied by the values $\overline{\overline{u}} = 1$ and $\overline{\overline{u}} = 0$ under hypotheses and notations (HN)), but also $f(a) \geq g(a)$ for all $a \in [\overline{\overline{u}}, 1]$ and $f(a) \leq g(a)$ for all $a \in [0, \overline{\overline{u}}]$ because of the monotonicity of G. An easy counter example is obtained with $g(a) = 3a - 2a^2$, $a_\star = \frac{1}{2}$, $f(a) = 1 - (1-a)^\gamma$, with $\gamma > 3$.
Therefore, a study of the general case (i.e. when no $\overline{\overline{u}}$ and G_I can be found) has to be led. Using some estimates proved in section 2, some compactness arguments are derived in section 3 and, obtaining the

convergence to Young measures entropy solutions in section 4, the results of [Vov02] are sufficient to state the following theorem:

Theorem 1 *Let $\xi \in (0,1)$ be given. Under hypotheses and notations (HN), let us assume that the time step $k > 0$ is such that*

$$k \leq \xi \frac{h}{2\mathcal{L}}. \tag{14}$$

Then the function $u_{h,k}$ (defined by (6)) converges in $L^p_{loc}((0,L)\times(0,T))$ for all $T>0$ and all $p \in [1,+\infty)$, as $h \to 0$, to the unique entropy weak solution $u \in L^\infty((0,L)\times\mathbb{R}_+)$ of the problem (10)-(13) with $\overline{\overline{u}} = 1$ in (13), in the following sense:

$$\begin{aligned}
&\int_0^{+\infty}\int_0^L \big(\eta_\kappa^\top(u(x,t))\,\varphi_t(x,t) + \Phi_\kappa^\top(u(x,t))\,\varphi_x(x,t)\big)\,dx\,dt + \int_0^L \eta_\kappa^\top(u_0(x))\,\varphi(x,0)\,dx \\
&+\mathcal{L}\int_0^{+\infty} \big(\eta_\kappa^\top(\overline{u}(t))\,\varphi(0,t) + \eta_\kappa^\top(1)\,\varphi(L,t)\big)\,dt \geq 0, \\
&\forall \kappa \in (0,1),\ \forall \varphi \in \mathcal{C}_c^\infty(\mathbb{R}\times\mathbb{R},\mathbb{R}_+),
\end{aligned} \tag{15}$$

and

$$\begin{aligned}
&\int_0^{+\infty}\int_0^L \big(\eta_\kappa^\perp(u(x,t))\,\varphi_t(x,t) + \Phi_\kappa^\perp(u(x,t))\,\varphi_x(x,t)\big)\,dx\,dt + \int_0^L \eta_\kappa^\perp(u_0(x))\,\varphi(x,0)\,dx \\
&+\mathcal{L}\int_0^{+\infty} \big(\eta_\kappa^\perp(\overline{u}(t))\,\varphi(0,t) + \eta_\kappa^\perp(1)\,\varphi(L,t)\big)\,dt \geq 0, \\
&\forall \kappa \in (0,1),\ \forall \varphi \in \mathcal{C}_c^\infty(\mathbb{R}\times\mathbb{R},\mathbb{R}_+),
\end{aligned} \tag{16}$$

where, denoting by $a\top b$ the maximum value between a and b and by $a\perp b$ the minimum value between a and b, the entropy pairs of functions $(\eta_\kappa^\top,\Phi_\kappa^\top)$ and $(\eta_\kappa^\perp,\Phi_\kappa^\perp)$ are defined for all $(a,\kappa) \in [0,1]^2$ by $\left\{\begin{array}{l}\eta_\kappa^\top(a) = a\top\kappa - \kappa = (a-\kappa)^+ \\ \Phi_\kappa^\top(a) = g(a\top\kappa) - g(\kappa)\end{array}\right.$ *and* $\left\{\begin{array}{l}\eta_\kappa^\perp(a) = \kappa - a\perp\kappa = (a-\kappa)^- \\ \Phi_\kappa^\perp(a) = g(\kappa) - g(a\perp\kappa)\end{array}\right.$.

We must now comment on the physical meaning of the formal boundary conditions (12) and (13). The rigorous mathematical meaning of these condition is expressed by the conditions (15) and (16) for general irregular data $u_0 \in L^\infty(0,L)$, $\bar{f} \in L^\infty(\mathbb{R}_+)$ (see [Ott96], where the existence and uniqueness of the entropy solution $u \in L^\infty((0,L)\times\mathbb{R}_+)$ have been established). If the solution u is "regular" enough (we have in mind $u \in BV((0,L)\times(0,T))$,– sufficient conditions for that matter are exposed in Section 2.2), then, from the weak formulation (15)-(16) follows the Bardos, LeRoux, Nedelec condition [BlRN79] which writes

$$\mathrm{sign}(T_0u(t) - \overline{u}(t))(g(T_0u(t)) - g(\kappa)) \leq 0 \ \text{ for all } \kappa \in [\overline{u}(t)\perp T_0u(t), \overline{u}(t)\top T_0u(t)], \text{ for a.e. } t \in \mathbb{R}_+, \tag{17}$$

and

$$\mathrm{sign}(T_Lu(t) - 1)(g(T_Lu(t)) - g(\kappa)) \geq 0\,, \quad \text{for all } \kappa \in [T_Lu(t), 1]\,, \text{ for a.e. } t \in \mathbb{R}_+\ . \tag{18}$$

In the inequalities (17)-(18), the values $T_0u(t)$ and $T_Lu(t)$ respectively denote the traces on $x=0$ and $x=L$ of the function $u \in BV((0,L)\times(0,T))$, for a.e. $t \in [0,T]$. Under the hypotheses and notations (HN), the relation (17) is equivalent to

$$g(T_0u(t)) = \bar{f}(t), \ \text{ for a.e. } t \in \mathbb{R}_+, \tag{19}$$

and the relation (18) is equivalent to

$$g(T_Lu(t)) \leq \alpha, \ \text{ for a.e. } t \in \mathbb{R}_+. \tag{20}$$

We then remark that the condition (19) was expected from the physical point of view (the nature of the injected fluid is imposed). On the contrary, the condition (20) is more surprising from the engineering point of view:

- the function f has no influence on the limit problem inside the domain, and its numerical role is only to determine the value of the discrete unknown in the cell I,
- the condition (20) expresses the fundamental physical condition at $x = L$: the outwards flux of phase one is lower than the total outwards flux, which means that the flux of phase two is outwards as well.

The discussion of the consequences of the above remark in the three industrial cases is reported to section 5.

2 Estimates on the approximate solution

2.1 L^∞ estimate

We first establish the following L^∞ estimate, which is necessary from the physical point of view, since the discrete values u_i^n are meant to verify $u_i^n \in [0, 1]$.

Lemma 1 *Under hypotheses and notations (HN), let* $(u_i^n)_{i=1,\ldots,I,\, n\in\mathbb{N}}$ *be defined by the scheme (1)-(4). Let us assume that the CFL condition*

$$k \leq \frac{h}{2\mathcal{L}} \tag{21}$$

is satisfied. Then the following inequalities hold:

$$0 \leq u_i^n \leq 1,\, \forall i = 1, \ldots, I,\, \forall n \in \mathbb{N}. \tag{22}$$

Proof of Lemma 1: Using (4), one has $0 \leq u_i^0 \leq 1$ for all $i = 1, \ldots, I$. Let $n \in \mathbb{N}$. Let us assume by induction that $0 \leq u_i^n \leq 1$, for all $i = 1, \ldots, I$. The scheme (1) can be rewritten as

$$u_i^{n+1} = H(u_{i-1}^n, u_i^n, u_{i+1}^n),\, \forall i = 2, \ldots, I-1,\, \forall n \in \mathbb{N}, \tag{23}$$

with

$$\begin{aligned} H :\quad & [0,1]^3 \longrightarrow \mathbb{R} \\ & (a,b,c) \mapsto b + \frac{k}{h}\,[G(a,b) - G(b,c)]. \end{aligned} \tag{24}$$

Under the CFL condition (21), the function H is nondecreasing with respect to each of its arguments (see [EGH00] or [Vov02]) and satisfies $H(a,a,a) = a$. This enforces the relation $\min(u_{i-1}^n, u_i^n, u_{i+1}^n) \leq u_i^{n+1} \leq \max(u_{i-1}^n, u_i^n, u_{i+1}^n)$. In the case $i = 1$, the scheme (2) writes

$$u_1^{n+1} = \overline{H}(\bar{f}^n, u_1^n, u_2^n),\, \forall n \in \mathbb{N}, \tag{25}$$

with

$$\begin{aligned} \overline{H} :\quad & [g(0), g(1)] \times [0,1]^2 \longrightarrow \mathbb{R} \\ & (s,a,b) \mapsto a + \frac{k}{h}\,[s - G(a,b)]. \end{aligned} \tag{26}$$

Since $\overline{H}$ is nondecreasing with respect to each of its arguments under the CFL condition (21) and verifies $\overline{H}(g(0), 0, 0) = 0$ and $\overline{H}(g(1), 1, 1) = 1$, one gets $0 \leq u_1^{n+1} \leq 1$. In the case $i = I$, the scheme (3) gives

$$u_I^{n+1} = \overline{\overline{H}}(u_{I-1}^n, u_I^n),\ \forall n \in \mathbb{N}, \tag{27}$$

with

$$\overline{\overline{H}}:\quad \begin{aligned} &[0,1]^2 \longrightarrow \mathbb{R} \\ &(a,b) \mapsto b + \frac{k}{h}\,[G(a,b) - f(b)]. \end{aligned} \tag{28}$$

Since $\overline{\overline{H}}$ is nondecreasing with respect to each of its arguments under the CFL condition (21), and satisfies $\overline{\overline{H}}(0,0) = 0$ and $\overline{\overline{H}}(1,1) = 1$, one gets $0 \le u_I^{n+1} \le 1$. This proves that $0 \le u_i^{n+1} \le 1$, for all $i = 1,\ldots,I$, and concludes the proof of (22).

2.2 Strong BV inequality

The following estimate is not a necessary argument for the proof of convergence which is given in this paper, and it demands stronger hypotheses. It is however useful to give sufficient conditions on the data in order to obtain the BV regularity for the limit problem (as mentioned in the introduction to this paper).

Lemma 2 *One assumes hypotheses and notations (HN) and the following additional hypotheses:*

1. *the function g is strictly increasing on $(0,a_\star)$ and the reciprocal function of g on $(0,a_\star)$ is Lipschitz continuous with constant $\mathcal{L}_r$,*
2. *for all $(a,b) \in [0,a_\star] \times (0,1)$, $G(a,b) = g(a)$,*
3. *$u_0 \in BV(0,L)$,*
4. *$\bar{f} \in BV_{\mathrm{loc}}(\mathbb{R}_+)$.*

Let $(u_i^n)_{i=1,\ldots,I,\, n\in\mathbb{N}}$ be defined by the scheme (1)-(4), assuming that (21) holds.

Then, for all $T > 0$, there exists $C_1 \ge 0$, which only depends on $T, L, u_0, \bar{f}, G, f, \mathcal{L}, \mathcal{L}_r$ such that

$$\sum_{n\in\mathbb{N};nk<T}\ \sum_{i=1}^{I-1}\Big(k|u_{i+1}^n - u_i^n| + h|u_i^{n+1} - u_i^n|\Big) \le C_1. \tag{29}$$

Remark 1

1. *Lemma 2 could be used to derive the convergence in $L^1((0,L)\times(0,T))$ of the approximate solution $u_{h,k}$ to a function $u \in L^1((0,L)\times(0,T)) \cap BV((0,L)\times(0,T))$, but it demands more regularity hypotheses on the data u_0, $\bar{f}$ and g than those which are included in hypotheses and notations (HN).*
2. *Hypotheses 1, 2. in Lemma 2 are satisfied in the example of multi-phase flow in porous media.*

Proof of Lemma 2: For $n \in \mathbb{N}$, let u_0^n be defined by

$$g(u_0^n) = \bar{f}^n,\ \forall n \in \mathbb{N}. \tag{30}$$

Then, for all $n \in \mathbb{N}$, one has $0 \le u_0^n \le a_\star$. The additional hypotheses *2.* above ensures that $G(a,b)$ does not depend on b for $a \in [0,a_\star]$ and that $G(u_0^n, u_1^n) = g(u_0^n) = \bar{f}^n$. Therefore (2) can be rewritten in

$$u_1^{n+1} - u_1^n + \frac{k}{h}\,[G(u_1^n, u_2^n) - G(u_0^n, u_1^n)] = 0,\ \forall n \in \mathbb{N}, \tag{31}$$

which entails

$$u_i^{n+1} = H(u_{i-1}^n, u_i^n, u_{i+1}^n),\ \forall i = 1,\ldots,I-1,\ \forall n \in \mathbb{N}, \tag{32}$$

Let $n \in \mathbb{N}$ with $nk < T$. Using the monotonicity properties of the function H, one gets

$$u_i^{n+1} \top u_{i+1}^{n+1} \leq H(u_{i-1}^n \top u_i^n, u_i^n \top u_{i+1}^n, u_{i+1}^n \top u_{i+2}^n), \ \forall i = 1, \ldots, I-2, \tag{33}$$

and similarly

$$u_i^{n+1} \bot u_{i+1}^{n+1} \geq H(u_{i-1}^n \bot u_i^n, u_i^n \bot u_{i+1}^n, u_{i+1}^n \bot u_{i+2}^n), \ \forall i = 1, \ldots, I-2. \tag{34}$$

Subtracting (34) from (33), then yields

$$\begin{array}{l} |u_i^{n+1} - u_{i+1}^{n+1}| \leq |u_i^n - u_{i+1}^n| - \dfrac{k}{h} \left[\begin{array}{l} (G(u_i^n \top u_{i+1}^n, u_{i+1}^n \top u_{i+2}^n) - G(u_i^n \bot u_{i+1}^n, u_{i+1}^n \bot u_{i+2}^n)) - \\ (G(u_{i-1}^n \top u_i^n, u_i^n \top u_{i+1}^n) - G(u_{i-1}^n \bot u_i^n, u_i^n \bot u_{i+1}^n)) \end{array} \right], \\ \forall i = 1, \ldots, I-2. \end{array} \tag{35}$$

One now deals with the boundary conditions. The following proof could be slightly simplified using $G(u_0^n, u_1^n) = G(u_0^n, u_0^n)$, but the argument here which remains valid in more general cases. One has, setting $r_0^n = u_0^{n+1} - u_0^n + \frac{k}{h}(G(u_0^n, u_1^n) - G(u_0^n, u_0^n))$,

$$u_0^{n+1} = H(u_0^n, u_0^n, u_1^n) + r_0^n.$$

It leads to

$$u_0^{n+1} \leq H(u_0^n, u_0^n \top u_1^n, u_1^n \top u_2^n) + (r_0^n)^+, \tag{36}$$

and

$$u_0^{n+1} \geq H(u_0^n, u_0^n \bot u_1^n, u_1^n \bot u_2^n) - (r_0^n)^-. \tag{37}$$

Using again the monotonicity of H, one gets

$$u_0^{n+1} \top u_1^{n+1} \leq H(u_0^n, u_0^n \top u_1^n, u_1^n \top u_2^n) + (r_0^n)^+, \tag{38}$$

and

$$u_0^{n+1} \bot u_1^{n+1} \geq H(u_0^n, u_0^n \bot u_1^n, u_1^n \bot u_2^n) - (r_0^n)^-. \tag{39}$$

Subtracting (39) from (38) gives

$$|u_0^{n+1} - u_1^{n+1}| \leq |u_0^n - u_1^n| \quad \begin{array}{l} -\dfrac{k}{h} \left[\begin{array}{l} (G(u_0^n \top u_1^n, u_1^n \top u_2^n) - G(u_0^n \bot u_1^n, u_1^n \bot u_2^n)) - \\ (G(u_0^n, u_0^n \top u_1^n) - G(u_0^n, u_0^n \bot u_1^n)) \end{array} \right] \\ +|r_0^n|. \end{array} \tag{40}$$

Since the function G is decreasing with respect to its second argument, one has

$$G(u_0^n, u_0^n \top u_1^n) - G(u_0^n, u_0^n \bot u_1^n) = -|G(u_0^n, u_1^n) - G(u_0^n, u_0^n)|.$$

Using $|r_0^n| \leq |u_0^{n+1} - u_0^n| + \frac{k}{h}|G(u_0^n, u_1^n) - G(u_0^n, u_0^n)|$, (40) gives

$$|u_0^{n+1} - u_1^{n+1}| \leq |u_0^n - u_1^n| \quad \begin{array}{l} -\frac{k}{h}(G(u_0^n \top u_1^n, u_1^n \top u_2^n) - G(u_0^n \bot u_1^n, u_1^n \bot u_2^n)) \\ +|u_0^{n+1} - u_0^n|. \end{array} \tag{41}$$

One now turns to the study of the case $i = I$. Using (27), one gets

$$u_I^{n+1} \leq u_I^n \top u_{I-1}^n - \frac{k}{h}(f(u_I^n \top u_{I-1}^n) - G(u_{I-1}^n \top u_{I-2}^n, u_I^n \top u_{I-1}^n)), \tag{42}$$

and

$$u_I^{n+1} \geq u_I^n \bot u_{I-1}^n - \frac{k}{h}[f(u_I^n \bot u_{I-1}^n) - G(u_{I-1}^n \bot u_{I-2}^n, u_I^n \bot u_{I-1}^n)]. \tag{43}$$

Using (23) and (42), one gets

$$u_{I-1}^{n+1} \top u_I^{n+1} \leq u_{I-1}^n \top u_I^n - \frac{k}{h}\left[\begin{array}{l} \min(f(u_I^n \top u_{I-1}^n), G(u_{I-1}^n \top u_I^n, u_I^n \top 1)) - \\ G(u_{I-2}^n \top u_{I-1}^n, u_i^n \top u_{i+1}^n) \end{array}\right], \tag{44}$$

and similarly, using (43),

$$u_{I-1}^{n+1} \bot u_I^{n+1} \geq u_{I-1}^n \bot u_I^n - \frac{k}{h}\left[\begin{array}{l} \max(f(u_I^n \bot u_{I-1}^n), G(u_{I-1}^n \bot u_I^n, u_I^n \bot 1)) - \\ G(u_{I-2}^n \bot u_{I-1}^n, u_i^n \bot u_{i+1}^n) \end{array}\right]. \tag{45}$$

One has, for all a, b, $G(a, b) \geq f(a)$. Therefore, subtracting (45) from (44) gives

$$|u_{I-1}^{n+1} - u_I^{n+1}| \leq |u_{I-1}^n - u_I^n| - \frac{k}{h}\left[\begin{array}{l} (f(u_I^n \top u_{I-1}^n) - G(u_{I-1}^n \bot u_I^n, u_I^n)) - \\ (G(u_{I-2}^n \top u_{I-1}^n, u_i^n \top u_{i+1}^n) - G(u_{I-2}^n \bot u_{I-1}^n, u_i^n \bot u_{i+1}^n)) \end{array}\right]. \tag{46}$$

In the case $u_I^n \leq u_{I-1}^n$, one has

$$\frac{k}{h}(G(u_{I-1}^n \bot u_I^n, u_I^n) - f(u_I^n \top u_{I-1}^n)) \leq \frac{k}{h}(G(u_{I-1}^n, u_I^n) - f(u_I^n)),$$

since G is increasing w.r.t. its first argument and f is increasing. Since $u_I^{n+1} - u_I^n = \frac{k}{h}(G(u_{I-1}^n, u_I^n) - f(u_I^n))$, one has in both cases ($u_I^n \leq u_{I-1}^n$ or $u_{I-1}^n \leq u_I^n$)

$$\frac{k}{h}(G(u_{I-1}^n \bot u_I^n, u_I^n) - f(u_I^n \top u_{I-1}^n)) \leq u_I^{n+1} - u_I^n.$$

Introducing the previous inequality in (46) gives

$$\begin{array}{rl} |u_{I-1}^{n+1} - u_I^{n+1}| \leq |u_{I-1}^n - u_I^n| & +\frac{k}{h}\left[\; G(u_{I-2}^n \top u_{I-1}^n, u_i^n \top u_{i+1}^n) - G(u_{I-2}^n \bot u_{I-1}^n, u_i^n \bot u_{i+1}^n) \;\right] \\ & +u_I^{n+1} - u_I^n. \end{array} \tag{47}$$

Adding (35) for $i = 1, \ldots, I-1$, (41) and (47) gives

$$\sum_{i=0}^{I-1} |u_{i-1}^{n+1} - u_i^{n+1}| \leq \sum_{i=0}^{I-1} |u_{i-1}^n - u_i^n| + |u_0^{n+1} - u_0^n| + u_I^{n+1} - u_I^n. \tag{48}$$

Adding (48) for $n = 0, \ldots, m-1$ gives

$$\sum_{i=0}^{I-1} |u_{i-1}^m - u_i^m| \leq \sum_{i=0}^{I-1} |u_{i-1}^0 - u_i^0| + \sum_{n=0}^{m-1} |u_0^{n+1} - u_0^n| + u_I^m - u_I^0. \tag{49}$$

Using the definition (4), one gets

$$\begin{array}{rl} \displaystyle\sum_{i=0}^{I-1} |u_{i-1}^0 - u_i^0| & \displaystyle\leq \frac{1}{h}\int_0^{L-h} |u_0(x+h) - u_0(x)| dx \\ & \leq \|u_0\|_{BV((0,L))}, \end{array}$$

and using (21), (2) and the additional hypothesis on the Lipschitz continuity of the reciprocal function of g, one gets

$$\sum_{n=0}^{m-1} |u_0^{n+1} - u_0^n| \quad \leq \frac{\mathcal{L}_r}{k} \int_0^T |\bar{f}(t+k) - \bar{f}(t)| dt$$
$$\leq \mathcal{L}_r \|\bar{f}\|_{BV((0,T+k))}.$$

Therefore, one has

$$\sum_{n \in \mathbb{N}; nk < T} \sum_{i=0}^{I-1} k |u_{i+1}^n - u_i^n| \leq (T+k)(\|u_0\|_{BV((0,L))} + \mathcal{L}_r \|\bar{f}\|_{BV((0,T+k))}). \tag{50}$$

Using the scheme (1), one obtains, for $i = 1, \ldots, I-1$

$$h|u_i^{n+1} - u_i^n| \leq k\mathcal{L}(|u_{i-1}^n - u_i^n| + |u_i^n - u_{i+1}^n|), \ \forall i = 1, \ldots, I-1,$$

which gives (29).

2.3 Weak BV inequality

The following result provides an estimate which is necessary in the course of the convergence proof when the additional hypotheses on u_0, $\bar{f}$ and G given in Lemma 2 are not satisfied; it does not yield any compactness property for the approximate solution.

Lemma 3 *Let $\xi \in (0,1)$ and let us assume that $(u_i^n)_{i=1,\ldots,I,\, n \in \mathbb{N}}$ are defined by the scheme (1)-(4) within the hypotheses and notations (HN) and the condition (14).*

Then, for all $T > 0$, there exists $C_2 \geq 0$, which only depends on $T, L, u_0, \bar{f}, G, f, \mathcal{L}$ and ξ such that

$$\sum_{n \in \mathbb{N}, nk < T} \sum_{i=1}^{I} h \, |u_i^{n+1} - u_i^n| \leq \frac{C_2}{\sqrt{h}} \tag{51}$$

and

$$\sum_{n \in \mathbb{N}, nk < T} \sum_{i=1}^{I} k \max_{(c,d) \in \mathcal{C}(u_i^n, u_{i+1}^n)} \Big(|G(c,d) - G(c,c)| + |G(c,d) - G(d,d)| \Big) \leq \frac{C_1}{\sqrt{h}}. \tag{52}$$

where, for all $(a,b) \in [0,1]^2$, $\mathcal{C}(a,b)$ denotes the set $\mathcal{C}(a,b) = \{(c,d) \in [a \perp b, a \top b]^2 \,;\ (b-a)(d-c) \geq 0\}$.

The proof of Lemma 3 is obtained by multiplying the scheme (1) by $k u_i^n$, summing over i and n, and then following the method described in [EGH00] and [Vov02].

2.4 Approximate entropy inequalities

One now establishes discrete entropy inequalities which are used in the next section to get continuous entropy inequalities with an error term.

Lemma 4 *let us assume that $(u_i^n)_{i=1,\ldots,I,\, n \in \mathbb{N}}$ are defined by the scheme (1)-(4) within the hypotheses and notations (HN) and the condition (21).*

Then

$$(u_i^{n+1} - \kappa)^+ - (u_i^n - \kappa)^+ + \frac{k}{h} \left[\begin{array}{l} (G(u_i^n \top \kappa, u_{i+1}^n \top \kappa) - g(\kappa)) \\ -(G(u_{i-1}^n \top \kappa, u_i^n \top \kappa) - g(\kappa)) \end{array} \right] \leq 0,$$
$$\forall \kappa \in [0,1], \ \forall i = 2, \ldots, I-1, \ \forall n \in \mathbb{N}, \tag{53}$$

$$(u_1^{n+1}-\kappa)^+ - (u_1^n-\kappa)^+ + \frac{k}{h}\left[\begin{array}{l}(G(u_1^n\top\kappa, u_2^n\top\kappa)-g(\kappa))\\ -(\bar f^n\top g(\kappa)-g(\kappa))\end{array}\right]\le 0, \quad (54)$$
$$\forall\kappa\in[0,1],\ \forall n\in\mathbb{N},$$

$$(u_I^{n+1}-\kappa)^+ - (u_I^n-\kappa)^+ + \frac{k}{h}\left[\begin{array}{l}(G(u_I^n\top\kappa,\kappa)\bot f(u_I^n\top\kappa)-g(\kappa))\\ -(G(u_{I-1}^n\top\kappa, u_I^n\top\kappa)-g(\kappa))\end{array}\right]\le 0, \quad (55)$$
$$\forall\kappa\in[0,1],\ \forall n\in\mathbb{N},$$

$$(u_i^{n+1}-\kappa)^- - (u_i^n-\kappa)^- + \frac{k}{h}\left[\begin{array}{l}(g(\kappa)-G(u_i^n\bot\kappa, u_{i+1}^n\bot\kappa))\\ -(g(\kappa)-G(u_{i-1}^n\bot\kappa, u_i^n\bot\kappa))\end{array}\right]\le 0, \quad (56)$$
$$\forall\kappa\in[0,1],\ \forall i=2,\ldots,I-1,\ \forall n\in\mathbb{N},$$

$$(u_1^{n+1}-\kappa)^- - (u_1^n-\kappa)^- + \frac{k}{h}\left[\begin{array}{l}(g(\kappa)-G(u_1^n\bot\kappa, u_2^n\bot\kappa))\\ -(g(\kappa)-\bar f^n\bot g(\kappa))\end{array}\right]\le 0, \quad (57)$$
$$\forall\kappa\in[0,1],\ \forall n\in\mathbb{N},$$

and

$$(u_I^{n+1}-\kappa)^- - (u_I^n-\kappa)^- + \frac{k}{h}\left[\begin{array}{l}(g(\kappa)-G(u_I^n\bot\kappa,\kappa)\top f(u_I^n\bot\kappa))\\ -(g(\kappa)-G(u_{I-1}^n\bot\kappa, u_I^n\bot\kappa))\end{array}\right]\le 0, \quad (58)$$
$$\forall\kappa\in[0,1],\ \forall n\in\mathbb{N}.$$

Proof of Lemma 4: The proof of (53) is a consequence of

$$\kappa \le H(\kappa\top u_{i-1}^n, \kappa\top u_i^n, \kappa\top u_{i+1}^n)$$

and

$$u_i^{n+1} \le H(\kappa\top u_{i-1}^n, \kappa\top u_i^n, \kappa\top u_{i+1}^n).$$

The proof of (54) is obtained, writing

$$u_1^{n+1} \le \overline{H}(\bar f^n, u_1^n\top\kappa, u_2^n\top\kappa),$$

$$\kappa \le H(\kappa, \kappa\top u_1^n, \kappa\top u_2^n)$$

and $G(\kappa,\kappa\top u_1^n)\le g(\kappa)$.
One gets (55), writing

$$u_I^{n+1} \le \overline{\overline{H}}(\kappa\top u_{I-1}^n, \kappa\top u_I^n),$$

and

$$\kappa \le H(\kappa\top u_{I-1}^n, \kappa\top u_I^n, \kappa).$$

Inequalities (56), (57) and (58) are obtained following a similar method.

3 Continuous entropy inequalities for the approximate solution

The discrete entropy inequalities (53) - (58) are used to derive continuous entropy inequalities. These inequalities are shown to include an error term which vanishes as $h\to 0$.

Lemma 5 *Let $\xi\in(0,1)$ and let us assume that the function $u_{h,k}$ is defined within the hypotheses and notations (HN) and the condition (14).*

Then for all $\varphi\in\mathcal{C}_c^\infty(\mathbb{R}\times\mathbb{R},\mathbb{R}_+)$, there exists a function $\varepsilon(h)$ which depends on $L,\varphi,u_0,\bar f,G,f,\mathcal{L}$ and ξ such that

$$\begin{aligned}&\int_0^{+\infty}\int_0^L \left(\eta_\kappa^\top(u_{h,k}(x,t))\,\varphi_t(x,t)+\Phi_\kappa^\top(u_{h,k}(x,t))\,\varphi_x(x,t)\right)dx\,dt\,+\int_0^L \eta_\kappa^\top(u_0(x))\,\varphi(x,0)\,dx\\&+\mathcal{L}\int_0^{+\infty}\left(\eta_\kappa^\top(\overline{u}(t))\,\varphi(0,t)+\eta_\kappa^\top(1)\,\varphi(L,t)\right)dt\geq-\varepsilon(h)\\&\forall\kappa\in[0,1],\end{aligned}\tag{59}$$

$$\begin{aligned}&\int_0^{+\infty}\int_0^L \left(\eta_\kappa^\perp(u_{h,k}(x,t))\,\varphi_t(x,t)+\Phi_\kappa^\perp(u_{h,k}(x,t))\,\varphi_x(x,t)\right)dx\,dt\,+\int_0^L \eta_\kappa^\perp(u_0(x))\,\varphi(x,0)\,dx\\&+\mathcal{L}\int_0^{+\infty}\left(\eta_\kappa^\perp(\overline{u}(t))\,\varphi(0,t)\right)dt\geq-\varepsilon(h)\\&\forall\kappa\in[0,1].\end{aligned}\tag{60}$$

and

$$\lim_{h\to 0}\varepsilon(h)=0.$$

Proof of Lemma 5: One defines, for all $i=1,\dots,I$ and $n\in\mathbb{N}$,

$$\varphi_i^n=\frac{1}{hk}\int_{nk}^{(n+1)k}\int_{ih}^{(i+1)h}\varphi(t,x)\,dx\,dt.$$

Multiplying inequality (53) by $h\varphi_i^n$ for $i=2,\dots,I-1$, (54) by $h\varphi_1^n$, (55) by $h\varphi_I^n$, summing the obtained inequalities on $n\in\mathbb{N}$ yields

$$T_0^\top+T_1^\top+T_2^\top+T_I^\top\leq 0,\tag{61}$$

with

$$T_1^\top=\sum_{n\in\mathbb{N}}\sum_{i=1}^{I-1}h\left[(u_i^{n+1}-\kappa)^+-(u_i^n-\kappa)^+\right]\varphi_i^n,$$

$$T_2^\top=\sum_{n\in\mathbb{N}}\sum_{i=1}^{I-1}k\left[G(u_i^n\top\kappa,u_{i+1}^n\top\kappa)-g(\kappa)\right](\varphi_i^n-\varphi_{i+1}^n),$$

$$T_0^\top=-\sum_{n\in\mathbb{N}}k\left[\bar{f}^n\top g(\kappa)-g(\kappa)\right]\varphi_1^n,$$

and

$$T_I^\top=\sum_{n\in\mathbb{N}}k\left[G(u_I^n\top\kappa,\kappa)\perp f(u_I^n\top\kappa)-g(\kappa)\right]\varphi_I^n.$$

Using the weak BV inequalities (51) and (52), one gets (see [Vov02])

$$T_1^\top=-\int_0^{+\infty}\int_0^L\eta_\kappa^\top(u_{h,k}(x,t))\,\varphi_t(x,t)\,dx\,dt-\int_{(0,L)}\eta_\kappa^\top(u_0(x))\varphi(x,0)dx+\varepsilon_1^\top\tag{62}$$

and

$$T_2^\top=-\int_0^{+\infty}\int_0^L\Phi_\kappa^\top(u_{h,k}(x,t))\,\varphi_x(x,t)\,dx\,dt+\varepsilon_2^\top,\tag{63}$$

with $\lim_{h\to 0}\varepsilon_1^\top=0$ and $\lim_{h\to 0}\varepsilon_2^\top=0$. One has

$$g(\kappa) - G(u_I^n \top \kappa, \kappa) \bot f(u_I^n \top \kappa) \le g(\kappa) - g(\kappa) \bot f(\kappa) = g(\kappa) - f(\kappa),$$

and $g(\kappa) - f(\kappa) \le \mathcal{L}(1-\kappa)$, since $\mathcal{L}$ is a Lipschitz constant for $g - f$. It leads to

$$T_I^\top \ge -\mathcal{L} \int_0^T \eta_\kappa^\top(1)\, \varphi(L,t)\, dt + \varepsilon_I^\top. \tag{64}$$

with $\lim_{h\to 0} \varepsilon_I^\top = 0$. Using the definition of $\bar{f}^n$, one gets

$$T_0^\top = - \int_0^T [\bar{f}(t) \top g(\kappa) - g(\kappa)]\, \varphi(0,t)\, dt + \varepsilon_0^\top.$$

with $\lim_{h\to 0} \varepsilon_0^\top = 0$ (note that this convergence result is obtained, remarking that the approximation of $\bar{f}$ converges to $\bar{f}$; this would not be true on approximations of $\overline{u}$). Since for a.e. $t \in \mathbb{R}_+$ one has $\bar{f}(t) = g(\overline{u}(t))$ and $\overline{u}(t) \in [0, a_\star]$, one gets $0 \le g(\overline{u}(t)) \top g(\kappa) - g(\kappa) \le \mathcal{L}(\overline{u}(t) - \kappa)^+$ and therefore

$$T_0^\top \ge -\mathcal{L} \int_0^T \eta_\kappa^\top(\overline{u}(t))\, \varphi(0,t)\, dt + \varepsilon_0^\top. \tag{65}$$

Inequalities (62)-(65) lead to (60). Similarly, one has

$$T_0^\bot + T_1^\bot + T_2^\bot + T_I^\bot \le 0, \tag{66}$$

with

$$T_1^\bot = \sum_{n\in\mathbb{N}} \sum_{i=1}^{I-1} h\, [(u_i^{n+1} - \kappa)^- - (u_i^n - \kappa)^-]\, \varphi_i^n,$$

$$T_2^\bot = \sum_{n\in\mathbb{N}} \sum_{i=1}^{I-1} k\, [g(\kappa) - G(u_i^n \bot \kappa, u_{i+1}^n \bot \kappa)]\, (\varphi_i^n - \varphi_{i+1}^n),$$

$$T_0^\bot = - \sum_{n\in\mathbb{N}} k\, [g(\kappa) - \bar{f}^n \bot g(\kappa)]\, \varphi_1^n,$$

and

$$T_I^\bot = \sum_{n\in\mathbb{N}} k\, [g(\kappa) - G(u_I^n \bot \kappa, \kappa) \top f(u_I^n \bot \kappa)]\, \varphi_I^n.$$

Using again the weak BV inequalities (51) and (52), one gets

$$T_1^\bot = - \int_0^{+\infty} \int_0^L \eta_\kappa^\bot(u_{h,k}(x,t))\, \varphi_t(x,t)\, dx\, dt - \int_{(0,L)} \eta_\kappa^\bot(u_0(x)) \varphi(x,0) dx + \varepsilon_1^\bot \tag{67}$$

and

$$T_2^\bot = - \int_0^{+\infty} \int_0^L \Phi_\kappa^\bot(u_{h,k}(x,t))\, \varphi_x(x,t)\, dx\, dt + \varepsilon_2^\bot. \tag{68}$$

with $\lim_{h\to 0} \varepsilon_1^\bot = 0$ and $\lim_{h\to 0} \varepsilon_2^\bot = 0$.
Since f is nondecreasing, one gets $G(u_I^n \bot \kappa, \kappa) \top f(u_I^n \bot \kappa) \le G(u_I^n \bot \kappa, \kappa) \top f(k)$.
Using $f \le g$, one gets $G(u_I^n \bot \kappa, \kappa) \top f(k) \le G(u_I^n \bot \kappa, \kappa) \top g(\kappa)$. Using the fact that G is nondecreasing w.r.t. its first argument, one gets

$$T_I^\bot \ge 0. \tag{69}$$

One has

$$T_0^{\perp} = -\int_0^T [g(\kappa) - g(\kappa)\perp \bar{f}(t)]\,\varphi(0,t)\,dt + \varepsilon_0^{\perp}.$$

with $\lim_{h\to 0} \varepsilon_0^{\perp} = 0$. Since for a.e. $t \in \mathbb{R}_+$ one has $\bar{f}(t) = g(\overline{u}(t))$ and $\overline{u}(t) \in [0, a_\star]$, one gets $0 \leq g(\kappa) - g(\kappa)\perp g(\overline{u}(t)) \leq \mathcal{L}(\overline{u}(t) - \kappa)^-$. It leads to

$$T_0^{\perp} \geq -\mathcal{L}\int_0^T \eta_\kappa^{\perp}(\overline{u}(t))\,\varphi(0,t)\,dt + \varepsilon_0^{\perp}. \tag{70}$$

Inequalities (67)-(70) yield (60).

4 Convergence of the scheme

We let $h \to 0$ in Lemma 5, which implies $k \to 0$ under CFL condition (14). We thus get, up to a subsequence, the convergence of $u_{h,k}$ in the nonlinear weak * sense to an entropy process solution $u \in L^\infty((0,L)\times \mathbb{R}_+ \times (0,1))$ of problem (10)-(13) (see [EGH00] or [Vov02]). Indeed, this nonlinear weak * limit u verifies

$$\begin{array}{l}\displaystyle\int_0^{+\infty}\int_0^L\int_0^1 \big(\eta_\kappa^{\top}(u(x,t,a))\,\varphi_t(x,t) + \Phi_\kappa^{\top}(u(x,t,a))\,\varphi_x(x,t)\big)\,da\,dx\,dt + \int_0^L \eta_\kappa^{\top}(u_0(x))\,\varphi(x,0)\,dx\\ \displaystyle+\mathcal{L}\int_0^{+\infty} \big(\eta_\kappa^{\top}(\overline{u}(t))\,\varphi(0,t) + \eta_\kappa^{\top}(1)\,\varphi(L,t)\big)\,dt \geq 0,\\ \forall\kappa \in (0,1),\ \forall\varphi \in \mathcal{C}_c^\infty(\mathbb{R}\times\mathbb{R},\mathbb{R}_+),\end{array} \tag{71}$$

and

$$\begin{array}{l}\displaystyle\int_0^{+\infty}\int_0^L\int_0^1 \big(\eta_\kappa^{\perp}(u(x,t,a))\,\varphi_t(x,t) + \Phi_\kappa^{\perp}(u(x,t,a))\,\varphi_x(x,t)\big)\,da\,dx\,dt + \int_0^L \eta_\kappa^{\perp}(u_0(x))\,\varphi(x,0)\,dx\\ \displaystyle+\mathcal{L}\int_0^{+\infty} \big(\eta_\kappa^{\perp}(\overline{u}(t))\,\varphi(0,t) + \eta_\kappa^{\perp}(1)\,\varphi(L,t)\big)\,dt \geq 0,\\ \forall\kappa \in (0,1),\ \forall\varphi \in \mathcal{C}_c^\infty(\mathbb{R}\times\mathbb{R},\mathbb{R}_+),\end{array} \tag{72}$$

using $\eta_\kappa^{\perp}(1) = 0$ for all $\kappa \in (0,1)$. The uniqueness theorem of such a solution (see [Vov02]) concludes the proof of the convergence theorem 1.

5 Industrial examples of one-dimensional two-phase flow problems

5.1 Two-phase flow in porous media

We consider waterflood experiments on a core extracted from an oil reservoir, made with the purpose to fit the reservoir data. The process can be roughly described as follows: the fit is achieved using a lab simulator, based on a coupled finite volume scheme for the two conservation equations of water and oil using Darcy's law and a phase-by-phase upstream weighting. It can be shown ([Pfe87] or [BJ91]) that, after elimination of the discrete pressures, this scheme yields (1)-(4) with the following interpretation of the data:

- The ratio u between the two phases is in this case the saturation of the water phase in the porous medium.

- The volumic flux of water, injected at $x = 0$, is defined by $\bar{f}(t) = \alpha > 0$ for all $t \in \mathbb{R}_+$.
- The function $G(a, b)$ is given by

$$\begin{aligned} G(a,b) &= \frac{M_w(a)(\alpha + \beta M_o(a))}{M_w(a) + M_o(a)} \text{ if } -\alpha + \beta M_w(a) \le 0 \\ G(a,b) &= \frac{M_w(a)(\alpha + \beta M_o(b))}{M_w(a) + M_o(b)} \text{ if } -\alpha + \beta M_w(a) > 0, \end{aligned} \tag{73}$$

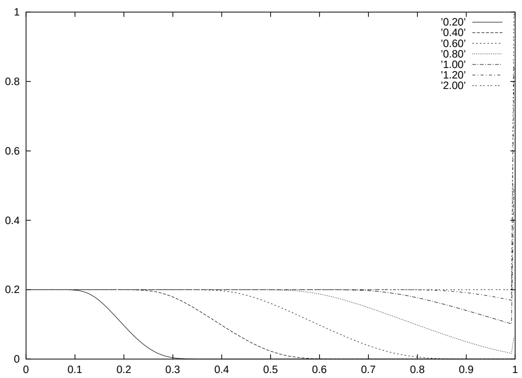
  where the function M_w is a non decreasing function with $M_w(0) = 0$ and the function M_o is a non increasing function with $M_o(1) = 0$, and the real positive value β results from the difference of density between water and oil.

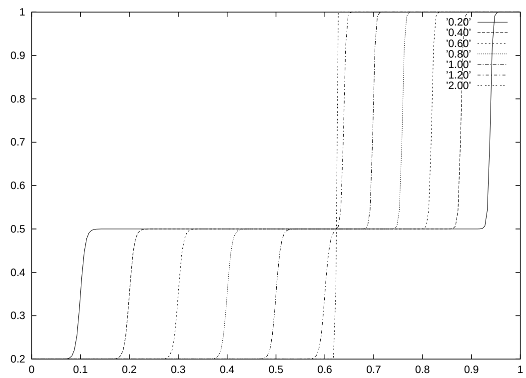
- The function $f(a)$ which computes the outwards flux of water is given by

$$f(a) = \frac{M_{wL}(a)\alpha}{M_{wL}(a) + M_{oL}(a)}, \tag{74}$$

  where the function M_{wL} is a non decreasing function with $M_{wL}(0) = 0$ and the function M_{oL} is a non increasing function with $M_{oL}(1) = 0$. These functions can a priori differ from M_w and M_o, because of specific physical phenomena occuring at the end $x = L$ of the core.

The theorem 1 shows that at the limit $h \to 0$, neither the saturation inside the core nor the values of the outwards fluxes of water and oil as functions of the time variable depend on the choice of the function f. Some numerical results give indications of the physical phenomena involved here. We consider the case $M_w(a) = a$, $M_o(a) = 1 - a$, $\alpha = 0.2$, $\beta = 1$ and $f(a) = a\alpha$ (this is an example where gravity effects are important in front of the flows imposed at the boundary). The numerical parameters are $L = 1$, $I = 200$ and $k = 0.0001$. The following figures present the results obtained at different times ($t = 0.2$, 0.4, 0.6, 0.8, 1.0, 1.2 and 2.0): the left figure corresponds to the case $u_0 = 0$ and the right figure to the case $u_0 = 0.5$.





The problem solved in the case $u_0 = 0$ is a Riemann problem yielding a unique rarefaction wave: oil and water phases flows are both positive. One observes in that case that the value of the saturation in the last control volume I is not used for computing the flow with $I - 1$. On the contrary, with the initial data $u_0 = .5$, oil flow is negative when water flow is positive until the time at which the injected fluid imposes its composition. After this time, both flows become positive.

5.2 Two-phase flow in a pipe

The general problem of two-phase (liquid and gas) flow in a pipe is quite complex. In the physico-mathematical description of the various phenomena are taken into account the equations of conservation of the masses of the liquid and the gas, the equation of conservation of the total impulsion, thermodynamic

laws for the phase transitions and a hydrodynamical law describing the fluid mechanics involved by this flow. We refer to [PT96] for an overview on the simulation of a two-phase flow in a pipe.
It has recently been shown in [BFT02] that a simplified scalar model can be used in order to understand with more accuracy some of the physical phenomena due to the transport features of the problem and, in particular, the numerical treatment of the boundary conditions. In [BFT02], the geometry of the pipe is characterized by its length L, its diameter D and its angle with the horizontal θ (see Fig.2).

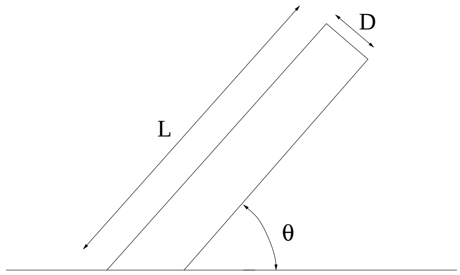


Figure 2: The pipe geometry

The flow of two species, one in the liquid phase, one in the gas phase is considered and the following equivalence between hypotheses and notations (HN) holds:

- We denote by u the fractional superficial mass of gas in the pipe.
- The value α is the total superfical speed of the fluids.
- The function g is defined by $g(u) = [(1+\mu)\alpha + \nu]u - (\mu\alpha + \nu)u^2$, where μ and ν are defined by $\mu = 0.2 \sin\theta$, $\nu = 0.35\sqrt{\gamma D}\sin\theta$, $\alpha = \beta\frac{\nu}{1-\mu}$ with $\beta = 0.5$ and the gravity acceleration is $\gamma = 9.81 m/s^2$. We have represented in figure 3 the case $D = 0.144$m, $\theta = \pi/4$.

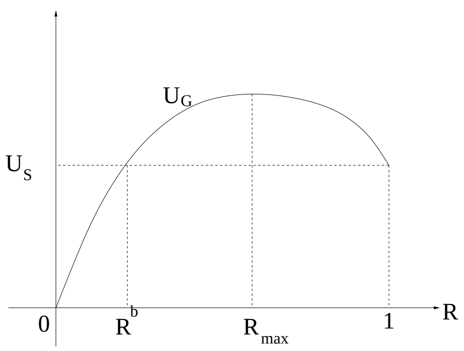


Figure 3: The function g

- The function G is defined by $G(a,b) = \frac{1}{2}\left(g(a) + g(b)\right) + \frac{1}{2}[(1+\mu)\alpha + \nu](a-b)$.
- In (2), the imposed flux $\bar{f}^n$ is replaced by the standard boundary condition $G(\overline{u}, u_1^n)$, corresponding to an imposed fractional superficial mass of gas $\overline{u}$ at $x = 0$.

The heart of the problem is the choice of the numerical boundary condition at the last control volume of the mesh (at $x = L$). For engineers, physical considerations lead to the following expression of the boundary condition: the superficial speed of water at the outward of the pipe is non-negative.

Notice that this is a boundary condition which is expressed via the unknown of the *continuous equation* $u_t + (g(u))_x = 0$: this fact hampered the determining of the accurate numerical boundary conditions for a long time, because making the link between the boundary condition of the continuous problem and the numerical boundary conditions of the associated scheme is not straighforward. Now, with the notations designed by (HN), the condition "the superficial speed of water at the outward of the pipe is non-negative" is equivalent to the condition $g(u)(L,T) \leq \alpha$. Therefore, in view of Theorem 1, it appears that a convenient choice for the numerical boundary condition is Eq. (3) where the function f is non-decreasing and such that $f(0) = 0$ and $f(1) = \alpha$. In fact, the numerical boundary condition that has been selected by petroleum engineers is Eq. (3) with the function $f(a) = \min(g(a), \alpha)$. The theorem 1 thus ensures that it is an accurate choice.

5.3 Separation of phases in binary distillation columns

In this section, we study the boundary conditions which must be applied to the study of a binary distillation column. We refer to [LR91] and [Rou90] for precise descriptions of the physical background and references. A binary column is a distillation column used to separate two components. At the top of the column is produced the light component (vapor) together with few of the heavy component (liquid). At the bottom of the column, it is the converse: the heavy component is released out together with few of the light component. For control purposes, a semi-discrete model is introduced, the Lewis model. Since the fluids are introduced between the top and the bottom of the column, two one-dimensional problems can be developped. Keeping in view the fact that we are interested in the interpretation of the boundary conditions at the top and the bottom of the column, the models which are considered can be described as follows.
The first one is (1), (3) and (4) where

- L is the distance between the top of the column and the introduction point,
- the liquid molar fraction is represented by u,
- the function G is defined by $G(a,b) = Vk(b) - Ma$, with $0 < M < V$ and the thermodynamical equilibrium function k is smooth, convex, increasing and such that $k(0) = 0$ and $k(1) = 1$. The function g is defined by $g(a) = Vk(a) - Ma$ and $\alpha = 0$,
- the function f is defined by $f(a) = \alpha a$.

The second one is (1), (3) and (4) where

- $\tilde{L}$ is the distance between the top of the column and the introduction point,
- the liquid molar fraction is represented by $\tilde{u}$,
- the function $\tilde{G}$ is defined by $\tilde{G}(a,b) = (L+M)a - Vk(b)$, with $0 < M < V < L+M$. The function $\tilde{g}$ is defined by $\tilde{g}(a) = (L+M)a - Vk(a)$ and $\tilde{\alpha} = L + M - V$,
- the function $\tilde{f}$ is defined by $\tilde{f}(a) = \tilde{\alpha} a$.

For the sake of simplicity, the numerical boundary condition at the first control volume is supposed to be classical. That is to say: the equation (2) is replaced, for the first model, by

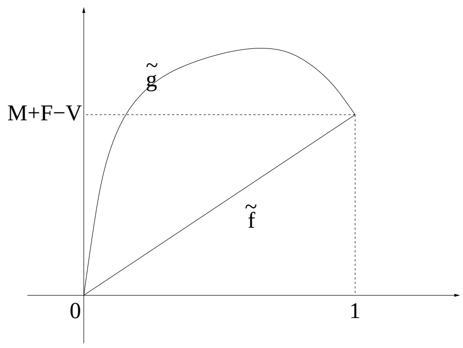
$$\frac{h}{k}[u_1^{n+1} - u_1^n] + G(u_1^n, u_2^n) - G(\overline{u}^n, u_1^n) = 0, \forall n \in \mathbb{N}, \tag{75}$$

and for the second model by

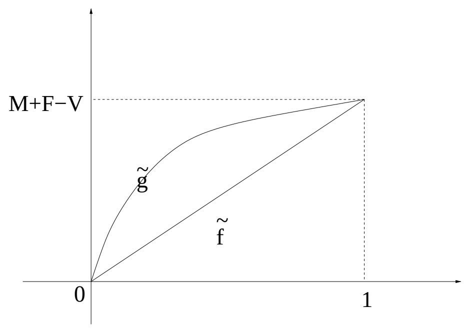
$$\frac{h}{k}[\tilde{u}_1^{n+1} - \tilde{u}_1^n] + \tilde{G}(\tilde{u}_1^n, \tilde{u}_2^n) - \tilde{G}(\overline{\tilde{u}}^n, \tilde{u}_1^n) = 0, \forall n \in \mathbb{N}\,. \tag{76}$$

Study at the bottom of the column

we make the distinction between two cases (see Fig.5.3): indeed, the function $\tilde{g} : u \mapsto (M+F)u - Vk(u)$ is concave (because the function k is convex) and satisfies $\tilde{g}(0) = 0 < M + F - V = \tilde{g}(1)$, therefore it reaches its maximum at a point u_m which is either 1 or in $[0, 1)$:
- CASE A: the function $\tilde{g}$ reaches its maximum at $u_m \in [0, 1)$,
- CASE B: the function $\tilde{g}$ reaches its maximum at $u_m = 1$.



CASE A



CASE B

In the case B, the flux function $\tilde{g}$ is non-increasing, therefore the boundary $\{x = \tilde{L}\}$ is not active: *no boundary condition is needed* (to define properly the solution of the problem) and one can prove that the scheme converges to the solution of the (well-posed) problem

$$\left\{\begin{array}{rcll} \tilde{u}_t(x,t) + (\tilde{g}(\tilde{u}))_x(x,t) &=& 0 & 0 < x < L\,,\ t > 0 \\ \tilde{g}(\tilde{u})(0,t) &=& \tilde{g}(\tilde{\overline{u}})(t)\,, & \\ \tilde{u}(x,0) &=& \tilde{u}_0(x) & 0 < x < \tilde{L}\,. \end{array}\right.$$

In the case A, Theorem 1 applies, to prove that the scheme converges to the solution of the problem

$$\left\{\begin{array}{rcll} \tilde{u}_t(x,t) + (\tilde{g}(\tilde{u}))_x(x,t) &=& 0 & 0 < x < L\,,\ t > 0 \\ \tilde{g}(\tilde{u})(\tilde{L},t) &\leq& \tilde{\alpha} & t > 0\,, \\ \tilde{g}(\tilde{u})(0,t) &=& \tilde{g}(\tilde{\overline{u}})(t) & t > 0\,, \\ \tilde{u}(x,0) &=& \tilde{u}_0(x) & 0 < x < \tilde{L}\,. \end{array}\right.$$

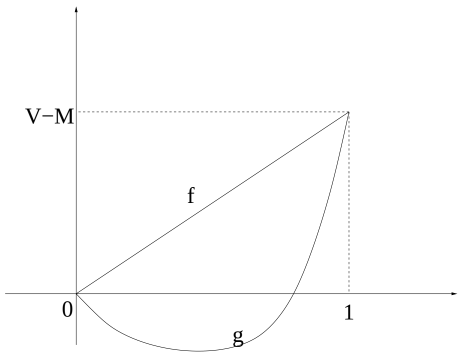
Here, we have written the boundary condition in accordance with the notations of Theorem 1.

Notice that, in both cases, the boundary condition on $\{x = \tilde{L}\}$ can be written $\tilde{g}(\tilde{u})(\tilde{L},t) \leq \tilde{\alpha}$ (this make sense from the physical point of view).

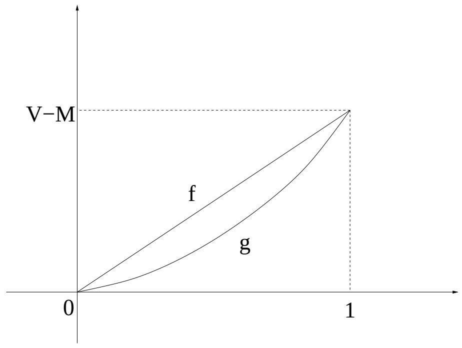
Study at the top of the column

Here, we lead a study very similar to the precedent one, and draw the same conclusions: again, we make the distinction between two cases (see Fig.5.3): indeed, the function $g : u \mapsto Vk(u) - Lu$ is convex (because the function k is convex) and satisfies $g(0) = 0 < V - M = g(1)$, therefore it reaches its minimum at a point u_m which is either 0 or in $(0, 1]$:
- CASE A: the function g reaches its minimum at $u_m \in (0, 1)$,

- Case B: the function g reaches its minimum at $u_m = 0$.



Case A



Case B

In the case B, the flux function g is non-increasing, therefore the boundary $\{x = L\}$ is not active: *no boundary condition is needed* and one can prove that the scheme converges to the solution of the (well-posed) problem

$$\left\{\begin{array}{rcll} u_t(x,t) + (g(u))_x(x,t) & = & 0 & 0 < x < L\,,\ t > 0 \\ g(u)(0,t) & = & g(\overline{u})(t) & t > 0 \\ u(x,0) & = & u_0(x) & x < 0\,. \end{array}\right.$$

In the case A, Theorem 1 (slightly adapted) applies, to prove that the scheme converges to the solution of the problem

$$\left\{\begin{array}{rcll} u_t(x,t) + (g(u))_x(x,t) & = & 0 & 0 < x < L\,,\ t > 0 \\ g(u)(0,t) & \geq & 0 & t > 0\,, \\ g(u)(0,t) & = & g(\overline{u})(t) & t > 0 \\ u(x,0) & = & u_0(x) & x < 0\,. \end{array}\right.$$

Here, we have written the boundary condition in accordance with the notations of Theorem 1.

Notice that, in both cases, the boundary condition on $\{x = L\}$ can be written $g(u)(L,t) \geq 0$ (this make sense from the physical point of view).

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